EXCITATION EQUILIBRIA IN PLASMAS
—a classification—

PROEFSCHRIFT

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Aan allen die er voor waken
dat de technische wetenschap
ons tot slaven maakt
van bewapening.
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I Introduction

1.1 The plasma state

If sufficient heat is supplied to matter in solid state, molecules will leave their initially fixed positions, and a state or phase transition takes place. This state transition known as melting, leads matter from the first or solid state to the second or liquid state, in which molecules crawl through each other but stay together. Supply of more heat will result in the fact that the mutual van der Waals forces are no longer able to keep the molecules together. A second state transition known as boiling takes place by which the liquid state turns into the gaseous state. The molecules in the gas are free and in search of the greatest volume available, they will drift apart and every wall which limits the gas will be subjected to a bombardment of molecules.

If even more heat is supplied, part of this energy will be transferred to the internal state of the particles. Molecules will dissociate in atoms and atoms will be excited and ionized i.e. they lose one or more electrons. We have reached the fourth state of matter, the plasma state: a chaotic mixture of molecules, atoms, ions and electrons with a lot of microscopic activity.

Although more than 99% of the visible matter in the universe is in the plasma state, this state is not generally recognized as a full-fledged fundamental state of matter like the solid, the liquid and the gaseous state. Sometimes, it is even classified as a pseudo state like the amorphous state of glass and the colloidal state of pudding.

This lack of acceptance is probably due to the fact that it is difficult to give good boundaries for the plasma state. In contrast with the first two state transitions like melting and boiling, the transition from gas to plasma state is difficult to define.

Other reasons may be that the science of plasma physics is relatively young and deals with the most complicated and chaotic state of matter. All types of molecules, radicals, atoms, electrons and ions interact with each other. The motions of the charged particles are influenced by electric and magnetic fields and waves and turbulences may arise. Thus it is an enormous problem to classify plasmas and in this respect plasma physics seems to be in the same preliminary stage of
development as botany was in the time before 1753 when Linnaeus published his 'Species Plantarum'.

With this study we will attempt to find a more transparent structure in the wild variety of plasmas. In this classification we are guided by and focussed at the specific question: How can we recognize the plasma by the way atoms and ions are distributed over their various excited states? In other words, which information is present in the bound state distribution function and what can we learn from it to classify the plasma? Since the distribution function is created by all kinds of microscopic processes, this activity must be reflected in the distribution function, which in this way can give a good image of the plasma. Almost all information about the distribution functions can be obtained from spectroscopy, so this classification can be effectuated with the help of a relatively old technique, already used in the last century in both physics and astrophysics. In our classification, we ignore the artificial boundary between physics and astrophysics. Both laboratory- and space plasmas will be considered.

1.2 Thermodynamic equilibrium and the principle of detailed balancing

The behaviour of particles of the kind \( \pi \) can in principle be described with the Boltzmann equation

\[
\frac{\partial f_\pi}{\partial t} + v_\pi \cdot \nabla f_\pi = \frac{(\partial f_\pi)}{\partial \mathbf{v}} + \int \frac{\partial f_\pi}{\partial \mathbf{v}} d^3 \mathbf{v} = \frac{\partial f_\pi}{\partial \mathbf{v}} \mid_{\text{CR}},
\]

in which \( f_\pi(E, v, t) d^3 v \) is the number of particles which, at time \( t \), are in the volume \( d^3 v \) at location \( \mathbf{r} \), with velocities lying in a velocity-space element \( d^3 \mathbf{v} \), centered around \( \mathbf{v} \). The first term in eq. (1.1) describes the temporal behaviour, the second the influence of homogeneous, and the third the velocity changes due to the presence of macroscopic forces. The CR deals with the production and destruction of the considered particles, due to elementary collisional and radiative (CR) processes.

With his H-theorem it was shown by Boltzmann that for an isolated system, the phase space distribution function \( f_\pi(E, v, t) \) of material particles tends towards a value that is independent of spatial position and time. This is the well-known Maxwellian translational velocity distribution function, completely determined by the temperature. The system has reached a uniform steady state of Thermodynamic Equilibrium (TE) in which there is an overall balance in the collision processes suffered by the particles. Moreover the
\( H \)-theorem shows that there is a detailed balancing in the elastic collisions, which means that the number of any specific collision is balanced by the number of its inverse process.

This detailed balancing (DB) also exists for inelastic collisions and for the interactions of matter with radiation, provided that the plasma has reached the state of TE.

The description of a plasma in TE is relatively simple. Macroscopic properties are interrelated by the equation of state which reduces the number of independent macroscopic parameters drastically. The state of the plasma is fully described by the mass density, temperature and chemical composition. Information about the particles can be obtained from the laws of statistical mechanics. Apart from the velocity distribution as given by Maxwell, the distribution of ions and atoms over their various excited states is given by the Boltzmann distribution law, the relation between the number densities of subsequent ionic states is given by the Saha equation, while the distribution of the photon gas obeys Planck's radiation law. If TE is present all these distribution functions for different types of particles are characterized by the same temperature.

Although the presence of TE implies that there are no changes on the macroscopic level, this is certainly not the case on a microscopic level. But specific for TE is that every detailed microscopic process is balanced by its inverse process.

It was pointed out in [OST.70] that the existence of DB is a sufficient condition for TE. We will see that the principle of DB can be used to relate rates of forward and backward processes even in certain non-equilibrium situations.

1.3 Equilibrium departure; proper and improper balances

In Table 1.1 we present the balances responsible for the establishment of Maxwell, Saha, Boltzmann, and Planck. These balances are so-called proper balances, i.e. they consist of forward and corresponding backward processes. If all these balances are affected for all particle states, this DB implies TE and the distribution functions are known. If some of the processes are not balanced, this can involve a TE departure and information is needed to calculate the distribution functions. The new situation can be classified by means of the affected balances. The degree of equilibrium departure is called a phase. We give some examples of phases (cf. table 1.2).

In laboratory plasmas, limited in dimension and mostly with a
Table 1.1
Proper balance. The symbol $u$ refers to a particle for which internal energy is not relevant. The symbol $A_p$ denotes the atom or ion in internal state $p$. The symbol $[\text{ and } \text{ ]}$ denote to which particles the energy belongs.

\[
\begin{align*}
\text{Maxwell balance} & \quad \nu_1 + \nu_2 \quad \xrightarrow{\text{M}} \quad \nu_1' + \nu_2' \\
& \quad \nu_1' + \nu_2' = \nu_1 + \nu_2 \\
\text{kinetic energy exchange and conservation} & \quad \text{B} \\
\text{Boltzmann balance} & \quad A_p + \pi + (E_{1u} + E) \quad \xrightarrow{\text{B}} \quad A_p + \nu + (E) \\
& \quad \text{deexcitation } \longleftrightarrow \text{ excitation} \\
\text{Saha balance} & \quad A_p + \pi + (E_{1u} + E) \quad \xrightarrow{S} \quad A^+ + \pi + c + (E) \\
& \quad \text{recombination } \longleftrightarrow \text{ ionization} \\
\text{Planck balance} & \quad A_p \quad \xrightarrow{\text{P}} \quad A_1 + h\nu \\
& \quad \text{absorption } \longleftrightarrow \text{ decay} \\
A_p + h\nu & \quad \xrightarrow{\text{}} A_1 + \text{2h}\nu \\
& \quad \text{stimulated emission}
\end{align*}
\]

cylindrical configuration, it often occurs that radiation escapes and gradients are present. Since photons are more liable to escape than material particles, it is well possible that Planck's photon distribution is strongly affected, while energy exchange between material particles remains so effective that locally Boltzmann, Saha and Maxwell are retained and that atoms, ions and electrons have the same temperature. This phase of equilibrium is known as Local Thermal Equilibrium (LTE). Thermodynamic properties like temperature and pressure have to be specified locally (and instantaneously) cf. table 1.2. Essential for LTE is that matter and radiation cannot be
Table 1.2
Phases of equilibrium departure. Going downwards equilibrium departure becomes more complete. More phenomena will be decoupled. Abbreviations: M, E, S and P see table 1.1. Other abbrev. are explained in the text.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Balances</th>
<th>Temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>T.E.</td>
<td>$\frac{1}{2} = 0 - 0$</td>
<td>$T_{h0} - T_a = T_e = T_{\infty} = T_{\infty}$</td>
</tr>
<tr>
<td>L.T.E.</td>
<td>$\frac{3}{2} \neq 0 \neq 0$</td>
<td>matter $\leftrightarrow$ radiation</td>
</tr>
<tr>
<td>P.L.T.E. (top)</td>
<td>$\frac{3}{2} \neq 0 \neq 0$</td>
<td>$T_a = T_e = T_{\infty} = T_{\infty}$</td>
</tr>
<tr>
<td>O.S.S. (bottom)</td>
<td>$\frac{3}{2} \neq 0 \neq 0$</td>
<td>$T_{h0} \neq T_e$</td>
</tr>
</tbody>
</table>

Described with the same temperature. We state that matter and radiation are 'decoupled' from each other. Apart from that, there is also a spatial decoupling possible in LTE: the plasma may have different temperatures at different locations.

A further departure from LTE can be realized if the gradients are so large that electrons are decoupled from heavy particles. Because of the small mass ratio the heating of the electrons is much faster than...
the transfer of energy from electrons to heavy particles. Another consequence of the small electron mass is that electrons are very effective in retaining Saha at least for the upper part of the atomic energy scheme. In this way the electrons impose their temperature on the internal state distribution of atoms. As a consequence the excitational and kinetic temperatures of the atoms may not be the same and the spectrum of the atoms reflects electron properties. In this phase denoted by Partial Local Thermal Equilibrium (PLTE), the equilibrium of Saha is established in the upper part of the energy scheme. The energy gaps between the lower lying levels are usually too large for retaining the equilibrium of Boltzmann. In this way the atomic energy scheme is decoupled in an upper and a lower part; in a bottom and a top.

Although this decoupling between lower and higher levels is essentially different from that of electron and heavy particle temperatures, both decoupling phenomena mostly accompany each other.

In this way we can proceed. The more we leave TE, the more phenomena will be decoupled and the more information is needed to characterize the plasma.

We will confine ourselves to plasmas where upper levels are in PLTE and for which the population of lower excited levels are determined by balances of elementary processes only. That is, we suppose that radiative and collisional processes are more rapid than the decay or growth of the plasma. This simplifying assumption is used in the Quasi Steady State Solution (QSSS) and the model of level calculation is called a Collisional Radiative (CR) model since only collisional and radiative processes determine the level density for excited levels.

In the bottom forward and backward processes are not balanced in a proper way. A departure of the Saha and Boltzmann distribution can be expected and the level population will change such that a new balance of destruction and production is established. But in this new balance, production and destruction are not each other's opposites. The balance is a so-called improper balance and in contrast with proper balances we need information about the elementary processes of production and destruction in order to be able to calculate the distribution function.

An important feature of improper balances is that they are associated with an activity on the macroscopic level. For instance, in ionizing plasmas improper balances create a net flow of excitation in the system of atomic levels which is related to outward diffusion of
Table 1.3

Features of improper balances, \( n_e \) = the electron density, adj. = adjacent, \( b(i) \gg 1 \) means that the groundstate is largely over-populated i.e. the groundstate density is larger than the value needed to retain the Saha balance (\( b(i) = 1 \)), Abbr. cf. fig.1.1.

<table>
<thead>
<tr>
<th>Component</th>
<th>Production</th>
<th>Destruction</th>
<th>Found in Plasmas</th>
</tr>
</thead>
<tbody>
<tr>
<td>CB</td>
<td>exc. from groundstate</td>
<td>spontaneous emission</td>
<td>relative low ( n_e )-values ( b(i) \gg 1 )</td>
</tr>
<tr>
<td>ion</td>
<td>exc. from lower adj. level</td>
<td>exc. to higher adj. level</td>
<td>outward transport of charged particles ( b(i) \gg 1 )</td>
</tr>
<tr>
<td>rec</td>
<td>deexc. from higher adj. level</td>
<td>deexc. to lower adj. level</td>
<td>inward transport of charged particles or irradiated plasmas</td>
</tr>
<tr>
<td>CRC</td>
<td>capt. and casc.</td>
<td>decay (= sp.em.)</td>
<td>inward transport of charged particles or irradiated plasmas</td>
</tr>
</tbody>
</table>

charged particles. In recombining plasmas they create a net flow of deexcitation processes which may be related to inward diffusion of charged particles. Thus there is a relation between the transport phenomena in the configuration space on one hand and the improper balances in the excitation space on the other hand. A particular balance will generally dominate a particular limited (lower) part of the atomic levels. The part of the energy scheme dominated by that balance is the so-called Balance Domain. In figure 1.1 and table 1.3 we give four possible balances, the corona balance CB, the ionizing
Fig. 1.1

A comparison between the proper balances of Boltzmann (B), Saha (S) and Planck (P) on one hand and the improper balances of Corona (CB), the ionizing excitation saturation balance (ion. ESB), the recombinating excitation saturation balance (rec. ESB) and the capture radiative cascade (CRC) on the other hand.

Abbr.: (d)e=exc. (d)e=excitation; ion/rec.= ionization/recombination; sp.e. = spontaneous emission; st.e. = stimulated emission; abs. = absorption; capt. = capture = 2 particle rec.; casc. = cascade.

and recombinating Excitation Saturation Balance (ESB) and the Capture Radiative Cascade (CRC) balance. The features of these Balance Domains is the main subject of this study.

So we confine ourselves to the discussion of plasmas for which the QSSS can be applied, where Saha is valid for the top and Maxwell valid for at least the bulk of the electrons (cf. fig. 1.2). The Boltzmann and Planck distribution may be largely affected and replaced by improper balances.

In chapter II we will classify elementary processes and we shall see that in a large variety of plasmas the excitation kinetics is realized by a competition between electron collisions and radiative decay. Other elementary processes are less important. The plasmas with this property are the so-called Electron Excitation Kinetic (EEK) Plasmas. The features of the distribution functions of these EEK-plasmas are studied in this thesis. In Chapter III we discuss and classify atomic
energy schemes which will be split up in a full quantum mechanical bottom and a top where the classical limit of quantum mechanics is manifest by the correspondence principle. In chapter IV the radiative processes are studied in detail while chapter V is devoted to electron collisions. Chapter VI gives the general structure of CR models providing the basis of the plasma and domain classification of Chapter VII. In Chapter VIII recombining plasmas are discussed in detail while chapter IX is dedicated to ionizing plasmas. Chapter X is an illustration of experimental results from an argon plasma.

Resuming: we classify plasmas with the help of the distribution function. The shape of the distribution function is related to the underlying balances of production and destruction. If destruction and production are each other's inverse processes the balance is called proper and the shape of the distribution function is described by Saha-Boltzmann. If this is not the case we say that the production-destruction balance is improper and the shape of the distribution function will deviate from the equilibrium shape but reflects the underlying improper balances and gives information about the plasma.

Fig. 1.2
An example of separation of the atomic energy schemes in top and bottom. The production of excited atoms must be realized by electrons with large energy. For a low ionization degree this can affect the tail of the energy distribution function of the electrons.
Chapter II  Classification of elementary processes.

2.1 Introduction.

The atomic state distribution function results from all kind of elementary processes. These processes can be classified in for- and backward processes. In section 2.2 we consider the proper balances where the production of each elementary state is balanced by its reverse (backward) destruction process. It is shown how in this situation of detailed balancing (DB) the principle of microscopic reversibility makes the knowledge of rates unnecessary and the derivation of the equilibrium distribution functions of Maxwell (2.2.2), Boltzmann (2.2.3) Saha (2.2.4) and Planck (2.2.5) possible.

In section 2.3 the validity of the Maxwell distribution for electrons is investigated. Criteria for the ionization degree, temperature, electric field strength and frequency are discussed.

Section 2.4 is devoted to deviations from Boltzmann. Classifications of cross sections are given and rate coefficients are discussed. The competition between collisional and radiative processes will be expressed in critical densities.

Section 2.5 deals with deviations from Saha. The conclusion is that although deviations can be expected in the lower part of the system there must be equilibrium somewhere high enough in the system. Saha and Boltzmann are compared with each other. Differences between the two are originating from the asymmetry of the atomic energy scheme, i.e. large energy gaps in the bottom and a continuum approaching top.

Due to the lowering of the ionization potential only a finite part of the levels has to be considered.

Section 2.6 is devoted to deviation from Planck's radiation law which frequently occurs in plasmas. In contrast with collisional transitions, radiative transfer is not a local phenomenon. By the introduction of the escape factor a local treatment is possible. The escape factor is transition dependent and closely related to the optical depth of the transition. Radiative properties of the plasma as a whole can be classified in Case A and B of Waker and Menzel for radiative active plasmas. In addition we consider case C and D for radiative passive (irradiated) plasmas (or parts of plasmas).

General conclusions are presented in section 2.7. The most important is, that there is a large class of plasmas in which the excitation kinetics is determined by electrons only. This class is denoted by electron excitation kinetics plasmas, shortly: EEK plasmas.
2.2 The principle of detailed balancing

2.2.1 General

The principle of detailed balancing states that in a given volume \( V \), for any two energy or momentum states \( i \) and \( f \) of the system, the number of transitions per second leading from \( i \) to \( f \) must equal the number of transitions per second that lead back from \( f \) to \( i \).

This principle together with the conservation laws of energy and momentum can be used to derive the \( T \)E distribution functions of Maxwell, Boltzmann, Saha and Planck. We only need to know how energy and momentum states are distributed over the energy range.

Since these \( T \)E distributions are of importance as a reference-frame for non-\( T \)E distributions we give a brief sketch of this derivation.

For a more detailed approach we refer to Oster [OST.70].

In the volume \( V \) we consider two particles \( X \) and \( Y \) involved in the reactions

\[
\begin{align*}
X^i & \rightarrow X^f + Y^i \quad \text{and} \\
X^i & \rightarrow X^f + Y^f
\end{align*}
\]  

(2.1)

In the forward process (from left to right) the initial energies \( E_x^i \) and \( E_y^i \) are converted into \( E_x^f \) and \( E_y^f \). These energies can be kinetic or internal.

The derivation is based on the following principles:

- The energy is conserved which means that

\[
\Delta E = E_x^f - E_x^i = E_y^i - E_y^f,
\]  

(2.2)

the amount of energy (\( \Delta E \)) gained by particle \( X \) (in the forward process) equals the amount of energy lost by particle \( Y \).

- The energy is quantized. For bound states this is trivial. For the kinetic energy of free particles this quantization can be understood in relation with the Heisenberg uncertainty principle which predicts that in a given volume \( V \), the momentum of any free particle cannot be specified better than \( \delta p = \hbar^2 / V \) (\( \hbar \) is Planck's constant). This uncertainty can be regarded as a momentum quantization which via the relation \( E = p^2 / 2m \) leads to the quantization of the kinetic energy.

We come back to this in the derivation of the Maxwell distribution.

We further assume that the number of forward processes is proportional to

- the initial numbers of particles \( N_x(E_x^i) \) and \( N_y(E_y^i) \) with the
corresponding energies in the volume $V$,
- the final numbers of quantum states $\xi_x$ and $\xi_y$ of the corresponding energies in the volume $V$ and
- an elementary transition probability denoted by $\left\{ E_x, E_y \mid E_x, E_y \right\}$ for which the relation

$$\left\{ E_x, E_y \mid E_x, E_y \right\} = \left\{ E_x, E_y \mid E_x, E_y \right\}$$

holds. This condition of symmetry of the transition probability is known as microscopic reversibility and is valid if the transition matrix is Hermitian (cf. sect. 3.4). This is fulfilled in almost any process. Only in cases of transitions between different spin states this Hermitian condition can be violated [OST 70].

The number of forward processes can now be written as

$$N_{x \rightarrow y} = N_y (E_x, E_y) g_x (E_y) g_y (E_x) \left\{ E_x, E_y \mid E_x, E_y \right\},$$

and the number of backward processes (eq. (2.1) from right to left) can be obtained from this expression by interchanging the indices $i$ and $f$.

The demand of DB, i.e. that the number of forward processes equals the number of backward processes, now results in

$$N_{x \rightarrow y} = N_y (E_x, E_y) g_x (E_y) g_y (E_x) \left\{ E_x, E_y \mid E_x, E_y \right\},$$

where the elementary transition probability was eliminated as justified by the principle of microscopic reversibility (eq. (2.3)).

After the introduction of the number of particles per quantum state

$$\tilde{N}(E) = N(E)/G(E),$$

eq. (2.5) can be written as

$$\tilde{N}_x (E_x) \tilde{N}_y (E_y) = \tilde{N}_x (E_y) \tilde{N}_y (E_x).$$

Now we employ the conservation of energy (eq. (2.2)) and rewrite eq. (2.7) as

$$\tilde{N}_x (E_x + \Delta E) / \tilde{N}_x (E_x) = \tilde{N}_y (E_y + \Delta E) / \tilde{N}_y (E_y) = \Delta E,$$
in which (in a third member) the quantity \( W(\Delta E) \) is introduced. Since both \( E_x^f \) and \( E_y^g \) are arbitrary the quantity \( W(\Delta E) \) is independent of \( \omega_x \) and \( \omega_y \) and only depends on the energy difference \( \Delta E \).

The \( \Delta E = 0 \) value of the derivative with respect to \( \Delta E \) of eq. (2.9), gives for particle \( x \) the differential equation (cf. note 1)

\[
\frac{d\tilde{\pi}_x(E)}{dE} = \frac{\partial W(\Delta E)}{\partial \Delta E} \bigg|_{\Delta E = 0}
\]

with the solution

\[
\tilde{\pi}_x(E) = c_x \exp(-a_x E)
\]

(2.10)

In the same way we find for the particle \( y \) the relation

\[
\tilde{\pi}_y(E) = c_y \exp(-a_y E)
\]

(2.11)

The integration constant \( c_x \) is proportional to the total number of particles \( N_x \) in the volume \( \mathcal{V} \), and is determined by the condition that

\[
\sum_{E_1} \tilde{\pi}_x(E_1) G(E_1) = N_x
\]

(2.12)

The summation runs over all the possible energy values.

If particles \( x \) and \( y \) are of different kinds \( N_x \neq N_y \) and consequently \( a_x \neq a_y \) generally holds.

The constant \( a_x \) must be positive since \( \pi = 0 \) if \( E < 0 \) and is determined by the relation

\[
N_x^{-1} \sum_{E_1} \tilde{\pi}_x(E_1) G(E_1) = \langle \epsilon \rangle
\]

(2.13)

in which \( \langle \epsilon \rangle \) is the mean energy. From the derivation of eqs. (2.10) and (2.11) it becomes obvious that

\[
a_x = a_y = \left[ \frac{\partial W(\Delta E)}{\partial (\Delta E)} \right]_{\Delta E = 0}
\]

(2.14)

It is known from the textbooks on statistical mechanics that the condition (2.13) results in \( \omega^2 / kT \) and that relation (2.14) simply states that the constituents of a gas mixture in \( \mathcal{T} \) all have the same temperature i.e.

\[
T_x = T_y
\]

(2.15)
With the knowledge of the total number of particles $N$ and the mean energy $\langle E \rangle$ eq.(2.10) can be solved. For obtaining the particle distribution function we need to know the quantum state distribution function. In the next sections we will derive these quantum state distributions for free and bound states of material particles and photons. This leads to the distribution functions of Maxwell, Boltzmann, Saha and Planck.

2.2.2 Elastic collisions: Maxwell

Consider the back- and forward processes of the type

\[
\begin{align*}
\gamma_1 + \gamma_2 & \leftrightarrow \gamma_1 + \gamma_2 \\
E_1 + E_2 & \leftrightarrow E_1 + E_2
\end{align*}
\]  

(2.16)

where the role of the particles X and Y are played by the material particles for which the internal state is not important and where all the represented energies are kinetic.

In order to determine the distribution function we first need to know the quantum state distribution i.e. the number of quantum states per unit of volume and unit of energy range, $G_{E,V}(E)$. The determination of this quantity can be realized using the six dimensional phase space where each particle occupies a volume $h^3$. In this view the phase space has a cellular structure. The volume of the cell is $h^3$ and the number of states in one cell equals $g_v$, the number of spin states. So in the phase space volume $d\Gamma = d^3r d^3p$ the number of states is given by

\[
\frac{dG}{d\Gamma} = \left(\frac{d\Gamma}{h^3}\right) g_v,
\]

(2.17)

which means that the density of states in phase space is

\[
G_{\Gamma} = \frac{dG}{d\Gamma} = g_v h^{-3}.
\]

(2.18)

Transformation from the phase space to the configuration space can be effectuated applying $d^3p = 4\pi p^2 dp$, and $p^2 = 2mE$ which gives the quantum state distribution function

\[
G_{E,V}(E) = G_{\Gamma} 4\pi p^2 \left(\frac{d\Gamma}{dE}\right) = 2^{3/2} \pi m^{3/2} g_v h^{-3} \frac{1}{\sqrt{2\pi}}.
\]

(2.19)

The number of particles per unit of volume and unit of energy range can now be obtained by applying eqs. (2.6) and (2.19)

\[
N_{E,V}(E) = \delta(E) G_{E,V}(E),
\]

(2.20)
and the conditions (2.12) and (2.13) which in a continuous formulation can be written as

$$\int \delta(E) G_{E,V}(E) \, dE = n,$$  \hspace{1cm} (2.21)

in which $n = n_V$ is the number density, and

$$\frac{1}{n} \int E \, \delta(E) G_{E,V}(E) \, dE = \langle E \rangle,$$  \hspace{1cm} (2.22)

Making use of values of well-known definite integrals, and the relation between mean kinetic energy and temperature $\langle E \rangle = \frac{3}{2} kT$ we find that

$$\delta(E) = n \frac{h^3}{8\pi (2\pi mkT)^{3/2}} \exp(-E/kT)$$  \hspace{1cm} (2.23)

and consequently

$$N_{E,V}(E) = n \delta(E) = 2\pi^{-1/2} n(kT)^{-3/2} \exp\left(-\frac{E}{kT}\right)$$  \hspace{1cm} (2.24)

The function which gives the fraction of this equilibrium number of particles per unit energy range $p(E) = N_{E,V}(E)/n$ will be denoted with the Maxwell distribution function.

2.2.3 Excitation and deexcitation; Boltzmann.

The back- and forward processes are here represented by

$$A_1 + \pi + (E_{1u} + E) \rightarrow A_u + \pi + E.$$  \hspace{1cm} (2.25)

The forward process is a collision of a particle $\pi$ with an atom (or ion; cf. note 2) with as a result that the initial lower internal state $l$ of the atom $A_1$ is transferred into the final upper state $u$. In this endoergic process of excitation, kinetic energy is converted into the internal energy of the atom which increases with the same amount $K_{1u} = E_{1u} - E_{1l}$ (cf. note 3).

The backward process is the exoergic deexcitation process. The demand of DB results in

$$\hat{\delta}(E) \, \delta(E_{1u} + E) = \delta(E) \, \delta(E_{1u}).$$  \hspace{1cm} (2.26)

The same technique as given in the derivation of eq.(2.11) here results in
\[ \hat{\eta}_A(E_e)/\hat{\eta}_A(E_u) = \hat{\eta}_u(E)/\hat{\eta}_u(E_{1u} + E) = \exp(E_{1u}/kT) \]  

(2.27)

The number of quantum states is now given by the statistical weight \( g(1) \), of the level 1. In contrary with the \( G(E) \) of the free particle states, the number of internal states of the atom \( g(1) \) is not proportional to the volume. It is therefore useful to introduce the reduced population density \( \eta(1) \) i.e. the number density of state 1, \( n(1) \), per statistical weight i.e. \( \eta(1) = n(1)/g(1) \). This reduced number density is related to the number of particles per quantum state by

\[ \eta(1) = \hat{\eta}(E_u)/\gamma \]  

(2.28)

and eq. (2.26) can be written as

\[ \eta(u) = \eta(1) \exp(-E_{1u}/kT) \]  

(2.29)

the well-known Boltzmann relation, a relation between level densities. The density \( \eta^b(u) \) related to the ground-state density \( \eta_1 \) such that

\[ \eta^b(u) = \eta_1 \exp(-E_{1p}/kT) \]  

(2.30)

holds, will be referred to as "the Boltzmann density".

2.2.4 Ionisation and three particle recombination; Saha. The back- and forward processes are here represented by

\[ A_p + \pi + (\varepsilon_p + E_e + E) \leftrightarrow A^+ + \pi + e + (E_e + E) \]  

(2.31)

The forward process is a collision of a particle \( \pi \) with an atom (ion) initially in state \( p \). Due to the collision the atom is ionized. We consider the case in which the ionization leads to the ionic ground state. From the kinetic energy of the colliding particles an amount \( |\varepsilon_p| \) is used to liberate the electron and an amount \( E_e \) is transferred into kinetic energy of the free electron.

The backward process is exoergic. The kinetic energy \( E_e \), of the captured electron and the energy released in binding the electron are converted into kinetic energy of the atom and the particle \( \pi \).

In the same way which leads to eq. (2.7) we find that

\[ \hat{\eta}_A(p)\hat{\eta}_p(E_p + E_e + E) = \hat{\eta}_u \hat{\eta}_u(E_e)(E_u)^n \]  

(2.32)

where \( \hat{\eta}_A = \gamma \hat{\eta}_u/\eta_1 \) is the ion number density per statistical weight (cf. note 4). Since both the electrons and the particles \( \pi \) are
supposed to have a Maxwell distribution function we can substitute eq. (2.23), which results in
\[ n_A^e(p) = \frac{n^e}{2} \frac{n_1^e}{n_1^e} \frac{\hbar^3}{\pi^{3/2} \sigma^3} \exp \left[ \frac{\hbar^2}{8\pi m^2 kT} \right] \frac{n^e_A(p)}{\bar{s}(p)} , \]  
the well-known Saha equation.

2.2.5 Matter-radiation interaction, Planck.
Several types of interactions are involved in the establishment of Planck’s radiation law. For instance, in a plasma we have photon-electron and photon-atom interactions. The first processes like free-free transitions (Bremsstrahlung) will not be discussed in this study. In the second case we have bound-free, free-bound and bound-bound transitions. The establishment of equilibrium in the bound-bound processes (line radiation) will be discussed below.
We consider the decay of an atom from an upper state \( u \) to a lower state \( l \), under simultaneous emission of a photon with energy \( \hbar \nu = E_u - E_l \). The inverse process is absorption of a photon with energy \( \hbar \nu \) leading to the opposite atomic transition. For- and backward processes are represented by
\[ A_u \leftrightarrow A_l + \hbar \nu . \]  
In the case of a weak radiation field we can employ the classical technique given in the preceding for which \( \Phi \) demands that in the volume \( V \)
\[ Vn(u)g_{\nu}(1)G_{\nu} = Vn(l)g_{\nu}N_{\nu} \]  
In the presence of a dense radiation field this classical approach is no longer valid. The results of quantum statistics can be interpreted such that the number of forward processes is enhanced by the fraction of photon quantum states ‘already’ occupied (cf note 5). So we get the balance
\[ Vn(u)g_{\nu}(1)G_{\nu} (1 + \frac{N_{\nu}}{G_{\nu}}) = Vn(l)g_{\nu}N_{\nu} . \]  
This enhancement is known as stimulated emission and is usually represented by the reaction equation
\[ A_u + \hbar \nu \rightarrow A_l + \hbar \nu . \]  
The two photons at the r.h.s. belong to the same quantum state i.e.
they are coherent. By employing $\frac{n}{N}=\frac{\pi}{h}$ and $n=\frac{(\omega)/h}{(\exp(-\hbar\omega/kT))}$ we find that

$$n_{\nu} = (\exp(\hbar\nu/kT) - 1)^{-1}. \tag{2.38}$$

The photon distribution can be obtained from the quantum state distribution (the number of photon quantum states per unit volume and energy range) which in its turn can be deduced from the phase space density. In analogy with the case of material particles, the number density in phase space is given by $G_{\nu}=2\hbar^{-3}$ (the factor 2 corresponds with possible directions of polarization). Transformation to configuration space can be achieved by using $G_{\nu,\nu'}=\int_0^\infty \frac{d\nu'}{\nu'\nu} \exp(-\hbar\nu/kT)$ and the relations $\nu = E/c = \hbar\nu/c$. This results in

$$G_{\nu,\nu'} = 8\nu^2 c^{-3} \hbar^{-1}. \tag{2.39}$$

In this case of radiation the conditions expressed in the eqs. (2.12) and (2.13) are fulfilled in a natural way. The quantum states are optimally populated, that is to say according to the weight-factor $(\exp(\hbar\nu/kT)-1)^{-1}$ only.

So the photon distribution is given by

$$N_{\nu,\nu'} = 8\nu^2 c^{-3} \hbar^{-1} (\exp(\hbar\nu/kT)-1)^{-1}. \tag{2.40}$$

Planck's radiation law can now be obtained realizing that the energy density per unit of volume and frequency interval equals

$$\rho_{\nu} = N_{\nu,\nu'} \nu \frac{d\nu}{d\nu}, \tag{2.41}$$

and consequently that

$$\rho_{\nu} = 8\nu^3 c^{-3} (\exp(\hbar\nu/kT)-1)^{-1}. \tag{2.42}$$

Another important quantity is the equilibrium value of the spectral intensity, given by

$$I_{\nu} = 2\hbar^3 c^{-2} (\exp(\hbar\nu/kT)-1)^{-1}. \tag{2.43}$$

This spectral intensity $I$ is the energy per unit time, area, frequency range, and solid angle, emitted in the direction perpendicular to a surface embedded in a TE radiation field.
Note 1. The limit procedure to obtain the differential equation seems to be in contradiction with the quantum nature of energy. Dealing with the kinetic energy of free particles, the smallest energy change is small enough (provided $\psi$ is large enough). For bound states another technique should be used (cf. [OST 70]) which gives the same result.

Note 2. We use 'atom' to refer to atoms as well as ions. A neutral atom will be denoted by the term 'neutral'. In general the groundstate density $n_\gamma$ will refer to that of an ion with core-charge number $Z$ and the ion density $n_\gamma^+$ to that of the subsequent ion state with charge number $2Z+1$.

Note 3. The internal energy of the atom in state $p$ is denoted by $E_p^p$, which is a negative quantity defined as $E_p^p = -|E_p|$. The positive quantity $|E_p|$ is the ionization potential of the atomic state $p$.

An analogous concept of $E_p^p$ is that of the energy of the bound outer electron. Evidently $E_p^p = 0$ corresponds with a free electron without kinetic energy. The energy difference $E_p^p - E_p$ is the excitation energy of the level $p$; the subscript 'I' refers to the groundstate.

Note 4. In eq. (2.32) the kinetic energy of the atom and ion was ascribed to the particles $\pi$ and $\tau$. A proper treatment in which the kinetic energy of $\pi$ and $\tau$ are considered separately would have introduced a further splitting of the kinetic energy. The exponential factors created in this way would have been eliminated in the division leading to eq. (2.33) and thus the same result is obtained.

Note 5. In the case of fermions the fraction of occupied quantum states will not result in an enhancement but in a diminution. Exclusion of fermions is the opposite of stimulation of bosons. This puts an upper limit to the electron densities to be considered, in such a way that $\Phi$ in eq. (2.23) should be less than unity in order to justify a classical, Maxwellian treatment. Numerically this results in

$$n_e < 6 \times 10^{27} \frac{T_s^{3/2}}{\alpha} \exp \left( \frac{E}{kT_e} \right)$$

(2.44)

with $\frac{T_s}{\alpha}$ in eV and $n_e$ in $\text{m}^{-3}$. 
2.3 Deviations from the Maxwell distribution.

2.3.1 General

In this section we will discuss equilibrium deviations from the balances of type

$$\dot{\pi}_1 + \pi_2 \rightarrow \dot{\pi}_1 + \pi_2,$$

$$E_1 \rightarrow E_2,$$

in which kinetic energy is exchanged between particles $\pi_1$ and $\pi_2$.

In an atomic plasma there are generally three different kinds of collision partners, electrons $e$, ions $i$, and neutrals $a$. So, formally the kinetic energy exchange between six different couples has to be considered ($e-e$; $i-i$; $a-a$; $e-i$; $e-a$; and $i-a$).

However, the goal of the present study is to classify non-LTE distribution functions of atomic states, and as we will see in section 2.4.7, these are primarily determined by electron collisions (or radiative processes). Thus, we can restrict ourselves to the study of the possible deviations from a Maxwellian distribution function of the electron gas, for which the $e-e$ interactions are the equilibrium restoring processes. Elastic collisions of the type $e-a$ and $e-i$ can disturb the Maxwellisation. Other elastic collisions will not be discussed in this section since the distribution functions of ions and neutrals are not of interest in this study.

In the study of the Maxwell-validity of the electron gas it turns out that it is useful to distinguish between Maxwell for the whole energy range and Maxwell for the energies smaller than the first excitation energy gap $E_{12}$ only. These two regions are denoted by case MA and case MB. The corresponding validities depend on the ionization degree, the electron temperature, electric field strength and frequency and the plasma dimension. We focus our attention on sufficient conditions for the Maxwellisation of electrons. These conditions are not always necessary.

2.3.2 Maxwell criteria for the electron gas

The discussion of the validity criteria for the Maxwellization of the electron gas will be guided by the Boltzmann equation (cf. eq. (1.1))

$$\frac{\partial f_e}{\partial t} = v \cdot \nabla f_e + \left( \frac{\partial f_e}{\partial E} \right) \nabla E = \left( \frac{\partial f_e}{\partial E} \right)_{\text{el}} + \left( \frac{\partial f_e}{\partial E} \right)_{\text{exc}} + \left( \frac{\partial f_e}{\partial E} \right)_{\text{ion}} + \left( \frac{\partial f_e}{\partial E} \right)_{\text{ele}} $$

$$+ \left( \frac{\partial f_e}{\partial E} \right)_{\text{exc}} + \left( \frac{\partial f_e}{\partial E} \right)_{\text{ion}} + \left( \frac{\partial f_e}{\partial E} \right)_{\text{ele}} $$. (2.46)
in which all processes compete with each other in the determination of the electron energy distribution. The Maxw ellization is affected by the first term at the rhs of eq.(2.46). The other terms reflect equilibrium disturbing processes. The Maxwell validity criteria can be traced back to these terms by the demand that they should be much smaller than the equilibrium restoring term for the elastic e-e interaction. In practice 'much smaller' will be replaced by smaller than or equal to one tenth.

1) The most important collision term \(\frac{\partial f}{\partial t}\) reflects the elastic e-e interaction. If these processes are dominant the Maxwell distribution will be established as described in sect.2.2.1. This happens within the typical Maxwellization time ([BR 65] and [SFT 56])

\[
\tau_{ee} = 3.4 \times 10^{11} \frac{\sigma_{ee}^{3/2}}{T_e^{3/2}} \left( \frac{n_e}{\ln \Lambda_e} \right)^{-1}.
\]  

(2.47)

The electron temperature \(T_e\) is in eV, the electron density \(n_e\) in \(m^{-3}\), and \(\ln \Lambda_e\) is the Coulomb logarithm (with a typical value of \(\ln \Lambda_e=10\)). It should be noted that eq.(2.47) gives a mean value. The time needed to 'cool' an electron with energy \(E \gg kT_e\) is according to [KRL 78] given by

\[
\tau_{eq} = 1.3 \times 10^{11} \frac{\sigma_{ee}^{3/2}}{T_e^{3/2}} \left( \frac{n_e}{\ln \Lambda_e} \right)^{-1}.
\]  

(2.48)

with \(\bar{E}\) in eV.

2) The relaxation time for energy transfer to ions is \(m_i/m_e\) longer than the value given by eq.(2.47). Since \(n_e = n_i\) (charge neutrality) we can neglect the second collision term.

3) The third collision term reflects the elastic collisions between electrons and neutrals and can be characterized by the e-a collision frequency for kinetic energy transfer \(2(\sigma_{ea}/m_a) n_e v_e\) the CEA in which \(v_e\) is the e-a cross section for momentum transfer. The validity of Maxwell for the bulk of the electrons implies that within \(\tau_{ee}\) the number of e-a collisions is much smaller than unity. So employing eq.(2.47) for \(\tau_{ee}\) and using \(v_e = \sqrt{2m_e\bar{E}}\) this validity criterion results in

\[
\frac{n_e}{n_a} \geq 2.7 \times 10^{-6} \frac{\sigma_{ea}}{M_a} \frac{M_a}{m_e} \left( \frac{n_e}{n_a} \right)_{cr}^{1/2},
\]  

(2.49)
in which $\tilde{M}$ is the mass in amu and $\sigma_{ea}$ the cross section in $10^{-20} m^2$. We used $M_e = 3.6$ and the symbol $>>$ is replaced by $\geq 10$. By means of the $\tilde{M}$ symbol we introduced a critical ratio. In fig. 2.2 this critical ratio is sketched for $\tilde{M}_{ea} = \tilde{M}_{12} = 1$.

Calculation of the electron distribution function in a medium pressure neon discharge [SNI 79] shows that the Maxwellian form of the bulk is established if $n_e/n_a \geq 4 \times 10^{-6}$ for $T_e = 3eV$. This is in accordance with the criterion formulated in eq. (2.49). For a further study along this line we refer to [MIT 79].

It should be noted that this condition is not in all cases necessary.

In the absence of electric fields and $T_e = T_a$ lower ionization degrees can be permitted.

4) The fourth collision term reflects the inelastic excitation collisions of electrons with atoms. We consider the worst case in which the atomic energy scheme is not in equilibrium, and excited states are largely underpopulated with respect to Boltzmann. Consequently the reverse process of deexcitation is not present to balance the energy loss of the electrons.

To get a validity criterion for the Maxwell distribution we employ a model based on the assumptions that

- there are no molecules in the plasma so that vibrational and rotational excitation can be neglected.
- only the energy gap (cf. [SMA 70]) between groundstate and first excited state will be considered. Cross sections of other transitions (including direct ionization) are ascribed to the transition $1\rightarrow 2$.
- the energy gap is larger than the temperature, i.e. $\hbar \omega > 2kT$ and that
- hydrogenic cross sections and rate coefficients can be employed.

In this model the electrons are divided into two groups: a small tail and a large bulk (cf. fig. 2.1). If a tail-electron excites an atom, it loses energy and it is removed from the tail. On the other hand, the tail is populated due to $e-e$ interactions. A deviation from Maxwell
can be expected if the rate of inelastic tail output processes exceeds the Maxwell value of the rate of the elastic tail input processes. The equilibrium number density of the tail electrons equals

$$n_T = n_e \int_{E_{12}}^{\infty} P(E) \, dE \approx n_e \left( E_{12} / kT \right)^0.5 \exp(-E_{12} / kT) .$$

(2.50)

The rate of excitation processes in equilibrium equals

$$n_e n_e K(1,2) = 4.4 \times 10^{-12} n_e n_e \tau_0^{-0.5} E_{12}^{-1/2} \exp(-E_{12} / kT) .$$

(2.51)

This is eq.(3.44) in which we take the sum of the oscillator strength

$$\alpha_{12} = \alpha_{12}^0$$

is a form factor according to [58A 77] (cf. eq.(5.63) and fig. 9.7) and $E_{12}$ is expressed in eV. So, the mean excitation frequency for an electron in the tail is given by

$$\nu_{12} = n_e n_e K(1,2)/n_e \approx 4.4 \times 10^{-12} n_e^{-3/2} E_{12}^{-1/2} .$$

(2.52)

The rate at which the tail is supplied via elastic processes from the bulk, equals (in equilibrium) the rate at which tail electrons lose energy due to elastic collisions with bulk electrons. In order to estimate the rate of energy transfer we use eq.(2.48) and we get

$$\nu_{\text{eq}} = 7.7 \times 10^{-11} n_e n_e \tau_0^{-3/2} E_{12}^{-1/2} .$$

(2.53)

The validity condition for Maxwell now reads that $\nu_{\text{eq}} / \nu_{12} > 10$ which gives the relation

$$n_e / n_+ \geq 6 \times 10^{-2} \nu_0 \approx (n_e / n_+)^{\text{exc}} .$$

(2.54)

between the ionization degree and the temperature. Again we used $n_+ = n_e$.

The critical value $(n_e / n_+)^{\text{exc}}$ is shown in fig.2.2 for $E_{12} = 10$eV (hydrogen); we see that for low temperatures low ionization degrees can be allowed whereas for high temperatures the ionization degree must be larger. It should be emphasized that for high temperatures, i.e. $kT > 1/2 E_{12}$, this model cannot be employed. Then the division in bulk and tail electrons is no longer a realistic approach. However, for higher temperatures all systems, except hydrogen, will move to the new ionization stage where the core of the 'groundstate' has charge number $Z=2$. Since charge neutrality implies that $n_e = n_+$, the Maxwell
distribution is usually assured (cf. fig. 2.2 where the critical ratios are much smaller than one). For the hydrogen system at high temperatures (as in tokamaks) the ratio of electron density to atom density is usually very large. Also here, the disturbance of the Maxwell distribution function by inelastic processes can be ignored.

From fig. 2.2 and the preceding text we may conclude that
- Excitation processes put a more severe demand on the Maxwell validity than elastic collisions.
- We can distinguish two regions.

MA, with \( n_e / n_a > (n_e / n_a)^{\text{exc}} \)  
and MB, with \( (n_e / n_a)^{\text{el}} \leq n_e / n_a < (n_e / n_a)^{\text{exc}} \)  

- In case MA the complete distribution is Maxwellian. In case MB the tail is affected due to non-equilibrium excitation processes, but since \( E_{\text{el}} / kT > 2 \) the tail contains much less electrons than the bulk. So the tail depletion is of no importance for the bulk which keeps a Maxwellian form. This is in accordance with the theoretical results presented in [SHA 70].

Fig. 2.2
Critical values of the ratio \( (n_e / n_a) \) as a function of temperature. 
\( (n_e / n_a)^{\text{el}} \) belongs to elastic collisions with neutrals (eq. (2.49) with \( \delta = \delta_a = 1 \)), and 
\( (n_e / n_a)^{\text{max}} \) belongs to excitation processes (eq. (2.54)). In the calculation of \( (n_e / n_a)^{\text{exc}} \) we applied \( E_{\text{el}} = 10 \) eV which refers to the hydrogen system.

If other systems are considered we should replace 10 eV by the first energy gap of that system and the second horizontal axis \( (E / E_{\text{el}}) \) should be used for \( (n_e / n_a)^{\text{max}} \). The curve of \( (n_e / n_a)^{\text{max}} \) is intersected for \( T / E_{\text{el}} > 0.5 \) since the model loses validity for higher \( T_e \)-values.

Case MA refers to Maxwell for the entire \( T \)-range and case MB to Maxwell for the bulk only. (cf. text and table 2.1)
It is still useful to maintain case MB as a possibility in our plasma classification. Surely we lose information about the 1 + 2 excitation process, but due to the Maxwellian form of the bulk, the rate of electron induced transitions between excited levels is determined to atomic properties and the bulk temperature. Thus case MB can still be treated to study the shape of the distribution function. In the calculation of the absolute value of the distribution function of excited states, the additional information of the tail is needed in order to calculate the rate of the ground state excitation-and ionization rates.

5) From fig. 5.2 it can be deduced that excitation of ions will not affect the Maxwellian of electrons since \( n_e^0/N_e^0 = 1 \) (charge neutrality). This value is much larger than the critical ratio derived for \( n_e^0/N_e^0 \).

6) In the lth of the Boltzmann equation the influence of the electric field strength is expressed by the third term \( \frac{eE}{m_e} \lambda_{ee} \). By comparing this term with the e-e interaction we find that the electric field is not important provided that

\[
\frac{eE}{m_e} \lambda_{ee} \ll 1 \quad \text{or} \quad \frac{eE}{m_e} \ll \lambda_{ee} \ll 0.1 \tag{2.56}
\]

which merely expresses that the energy gain of an electron due to the acceleration over a mean free path (mfp) must be much smaller than the thermal energy \( (1/2 \ kT) \) in the degree of freedom along the field lines.

By inserting \( \lambda_{ee} = \frac{4\pi}{3} \frac{\kappa T_e}{m_e} \) and eq. (2.47) for \( \lambda_{ee} \), we find that

\[
\epsilon \leq 7 \times 10^{-18} \ n_e \frac{\pi}{T_e} \ \text{cm}^{-1} \ \text{V}^{-1} \ \text{m}^{-1} \ . \tag{2.57}
\]

It should be noted that this condition is formulated for the average electron. Specified to an electron with energy \( E \) we find an \( T^{-1} \) dependence. So tail electrons are more sensitive to acceleration than bulk electrons are. This is closely related to the phenomenon of run away electrons which is studied in [DRE 59].

7) If the electric field is oscillatory this creates another problem expressed by the first term of eq. (2.46). Validity of Maxwell implies that the frequency of the applied \( \epsilon \) -field must be much smaller than \( \lambda_{ee} \) i.e.

\[
\epsilon \leq 3 \times 10^{-12} \ \text{n_e} \pi^{-3/2} \ . \tag{2.58}
\]
In that case a quasi stationary treatment of the distribution function is possible which means that a Maxwellian description is possible at any moment, although the distribution function can change in time. The frequency dependency of RF plasmas is investigated in [VAL 85] and [WIN 84].

8) The effect of inhomogeneity is reflected in the \( \nu \sqrt{\nu} \) term. Here we have the demand that

\[
\nu \sqrt{\nu} \frac{\rho}{e} \lesssim \nu \frac{f_{ee}}{e} \leq f_{ee} \frac{1}{\lambda_{ee}} \text{ or } \lambda \lesssim 10 \lambda_{ee},
\]  

(2.59)

which imposes the restriction that the linear dimension \( \lambda \) of the plasma should be much larger than the mfp of the e-e interaction. Under that condition a local Maxwellian description is possible. Numerically we find

\[
\lambda \gtrsim 1.4 \times 10^{17} n_{e}^{-1} E_{e}^{2} \text{ (m)},
\]

(2.60)

which must be satisfied to make a local treatment possible.

It should be noted that the demand expressed by eq.(2.60) is not in all cases necessary. In a magnetized plasma the mfp can be replaced by the cyclotron radius.

2.3.3 Summary

From the preceding study of the Maxwellization of the electron gas we may conclude that:

- The tail is most sensitive to equilibrium disturbing processes. The electric field can cause an enhancement of the tail due to the creation of runaway electrons, whereas the excitation collisions with neutrals can cause a depletion of the tail.
- The interaction of the type e-i can be ignored.
- Only low temperatures, i.e. \( kT \leq \frac{1}{2} \epsilon_{12} \), in which \( \epsilon_{12} \) is the first excitation gap of the neutral system have to be regarded. For increasing temperatures the system will move to the next ionization stage, which implies an elimination of the neutral particles.
- An important exception to this rule is the hydrogen plasma. Maxwellization of the electron gas of fusion reactors lies beyond this classification.
- It is useful to distinguish between Maxwell for the whole energy range and for the bulk alone. This decoupling of tail and bulk introduces a decoupling in the bottom and top of the system.
Table 3.1
Sufficient conditions for the validity of the Maxwellation of the electron gas. Most conditions are generally not necessary. Column 5 gives extenuating meronamenon. A * sign in the column headed with 'effect on tail' indicates that the Maxwell-departure implies an enhancement of the tail.

Note: The critical values of $\lambda, f_c$, and $\varepsilon$ are valid for the bulk of the electron gas. If Maxwellation is requested for electrons with energy $E \gg T$ one should enhance the given critical value of $\lambda$ with $(E/T)^{3/2}$ and reduce the critical value of $f_c$ and $\varepsilon$ with $(E/T)^{3/2}$.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Condition</th>
<th>effect on tail less necessary in</th>
<th>eq.</th>
<th>ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>linear dimension</td>
<td>$\lambda$</td>
<td>$\lambda \geq 10 \lambda_{ee}$</td>
<td>presence B field</td>
<td>(2.60)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\lambda \geq 1.4 \times 10^{17} \frac{n_{ee}}{n_e^2}$</td>
<td></td>
<td></td>
<td>[WAL 85]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$f_c \leq 0.1 \frac{\varepsilon}{\varepsilon_{ee}}$</td>
<td></td>
<td>(2.58)</td>
<td>[WAL 85]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$f_c \leq 3 \times 10^{-12} \frac{n_{ee}}{n_e^2}$</td>
<td></td>
<td></td>
<td>[WIN 84]</td>
</tr>
<tr>
<td>electric f. frequency</td>
<td>$\varepsilon$</td>
<td>$\varepsilon \leq 0.1 \frac{\varepsilon}{\varepsilon_{ee}}$</td>
<td>presence excitation</td>
<td>(2.57)</td>
<td>[DRE 59]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\varepsilon \leq 7 \times 10^{-18} \frac{n_{ee}}{n_e^2}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ionization degree ($n_i/n_e$)</td>
<td></td>
<td>Case A: $\geq (n_i/n_e)^{0.53c}$</td>
<td>Boltzmann capture of radiation</td>
<td>(2.54)</td>
<td>[SHA 70]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Case B: $\leq (n_i/n_e)^{0.53c}$</td>
<td>absence of radiation</td>
<td>(2.49)</td>
<td>[BRA 79]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$T_e = T_a$</td>
<td></td>
<td></td>
<td>[MIT 73]</td>
</tr>
</tbody>
</table>
2.4 Deviation from the Boltzmann distribution

2.4.1 general

In this study, which is focussed on the distribution function of atomic states, the deviations from the Boltzmann distribution are of great interest. Only in TE and LTE the distribution is sufficiently close to the Boltzmann equilibrium to be characterized by a temperature. In all other cases in which classification is needed there will be departure from the proper Boltzmann balance:

\[ A_1 + \pi + (E_{1u} + E) \leftrightarrow A_u + \pi + (E) \]  \hspace{1cm} (2.61)

Excitation and deexcitation are in general not balanced and we have to consider flows, sources and sinks in the excitation space which are caused by improper balances. To calculate the distribution function in the absence of LTE, information is needed about the various rate coefficients for production and destruction processes.

In this section we will study rate coefficients of transitions of type (2.61) in which the role of the particle \( \pi \) can be played by an electron \( e \), ion \( i \) or neutral \( n \). These rate coefficients will be compared with each other and with the rate for radiative decay.

The rate of forward process of the type (2.61) equals the product \( n_p n(1) K_x(1,u) \) in which \( n_p \) and \( n(1) \) are the number densities of the particles \( p \) and the atoms in state \( 1 \).

The rate coefficient \( K_x(1,u) \) is the product of the cross section \( \sigma_x(1,u,E) \), and the velocity \( v = \sqrt{2E/m} \) averaged over the Maxwellian distribution function, i.e.

\[ K_x(1,u) = \langle \sigma_x(1,u,E) v \rangle = \int_{p1}^{P} \frac{e^{P(E)/\sqrt{2E/m}}} {\sqrt{2E/m}} \sigma_x(1,u,E) dE \] \hspace{1cm} (2.62)

In fact we should integrate over the relative velocity and two distribution functions are involved. In the case of electron excitation the relative velocity is determined by the electron and only the electron distribution is of relevance. For ion-neutral collisions only the ion distribution and velocity are of importance if \( T_i > T_n \) so the representation of eq.(2.62) has a large range of applicability.

In the following we will study cross sections and rate coefficients of (endothermic) excitation processes. By the application of the principle of DB which states that in equilibrium the relation...
\[ n^b(u) K_n(u,1) = n^b(l) K_n(l,1) \] (2.63)

holds, the rate coefficient for the deexcitation process can be obtained. This relation (2.63) can be applied even in the absence of equilibrium. A sufficient condition is that the velocity distribution of particles \( n \) is Maxwellian.

2.4.2 Cross sections; main features

In this study we use the following concepts:

With 'atom' we refer to atoms as well as ions; a 'hydrogenic' is an atom which consists of a nucleus with charge number \( Z \) and one outer electron, whereas a 'hydrogen-like' atom (or state) consists of a core (nucleus and inner electrons) and one outer electron; the interaction between core and outer electron is negligible. A 'rydberg state' is a state in which the interaction between core and outer electron is not negligible but limited. Section 3.2 is devoted to the classification of atomic states.

It is useful to distinguish between neutral-atom (n-a) and charged particle-atom collisions (e-a) and (i-a). We first consider the main features of cross sections of collisions in which charged particles are involved. In section 2.4.5 n-a collisions will be considered, while chapter V is completely devoted to electron-atom collisions.

The shape of the cross section depends on the kind of excitation transition which for hydrogenics can be classified [DRA 66] in

1) optically allowed \( \Delta E = 0, \Delta n = 0 \),
2) parity forbidden \( \Delta E \neq 0, \Delta n = 0 \), and
3) spin forbidden \( \Delta n \neq 0 \).

In which \( \ell \) and \( s \) represent the orbital and spin quantum number.

1) The shape of the cross section as function of energy of optically allowed (i.e., dipole-) transitions varies relatively slowly. For instance the tail of the function decreases slowly with \( E^{-1} \ln E \)-dependence.

2) Parity forbidden transitions are rapidly increasing and decreasing compared to the dipole transitions. The tail has \( E^{-1} \)-dependence.

3) For the spin forbidden transitions the cross section is even more peaked; the tail has a typical \( E^{-3} \)-dependence.

In fig. 2.3 we compare the three shapes as function of \( U = E/E_0 \) as obtained from [DRA 66].

For non-hydrogenics this 3-fold classification can be obtained if the atom is composed of a core and one outer electron (a Rydberg state).
Fig. 2.3
A comparison between the shapes of the cross sections of an optically allowed $\sigma^0$, a parity forbidden $\sigma$ and a spin forbidden $\sigma^0$ transition as functions of $U_{ij} = E/E_{ij}$.

2.4.3 The threshold temperature ratio
In contrast with the tail of the cross section, the threshold behaviour is still a subject of theoretical discussion. Apart from the charges of the colliding particles it depends on the reduced mass of the colliding system. In the case of electron collisions with ions of large Z-values, the initially slow incident electron will be strongly accelerated and the probability of a transition is greater than that of a (Z-scaled) electron-neutral collision. In fig. (2.4) a sketch is given of $\sigma(E)$ as function of Z for electron collisions. It appears that for large Z-values the tail can be extrapolated to the threshold.

Fig. 2.4
A sketch of the threshold behaviour of the cross sections for the 1s-2p transitions in hydrogenics according to [SPA 66].
It depends on the threshold temperature ratio $E_{th}/kT$ how important the uncertainty behaviour of the threshold is in the determination of the rate coefficients. We therefore introduce the following classification.

1) Large threshold processes, $E_{th}/kT > 1$, are often found in the case of excitation from the ground state to excited states. The greater part of the rate coefficient $K(1,0)$ originates from the integration of the theoretically uncertain threshold part of the cross section over the tail of the distribution function (cf. fig. 1.5a). The use of experimental results (direct or in a semi-empirical way) for ground state excitation has to be preferred above that of pure theoretical calculations. A second feature typical for large threshold processes is that they are induced by particles in the tail of the velocity distribution. And especially this tail is sensitive to non-equilibrium situations, resulting from the fact that kinetic energy exchanges between tail- and bulk-particles are ineffective due to the large energy gap (cf. sect. 2.3).

For small temperatures the transitions between highly excited states can also be of the large threshold type. For a sufficiently high principle quantum number these processes can be described classically (cf. chapter V).

2) Small threshold processes, $E_{th}/kT < 1$, are often found between excited states. The $K(1,0)$ is mainly determined by the bulk of the distribution function and the well-known Born tail of $\sigma(E)$ (see fig. 1.5b). The smaller the threshold the more the uncertainty in the rising part loses its importance. On the other hand there is not much experimental evidence for excitation processes between excited states. So we have to rely upon at least one of the several semi-empirical (SE) approximations for cross sections like those given by [GTY 65], [JOH 72], [DRA 71], [GEE 76], and [TRE 80]. In chapter V these SE approximations for electron induced transitions will be discussed.

- By realizing that the cross section of charge particle-atom collisions is mainly determined by the velocity and loss by the mass of the colliding system we may conclude that both large and small threshold transitions are mostly electron induced.

3) Very small threshold processes $E_{th}/kT \ll 1$ are e.g. those of changing collisions for hydrogenic and transitions between sublevels of more complex systems (cf. fig. 1.5c).

For these transitions electron collisions lose their importance whereas ion collisions become more effective. This can be understood realizing that the cross section depends mainly on the velocity and
Fig. 2.5a
An example of a large threshold process \( \Delta E/kT \gg 1 \) from ground to excited state.

Fig. 2.5b
An example of a small threshold process \( \Delta E/kT \ll 1 \) between two excited states.

Fig. 2.5c
A very small threshold process \( \Delta E/kT \ll 1 \).

The energy scheme in the right upper corner of the figs. indicates the corresponding transition.

much less on the mass of the incident particle (cf. section 3.5 [SEA.64b] and [PEN.64]). In fig.(2.6) the distribution functions of both electrons and ions together with the cross section are given as functions of velocity \( v \) for \( T_e = T_i \). Since there are much more ions than electrons with small velocities, the rate coefficient for ion collisions is larger than those of electrons.

- Concluding we may state that very small threshold transitions are ion (heavy particle) induced
To compare the rate coefficient of transitions induced by ions with those induced by electrons we consider the case where electrons and ions have the same temperatures and write the rate coefficient as a product of thermal speed and a mean cross section \( \langle \sigma v \rangle = \langle v \rangle \sigma_{\text{th}} \). Then the ratio of the rate coefficients is given by

\[
\frac{K_e}{K_i} = \frac{v_{\text{th}} e}{v_{\text{th}} i} \frac{\sigma_e}{\sigma_i} = \frac{\sqrt{\frac{m_e}{m_i} \sigma_e}}{\sqrt{\frac{m_i}{m_e} \sigma_i}}.
\]

(2.64)

For the \( v^2 \) dependent processes (type II) this means that

\[
\frac{K_e}{K_i} = \frac{1}{\sqrt{\frac{m_i}{m_e}}}.
\]

(2.64a)

which e.g. for hydrogen implies that the proton collision rate is a factor 40 larger than that of electrons. For optically allowed transitions (type I) the ion dominance is less pronounced while for spin forbidden transitions, ion rates surpass those of electrons by a factor \((m_i/m_e)^{2.5}\).

From the literature it appears that the maximum cross section of spin forbidden transitions (type III) is generally not much larger than that of comparable transitions of type I and II. Moreover we see in fig. 2.3 that the area under \( \sigma^e \) is much smaller than that under \( \sigma^n \) and \( \sigma^P \). Thus we can conclude that electron induced spin forbidden transitions are only of importance for large threshold transitions.

2.4.4 Critical densities

The balance of type (2.61) can be disturbed by radiative decay processes with rate \( n(\nu)A(\nu,1) \). Since the rate for the collisional deexcitation process equals \( n_0 n(1) K(1,0) \), the decay processes will be important for small \( n_e \) values. The demand that the influence of radiative decay processes can be neglected puts a lower limit on \( n_e \), the critical density \( n_{e}^{C} \). Note that the critical density is state dependent.

We first consider in a hydrogen plasma the \( \lambda \) changing transitions between states with the same quantum number \( p \). The process

\[
\text{H}(p,\lambda) + H^+ \rightarrow \text{H}(p,\lambda + 1) + H^+
\]

(2.65)

has been investigated by Pengelly and Seaton [PEN64]. Since these processes are very small threshold transitions, they occur more frequently than due to electron collisions. It was found that very
Large impact parameters contribute to the cross section and that a cut off, depending on the density, has to be introduced. Comparing the rates of eq.(2.65) with those for radiative decay gives a critical value \( n^e \) of the proton density \( n_p \) such that for \( n_p > n^e \) the sublevels of states with \( p > p^* \) are populated according to Boltzmann. In this case of \( E_{\text{tot}} / kT \ll 1 \), for which the Boltzmann factor \( \exp(E_{\text{tot}} / kT) \) equals one, it implies a statistical distribution i.e.

\[
\frac{\partial n}{\partial p} = \frac{2L - 1}{p^2} n(p).
\]  

(2.66)

**Fig. 2.7**
Values of the product of the radiative lifetime and the rate coefficient for changes in azimuthal quantum number as function of \( k \) for different \( p \)-values. (from [WLI 64]).

Figure 2.7 shows the values of the product of the radiative lifetime of a state \( p \), and the collisional rate coefficient for change in orbit quantum number. It is in principle possible to introduce for every sublevel a critical ion density such that \( n^e(p,k) = (k^e \cdot \tau_{p,k}^{-1}) \).

The fact that \( n^e(p,k) \) is by no means constant for one \( p \)-value indicates that atomic processes are not homogeneously distributed over the substates and that collisions of type (2.65) are needed to establish a statistical distribution.
Fig. 2.8
The critical densities \( n_c^\alpha \) and \( n_c^\gamma \) as function of principal quantum number \( \ell \). The solid curve for which \( n_c^\alpha = n_c^\gamma \) is the average of the \( n_c^{\ell}(p,\ell) \) values as obtained from Fig. 7.7. The maximum of the \( n_c^{\ell}(p,\ell) \) value is represented by the dash-dot line.

For \( n_c = n_c^\alpha \), collisional destruction of the energy level occurs once in a mean radiative lifetime.

Fig. 2.8 shows in a log \( n_c^\alpha \) versus log \( p \) plot the results of the \( n_c^{\ell}(p) \) calculations for H found in [BEN 56]. The critical density varies markedly with the principal quantum number \( p \) it scales roughly with \( p^{-3} \). The \( n_c^{\ell}(p) \) values were obtained by taking the average of \( n_c^{\ell}(p,\ell) \) over the various \( \ell \) values. A better approach would be to take the maximum of \( n_c^{\ell}(p,\ell) \). These maximum values are also depicted in Fig. 2.8.

Applied to the He* system where the He*–He\(^+\) collisions are responsible for the \( \ell \)-mixing, the critical density should be multiplied with \( Z^6(n_e/n_{He})^{1/2} \) (the cross section scales with \( Z^2 \) and the radiative lifetime with \( Z^4 \) cf. Table 3.1), but from experimental results of a He* plasma [KOH 77] it appears that the statistical distribution between sublevels is not established for the \( \ell = 4 \) level when \( n_e \approx n_1 = 3 \times 10^{19} \) m\(^{-3} \), \( I_1 = 1 \) eV and \( T_e \approx 20 \) eV. This shows a lack of accordance between experimental and theoretical results.

Going to more complex systems the energy gaps between sublevels will increase, ion collisions will lose their efficiency and deviations from Boltzmann can be expected. Conditions under which Boltzmann holds for sublevel mixing deserve further investigation.

In the same fig. 2.8 we present the critical electron density \( n_c^\alpha(p) \) for an H plasma. This critical electron density is defined such that
for \( n_e \gg n^0_e \) electronic destruction of the energy level with \( p \) quantum number \( p \) occurs more frequently than ones in the mean radiative lifetime, i.e. \( n_e K_e \gg 1 \). This boundary condition for the transition from radiative to collisional dominance will be discussed in sect. 7.8.

2.4.5 Neutral-atom collisions.

We first consider transitions between sublevels. A scaling formula for \( l \)-mixing collisions is given in [MIC 81], from which it appears that collisions of Rydberg atoms with all kinds of (heavy) collision partners can globally be described in the same way. A typical dependence of the cross section as a function of \( p \) is given in fig. 2.9. From this we see that the cross section of an atom with low \( p \)-value is comparable to the geometrical cross section \( \sigma_{\text{g}} = \pi a^2 \). For larger \( p \)-values \( (p>10) \) the cross section lags behind \( \sigma_{\text{g}} \). So compared to \( \ell \)-a collisions where cross sections for \( \ell \)-mixing largely exceed the geometrical cross section, \( n-a \) collisions are less effective. However, the presence of \( n-a \) collisions implies support rather than competition in the establishment of Boltzmann, because even in the case of \( T_a \ll T_0 \) Boltzmann implies a statistical distribution if \( n_{1u}/kT \ll 1 \).

Transitions between energy levels due to \( n-a \) collisions were studied in [DEV 79]. They found experimentally for the destruction rates of \( \text{He} \) levels with \( \Delta p \leq 17 \) values of \( 3 \times 10^{-16} \text{m}^3\text{s}^{-1} \) and only a small \( p \)-dependence. If we give this value to the destruction rate of level \( p=2 \) (which is an overestimation) and compare this with the electron destruction rate of level \( p=2 \) according to

\[
K_e(p) = 10^{-13} p^4,
\]

(2.67)
we see that $n$-a collisions are more effective than e-a collisions if $n_e/n_a < 10^{-5}$ which is comparable to the Maxwell criteria MB.

Thus the conclusion may be drawn that as long as we consider plasmas with a sufficiently high ionization degree such that the bulk of the electrons have a Maxwellian distribution, we can ignore neutral collisions.

2.4.6 Molecular processes

Up to here only atomic particles are considered. In plasmas with molecules, molecular ions, and with several atomic species, other processes than excitation and radiation may influence the distribution of the excited states. Though these processes fall outside the scope of the present study we will make some remarks on this subject.

First in molecular plasmas with a substantial amount of molecules vibrational and rotational excitation is important and must be described. Processes as dissociation, dissociative recombination and attachment will be a function of the vibrational and rotational distribution. As dissociative recombination of a molecular ion is a fast process and usually ends in an excited atom, a disturbance of the excited state distribution cannot be ruled out a priori in plasmas with molecular ions. However if one confines oneself to plasmas with a substantial ionization degree, usually the relative abundance of molecules is small and the influence of molecular processes on the excitation distribution is negligible. An exception may be cool, recombining plasmas and plasmas at higher densities and pressures (e.g. exciplex and excimer laser plasmas).

A second important process in the non-resonant charge transfer reaction in plasmas with more than one kind of atoms and ions. A pertinent example here is the noble-gas/metal-vapor plasmas, as used in metal vapor lasers. An important reaction may be the charge transfer from the noble gas ion (e.g. Ar$^+$) to the metal atom, usually leading to an excited metal ion state. It is clear that this process will form a source somewhere in the excitation space of the metal ion and that this leads to a disturbance of the metal ion excited state distribution. A similar disturbance is present in the neon atomic systems in a He-Ne mixture as in He-Ne lasers.

Though these processes are not considered here it is likely that these processes can be added in the CR-formalism, by introducing a local source term in the equations for the relevant states.

As mentioned, we will confine ourselves to simple atomic plasmas.
2.6.3 Summary

- If the ionization degree is so large that the bulk of the electron gas is Maxwellian and an electron temperature can consequently be defined, the electrons are most effective in the transfer of kinetic into internal energy. In fact, we are faced with a remarkable situation in which energy is exchanged between identical particles in different situations, i.e., free and bound electrons.

- Thus, we may expect that the kinetics of the electron gas will in some way be imposed on the atomic energy scheme, provided that the radiative transitions are not important and that the energy gaps between levels are not much smaller than the mean kinetic energy of the electron gas. If we use as the typical energy gap of the system the ionization potential of the first excited level, \( E_2 \), this means that \( E_2 / kT \) should not be much smaller than one.

- Since a phenomenological fact is that most plasmas 'work' at \( kT \approx E_2 \), we realize that the excitation kinetics is in many cases electron determined.

- Only in the case of a high-temperature plasma, the electron temperature will exceed the typical energy gap by many orders of magnitude.

- More electron systems move to the next ionization stage.

- The decay processes are only important for low \( n_e \) and low \( p \) values; we have seen that the critical density \( n_c \) is a rapidly decreasing function of \( p \).

- Heavy particle collisions will be dominant in the establishment of the Boltzmann distribution between (quasi) degenerated sublevels. But, since for these cases \( \Delta E / kT \ll \), the Boltzmann factor equals unity i.e. \( \exp(\Delta E / kT) \approx 1 \) and a statistically distribution will be the result.

- So, the inequality \( T_e \neq T_1 \neq T_0 \) has no consequences in the study of non-TE distribution functions.

- We can even permit situations in which the temperature of the heavy particles is not defined.
2.5 Deviations from Saha

2.5.1 General

In the class of plasmas where atoms are less effective than electrons in realizing (de)excitational transitions, this also applies to ionization/recombination processes. Since the role of ions can also be ignored, we can restrict ourselves to the balance (eq. (2.33)) in which the third particle \( \omega \) is an electron, i.e.

\[
A_p + e + (|E_p| + E) \rightarrow A^+ + e + \overset{\rightarrow}{e} + (E),
\]

(2.66)

In analogy with the excitation process, the reaction can be characterized by the cross section as a function of energy \( \sigma_{pl}(E) \). The ionization rate coefficient \( S(p) \) is defined in the same way as \( K(p,q) \) (of eq. 2.62)

Once the ionization rate is determined, the recombination rate \( K_p(p) \) can be obtained using the principle of DB by

\[
K_p(p) = \frac{u^b(p)}{[n_e n_p]} S(p),
\]

(2.69)

in which \( n^b(p) \) is the Saha density given by eq. (2.33)). Note that even for levels where ionization and recombination are not balanced, this relation can be employed. The only demand is that the distribution of free electrons is Maxwellian.

2.5.2 On the difference between Saha and Boltzmann

It is instructive to compare the Boltzmann and the Saha distribution with each other. Boltzmann originates from the proper balances of forward and backward processes between levels. It consequently gives (in LTE) a relation between populations of excited states, and (in LTE) between excited states and the ground state. Saha originates from the proper balances of processes from a level at one side and the ion state and continuum at the other side; it consequently relates that level population with that of the ion ground state and the continuum. So Saha contains more information.

In both distributions the exponential factor appears, which means that

\[
\frac{n^b(p)}{n^b(q)} = \frac{n^a(p)}{n^a(q)}
\]

(2.70)

and we can state that if two levels are populated according to Saha,
their population densities are related to each other according to Boltzmann.
The opposite statement is not always valid (cf. section 9.3). Boltzmann does not imply Saha.

As stated before Boltzmann's relation will not be assumed to be valid in general. This implies that the Saha distribution is not generally valid either, especially not for lower lying levels. But somewhere high in the atomic energy spectrum there will be a level \( N \) with such a small separation from the ion ground state that reactions of type (2.68) occur more frequently than other balance disturbing processes. This upper part of the system \( \{ p \geq N \} \) is said to be in the partial local thermal equilibrium (PLTE) and the levels are populated according to Saha. Here an important difference between the ground and ion state manifests itself. The ground state is isolated from the rest of the system by the large energy gap \( E_{12} \) whereas the ion state is approached infinitely close by the upper part of the atomic system. So we can say that the greater part of the system is in equilibrium and that deviations from the equilibrium manifest themselves in a finite lower part of the system.

2.5.3 The equilibrium departure factor \( b \) and relative overpopulation \( \delta b \).

It is useful to relate the population of the lower levels with that of the upper PLTE part by introducing the equilibrium departure factor

\[
b(p) = \frac{n(p)}{n^e(p)},
\]  

(2.71)

Levels for which \( b(p) < 1 \) are said to be underpopulated whereas levels with \( b(p) > 1 \) are overpopulated. In the astrophysical literature (mostly concerning underpopulations) this \( b \)-factor is often called the Saha decrement; in the case of \( b > 1 \) the same increment is more appropriate.

Another useful quantity is the relative overpopulation denoted by

\[
\delta b(p) = b(p) - 1,
\]  

(2.72)

scaling in the range \( \delta b \geq -1 \). Underpopulated levels have negative and overpopulated levels positive \( \delta b \)-values.

2.5.4 The maximum number of bound states.

There is a limit on the number of bound states which have to be
considered. This can be understood by realizing that the size of the atom is an increasing function of the pgn; classically the radius of an atom with pgn p is given by \( a_p = a_0 n_p^{-1} \). If the p-value is so high that the corresponding atomic size exceeds the mean particle distance between ions \( n_e^{-1/3} \), it is not useful to consider the atomic state as a bound state. The electron is common property of more than one ion. The boundary value of \( p \) must satisfy \( a_0 n_e^{2} p^2 = \frac{1}{2} \) \( n_e^{-1/3} \), which results in

\[
\rho_{\text{max}} = a_0^{-1/2} \sqrt{\frac{1}{2}} \frac{1}{2} \frac{1}{6} = 1.4 \times 10^5 \sqrt{\frac{1}{2}} \frac{1}{6} \frac{1}{6} .
\]

(2.73)

In this formula the ion density is in \( \text{m}^{-3} \).

Another value of \( \rho_{\text{max}} \) can be obtained from the lowering of the ion potential

\[
\Delta E_I = 2.74 \times 10^{-13} \sqrt{\frac{n_i}{n_e}} \text{ (eV)} ,
\]

(2.74)

with \( \frac{n_i}{n_e} \) in eV. The level for which this equals the ionization potential is the last bound state. The p-value for this level equals

\[
\rho_{\text{max}} = 7.0 \times 10^5 \frac{1}{2} \frac{1}{6} \frac{1}{6} \frac{1}{6} .
\]

(2.75)

In practice we can use the lowest of the values given by eqs. (2.73) and (2.75).
2.6 Deviation from Planck's radiation law.

2.6.1 General

To study the deviation from the proper balance

\[ A_u \leftrightarrow A_1 + h\nu \]

\[ A_u \leftrightarrow A_1 + 2h\nu \quad \text{(2.76)} \]

we need information about the reaction rates which are given by \( n(u)A(u,1) \) for the spontaneous emission, \( n(1)B(1,u)\rho_\nu \) and \( n(u)B(u,1)\rho_\nu \) for the absorption and stimulated emission respectively. \( A(u,1) \), \( B(u,1) \) and \( B(1,u) \) are the so-called Einstein coefficients whereas the symbol \( \rho_\nu \) represents the spectral energy density.

The rate coefficients for back- and forward processes are related to each other by the principle of detailed balancing in

\[ e(u)B(u,1) = g(1)B(1,u) \quad \text{and} \quad B(u,1) = c^3(8\pi\nu)^{\frac{3}{2}}A(u,1). \quad \text{(2.77)} \]

Note that in the absence of equilibrium these relations can be employed. So, once the decay rate \( A(p,q) \) is known, \( B(p,q) \) and \( B(q,p) \) can be determined. However, the determination of the spectral density is in general not a simple task. Chapter IV is devoted to the study of decay rates \( A \). Here we will discuss the properties of radiative transfer in plasmas. In sect. 2.6.2 we discuss properties of individual radiative transitions like the escape factor and optical depth while sect. 2.6.3 is devoted to global properties for the plasma as a whole.

2.6.2 The escape factor and optical depth

Especially for laboratory plasmas where linear dimensions are small, equilibria of kind (2.76) are rare. This is inherent to the volatile character of radiation, i.e. to the relatively small cross sections for the interaction between radiation and material particles. So radiation created by spontaneous decay can in many cases escape from the plasma without giving rise to absorption or stimulated emission. In other situations it is possible that radiation created in one part of the plasma may be captured in another part. So contrary to electron-induced transitions which are local events, transitions due to the radiative transfer cannot be treated locally.

To be practical and to get generalized results needed in the framework of CE models, one can use the method of the escape factor which
decouples radiation from material particles and makes a local treatment possible.

We will use the concept of the escape factor \( \theta(u) \) such that in the balance equation of an upper level \( u \), all radiative processes to and from a lower level \( l \), can be written as a modified decay term, consequently \( n(u) A(u,l) \) will be replaced by

\[
\frac{\partial n(u)}{\partial t} + \int \left( \frac{\partial n(u)}{\partial x} A(u,l) - \frac{\partial n(l)}{\partial x} A(l,u) \right) dx = -n(u) \frac{\partial}{\partial x} \left( n(u) A(u,l) \right) dx .
\]

(2.78)

which implies that

\[
\theta(u) = 1 - \int \left( n(u) A(u,l) - \frac{\partial n(u)}{\partial x} A(u,l) \right) dx .
\]

(2.78b)

The integrations are carried out over the line profile.

From eq.(2.78) it can be deduced that

- \( \theta = 1 \) if absorption and stimulated emission can be neglected,
- \( \theta < 0 \) if the Planck balance (2.76) is in equilibrium,
- \( \theta > 1 \) if absorption precedes the local emission, and
- \( \theta > 1 \) if stimulated emission is dominant.

The concept of the escape factor as we use it here is also known as the \( \theta \)-factor. In astrophysical literature as the "net radiative bracket". It should be noted that different concepts and calculation methods of the escape factor can be found in literature. A review of this matter is given by Iben [197].

In this study of plasma classification only global properties of the escape factor will be discussed in relation with the radiative transfer in the plasma which in the \( s \) direction obeys the equation

\[
\frac{dI_s}{ds} = \beta_s - \kappa_s I_s ,
\]

(2.79)

in which \( I_s \) is the intensity in the \( s \) direction, \( \beta_s \) the volume emissivity related to decay processes by

\[
\beta_s = n(u) A(u,l) h v \Phi(v) (4\pi)^{-1} .
\]

(2.80)

The line profile factor \( \Phi(v) \) is normalized so that \( \int \Phi(v) dv = 1 \). The absorption coefficient is given by the formula

\[
\kappa_s = c^2 (\theta \omega v^3)^{-1} \left( \frac{n(l)}{n(u)} - g(u) \frac{A(u,l)}{\Phi(v)} \right) .
\]

(2.81)

The first part of this coefficient refers to absorption, the second to stimulated emission, which in this way can be regarded as a negative absorption. In most cases it is justified to assume that the shape of
the absorption profile equals that of the emission profile.
It is useful to relate radiative transfer to the LTE situation which
can be done by the introduction of the LTE values of $j^*$ and $k^*$ by
which we get

$$j = j^* b(u) \text{ and } k = k^* B_{ul},$$  \hspace{1cm} (2.82a)

where

$$B_{ul} = (\exp(hu/kT) - b(u)/b(1)) (\exp(hu/kT) - 1)^{-1}. \hspace{1cm} (2.82b)$$

Evidently, LTE corresponds with $B_{ul} = b(u)/b(1) = 1$
and consequently

$$j/k = j^*/k^* = 2hu^3 \exp(-2(\exp(hu/kT) - 1)^{-1}, \hspace{1cm} (2.83)$$

the Planck function for the spectral intensity (cf. eq. (2.43), a
solution of eq. (2.79) for the homogeneous case (as it should be).

Now we consider the simple
case of a homogeneous plasma
slab of linear dimension $\lambda$, 
irradiated by an external
source with intensity $I_0$ (see
fig. 2.10). Since homogeneity
implies that $\Delta I = \frac{\partial I}{\partial \delta} = 0$
the solution of eq. (2.79) can
be written as

$$\Delta I = I - I_0 = (j/k - I_0) (1 - \exp(-\kappa \lambda)). \hspace{1cm} (2.84)$$

An expression which gives the change in intensity due to the presence
of the plasma. The argument of the exponent $\kappa \lambda$ is the optical depth;
it more generally reads $\int_0^{\kappa \lambda} \kappa \delta s$ and is an important quantity to
characterize radiative transitions.

- For $\kappa \lambda \ll 1$ the plasma is optically thin (transparent) and
- for $\kappa \lambda \gg 1$ the plasma is optically thick (opaque) for the
  transition.

In order to understand the main features of the escape factor we first
consider the solution for an optically thin transition without
external source. Since $\kappa \lambda \ll 1$ and $\Delta I = 0$ the solution of eq. (2.79) reads

$$I_I = I = n(u) A(u, I) h \theta(v) (4\pi)^{-1} \lambda , \hspace{1cm} (2.85)$$
The line intensity turns out to be proportional to the number density of the upper level and the plasma dimension. This transparent intensity $I_T$ can be used as a standard to which non-transparent situations can be related. Here we use the ratio $I/I_T$ to get information about the escape factor. In the simple case of no external sources we find from eq. (2.84) that

$$\frac{I}{I_T} = \frac{\langle \sigma v \rangle}{\langle \sigma v \rangle} \left(1 - \exp(-\langle \sigma v \rangle)\right) = 0 \ .$$  \hspace{1cm} (2.86)

This happens to be a good approximation for the escape factor (cf. [IR 79]). In a proper treatment both $I$ and $I_T$ should first be averaged over the profile shape. But in the case of the relatively small Doppler broadened Gaussian profile the results of extensive calculations are not much different from those presented by the analytical eq. (2.86), (cf. fig. 2.11) if we take for optical depth of the line centre the value

$$\kappa_0 \lambda = n(1) g(1)/g(2) \exp(2 \Delta \nu_0^2) \lambda(n_1) \exp(3/2 \Delta 
u_0^2) \ .$$  \hspace{1cm} (2.87)

This is eq. (2.82) for the line centre multiplied with $\kappa_0$, where the stimulated part ($\eta(u)$) has been omitted, $\Delta 
u_0$ is the doppler width. For a cylinder with radius $R$ we apply $\kappa_0 = 1.27 R$.

If Stark effects dominate, then the profile is Lorentzian and the escape factor is considerably larger than the value given by eq. (2.87). The analytical approximation of the escape factor for a Lorentz profile as given by Holstein in [HOL 51] is

$$0 = 0.65 \left(\kappa_0 \lambda\right)^{-1/2} \ .$$  \hspace{1cm} (2.88)

This expression can be used if $\kappa_0 \lambda > 1$ (cf. fig. 2.11)

---

**Fig. 2.11**

The escape factor as a function of the optical depth of the line centre for an infinite plane parallel slab geometry.

---

[IR 79]  
[DI 40]  
[DI 40]  
[eq. 2.86]  
[eq. 2.88]
2.6.3 Classification of global radiative properties

In the classification of global radiative properties of the plasma as a whole we first distinguish between radiative active and radiative passive plasmas. The radiative active plasmas can be classified according to Baker and Mense (BAK 38) in opacity case A and case B. The radiative passive plasmas are irradiated plasmas. Temperature and other radiative features are imposed by an external source. We distinguish between case C and case D. So we consider the following cases A to D.

A) No external sources ($I_0 = 0$) and small dimension and densities, so that the plasma is transparent for all transitions. Case A is specified by

$$\theta = 1$$

for all transitions.

B) No external sources ($I_0 = 0$) and complete absorption of resonant radiation, i.e. radiation originating by decay to the ground state (for hydrogenics known as Lyman radiation). This situation offers a good approximation for a large variety of low temperature plasmas with large ground state densities. That is, if $\omega_\lambda$ can be very large for resonant radiation and small for all other transitions can be understood by realizing that the population of the ground state supercedes that of the excited states by many orders of magnitudes.

Case B can be specified by

$$\theta = 0$$

for resonant radiation, and

$$\theta = 1$$

for all other transitions.

C) A plasma irradiated by an external source for which $I_0 > j/\kappa$. We see that eq. (2.84) gives $1 - I_0 < \theta$, which results in a negative escape factor (remember that $\theta = \Gamma / \Gamma_0$). This negative escape factor reflects a situation in which the number of radiative processes from the lower to the upper level (absorption) exceeds the number of processes in the opposite direction (emission). Since the net number of processes is written as a modified loss term $n(u) B_{ul} \Delta \nu(u)$ and $\Lambda(u)$ of $u$ in favour of the production of $u$, the value of $\theta_{ul}$ must be negative since the actual situation is that of a production of $u$ at the expense of $l$.

If this is accompanied by a large optical depth and small electron densities the temperature of the radiation field will be imposed on the level population, i.e. $\theta_{ul}$ approaches zero from the negative side and we get
\[ \eta(\omega) = \eta(1) \exp(-\hbar \omega / k T_0) , \] (2.89)

where \( T_0 \) represents the temperature of the radiation field. In its course through the plasma the intensity of the incident radiation will be diminished.

As an example of this Case C we refer to planetary nebulae consisting of material ejected by an old star. The nebula is irradiated by the central star with a high effective temperature. Going from the inside to the outside the colour of the nebula shifts from blue to red. Another example can be found in many laboratory plasmas where a hot inner part irradiates a cooler outer shell.

As a third example we consider a plasma irradiated by a laser operating on a frequency which belongs to the transition \( p \rightarrow q \). The high intensity can be regarded as having a high temperature and we get

\[ \eta(p) = \eta(q) , \] (2.90)

D) If an external source irradiates the plasma at a frequency of a transition between inverted states \( (\eta(\omega) > \eta(\omega')) \), we find that since \( \omega \) has a negative value the intensity will be amplified, and \( 0 \) gets values larger than unity. Apart from the laser applications this situation can be found in \( H^+ \) regions where young stars illuminate clouds of recombining plasmas in which they are imbedded.

In our plasma classification we will mainly distinguish between Case A and Case B as far as global plasma properties are concerned. In some special circumstances we will refer to the classes C and D in order to understand more specific features of a plasma.
2.7 Conclusions: Electron excitation kinetics (EEK) plasmas

The analysis of elementary processes as given in this chapter shows that the electron is in most processes the leading collision partner. The fundamental reason for that is quite simple: The electron is a charged particle with small mass. So the long range interactions (large cross sections) take place with a large rate (large velocity). The consequence is that even in plasmas with rather small ionization degrees the bulk of the electrons is Maxwellian and that the kinetics of excited levels is determined by the electron gas only. The excitation kinetics of these plasmas can easily be described. In fact it is the description of the energy transfer between free and bound electrons, identical particles in different situations. The for- and backward processes can be related to each other by the application of the principle of DB. This study is devoted to the classification of this kind of plasmas, the so-called EEK plasmas. EEK stands for electron excitation kinetics. EEK plasmas are plasmas for which
- molecular processes are not important
- the energy gaps (especially $|E_2|$) are not much smaller than the electron temperature
- at least the bulk of the velocity distribution of electrons is Maxwellian
- sublevels are statistically distributed by ions (and/or neutrals)
- there is no need for Maxwellization of ions and neutrals
- the proper Saha balance is present somewhere high enough in the atomic energy scheme
- the proper Planck balance and the proper Boltzmann balance between groundstate and excited states is in most cases not present
- improper balances consist of radiative or electron induced transitions only and are established on a timescale much smaller than the growth or decay of the plasmas (QSS).

In the study of the elementary processes in this chapter we have seen several times that it is useful to split up the atomic energy scheme in a bottom and a top. Reasons for this are
- in the bottom energy gaps are large. The transitions are in many cases large threshold transitions for which the best approach is to use experimental results. In the top we can use semi empirical approximations, but
- in the top where the continuum is approached we expect that a classical treatment may be possible.
- In a lot of situations excitation from the ground state is caused
by the tail of the electron distribution function. If the Maxwell validity is restricted to the bulk this means that ground state excitations have to be treated separately: a treatment for which the tail distribution has to be known if the absolute value of the distribution function is requested. If we confine ourselves to the determination of the shape of the distribution function for $p>1$, this information is not needed.

- The competition between radiative and collisional transitions as expressed by the critical densities, is for increasing $p$-values rapidly in favour of the collisions.

In the study of EXC plasmas we can confine ourselves to two kinds of elementary processes:

- First the radiative decay, which is studied in chapter IV
- second the electronic collisions to which chapter V is devoted.

Collisional and radiative properties are related to other atomic properties. In chapter III attention is paid to different energy schemes of different atomic species in relation with atomic properties.
Chapter III  Properties of atomic states.

3.1 Introduction

Faced with the challenge of classifying plasmas we meet with the problem that different atomic systems have to be considered. This problem is twofold; how do we handle the simplest of all, the hydrogen system, and what are the implications of all possible deviations from the hydrogen system.

A useful approach of the hydrogen system is to split up the energy scheme in a bottom and a top. It already appeared in the preceding chapter that this distinction between top and bottom is practical with regard to collisional and radiative properties. Apart from that it also has a fundamental justification. In the bottom energy gaps are large and a quantum mechanical description is needed. In the top we are faced with small energy differences and it is expected that the classical limit of quantum mechanics is valid and makes a simple approach possible.

This split up of the energy scheme is also useful for other more complex systems. The wave function of a highly excited state can, under certain conditions, be separated into a wave function for the core and one for the outer or valence electron. This type of atomic states, denoted by Rydberg states, are dealt with in section 3.2. Since the wave function of the core is limited to a small region, only large eccentric orbits of the valence electron will 'feel' deviations from the Coulomb potential. This implies that for increasing energy the hydrogenic description of an energy shell will be progressively better. So any atomic system has a hydrogenic top.

In the top the classical limit of quantum mechanics is approached and we expect the correspondence principle (CP) to be applicable. This is discussed in sec. 3.3 where features and applications of the CP are studied. It turns out that the CP can be applied to stationary and statistical properties of highly excited atoms. But in the treatment of transitions the CP is less straightforward. We have to distinguish between jump processes for which the change in Quantum is comparable with or larger than $\Delta p$, i.e. $\Delta p/\rho \geq 1$ and step processes for which $\Delta p/\rho \ll 1$. For the latter the CP is not easily effectuated.

The distribution function of atomic states is determined by the statistical interference of all kinds of transitions. The result of this interference can be expressed in sum rules. In section 3.4 we discuss the sum rules of oscillator strengths. In section 3.5 we discuss specific values of the oscillator strength for hydrogenics.
3.2 Properties of Rydberg states

In a hydrogen atom (or hydrogenic ion) the electron moves in an attractive Coulomb field with potential energy

$$V(r) = -\frac{Z\epsilon^2}{r}.$$  \hspace{1cm} (3.1)

Quantum mechanics predicts that the bound electron can only be in a discrete number of states. The energy values of the states are

$$E_p = -\frac{Ry}{2} \frac{\epsilon^2}{p^2},$$  \hspace{1cm} (3.2)

in which \(p\) is the principal quantum number (pqn) of the state \(|l\). With the help of the wave function it is possible to calculate atomic properties. Several of these are listed in table 3.1 as a function of the principal quantum number (pqn) \(p\) and the charge number \(Z\). In this table and the rest of this study we use the term 'atom' to refer to atoms as well as ions.

If the atom is not hydrogenic the character of the atom is more complex. In order to make a classification in this complexity we consider the classical picture of an atom consisting of a core and one outer electron which moves in an elliptical orbit. The distance to the nuclicus, for eccentric orbits, lies between that of the 'perihelion' \(r_1 = (\lambda + \frac{1}{2})L\), and that of the 'aphelion' \(r_2 = 2p^2L\). The perihelion depends on an eccentricity parameter \(\epsilon\) which can be seen as the classical analogon of the orbital quantum number. We do not consider the spin of the electron.

In table 3.2 we give some properties of atomic states which we describe from left to right, i.e. in the direction of increasing complexity.

The single electron approximation is applicable to atomic states for which the interaction between core and electron is negligible. The radial part of the atomic wave function can then be written as a product of the wave function of the core and that of the outer electron

$$\psi_nl = \phi_n \psi_l.$$  \hspace{1cm} (3.3)

For the non-penetrating orbits (relatively large \(\lambda\)-values) only slight deviations from hydrogenic properties can be expected. Some minimum values (obtained from [FAB 83]) of \(\lambda\) for certain atoms are given in table 3.2.

Core penetrating states are more complex. The radiative lifetime
<table>
<thead>
<tr>
<th>Property</th>
<th>Scaling</th>
<th>Constants</th>
<th>Accuracy and remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
<td>$E_p = \frac{m_e Z^2 \alpha^2}{p^2}$</td>
<td>$\alpha = \frac{\hbar^2}{2m_e \varepsilon^2} = 13.6 \text{ eV}$</td>
<td>$m$ is the electron mass</td>
</tr>
<tr>
<td>Effective p-value</td>
<td>$p^* = p - \Delta L$</td>
<td></td>
<td>$\Delta L$ is the quantum defect ($\phi\Delta$)</td>
</tr>
<tr>
<td>Energy differences</td>
<td>$E_p - E_{p'} = \frac{Z^2 (p^2 - p'^2)}{2}$</td>
<td>$p_{p} = 2Z^2 p \sim 0.1 p$</td>
<td>For $\Delta p = 1: p = 5, 30%; p = 15, 15%$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Hydrogenic $p = 30%; 5%$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>For $\Delta p = 2: p = 5, 60%; p = 10, 30%$</td>
</tr>
<tr>
<td>Mean radius</td>
<td>$\bar{a} = a_0 Z^{-2} p^2$</td>
<td>$a_1 = a_0 Z^2 / (2\pi \varepsilon^2) = 5.3 \times 10^{-11} \text{ m}$</td>
<td>$\bar{a} = a^2 (4\pi \varepsilon^2)^{-1}$</td>
</tr>
<tr>
<td>Bohr cross section</td>
<td>$a_0 = a_0 Z^{-2} p^4$</td>
<td></td>
<td>For Hydrogenics $a_4 = 1$</td>
</tr>
<tr>
<td>Statistical weight</td>
<td>$g_p = 2g_4 p^2$</td>
<td></td>
<td>$a$ is the fine structure constant</td>
</tr>
<tr>
<td>Rms velocity</td>
<td>$v_p = v_0 \sqrt{p}$</td>
<td>$v_0 = 2 \sqrt{\hbar} = 0.1 \alpha$</td>
<td></td>
</tr>
<tr>
<td>Period</td>
<td>$\tau_p = \sqrt{(p+1) \hbar}$</td>
<td>$T_1 = 2\pi \hbar / v_0 = 1.5 \times 10^{-16} \text{ s}$</td>
<td></td>
</tr>
<tr>
<td>Angular momentum</td>
<td>$L_p = h \sqrt{(p+1) \hbar}$</td>
<td>$x \leq p \sim 1$</td>
<td></td>
</tr>
<tr>
<td>Bohr angular momentum</td>
<td>$\tilde{L}_B = \hbar \tilde{p}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Decay frequency</td>
<td>$A(p) = 3y^2 Z^2 (ln p - \xi / 2)$</td>
<td>$\gamma = \frac{3y^2}{2\pi^3} \approx 7.87 \times 10^{-9} \text{ s}^{-1}$</td>
<td>$\zeta = 0.23$ case A, $\zeta = 1.04$ case B, Radiation lifetime $\tau_\gamma = A(p)^{-1}$</td>
</tr>
</tbody>
</table>

Table 3.1: Magnitudes and scaling laws of atomic properties. Scaling parameters are the proton $p$, the charge number of the core $Z$, and the statistical weight of the core $g_4$. For non hydrogenic systems and low $p$-values the effective quantum number $p^*$ should be applied. In cases where $p$ is applied instead of $p^*$ it is not useful to make the difference.
Table 3.2
A classification of atomic states. From left to right is the direction of increasing complexity. $E_0$ is the kinetic energy of the bound outer electron. $C$ indicates the core; $r_1$ the perihelion; $r_2$ the aphelion.

<table>
<thead>
<tr>
<th>R-like</th>
<th>Single-electron</th>
<th>Multichannel</th>
<th>Planetary</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rydberg states</td>
<td>non-penetrating</td>
<td>penetrating</td>
<td></td>
</tr>
<tr>
<td>Energy</td>
<td>$E_e &lt; E_{exc} &lt; E_{ion}$</td>
<td>$E_{exc} &lt; E_e &lt; E_{ion}$</td>
<td>$E_{ion} &lt; E_e$</td>
</tr>
<tr>
<td>Q-defect</td>
<td>$\Delta_q = 0$</td>
<td>$\Delta_q \propto \epsilon^{-5}$</td>
<td></td>
</tr>
<tr>
<td>Decay rate</td>
<td>$\lambda \propto \rho^{-5}$</td>
<td>$\rho^{-5}$</td>
<td>$\rho^{-3}$</td>
</tr>
<tr>
<td>Wave $\ell$</td>
<td>$\ell \in {0, 2}$</td>
<td>$\ell \in {0, 2}$</td>
<td>$\ell \in {0, 2}$</td>
</tr>
<tr>
<td>Structure</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Core states
- $c_2 = c_1 + c_2$
- Outer orbit possible
- Core excitation possible
- Core ionization possible
scales with \( p^3 \) which is short compared to circular orbits where \( T_{\text{dep}}^5 \). This \( p^3 \)-dependency can be understood by realizing that decay is most probable during a core penetration, occurring each revolution period which scales with \( p^3 \) (Table 3.1).

In the multichannel case it is not possible to split the atom in one core and one outer electron. In this case the atomic wave function can be seen as an addition of products of eq. (3.3) [SEA 66]. This is the case when the excitation energy of the core is much smaller than the ionization energy (consequently the mean value of the kinetic energy) of the outer electron. Each core penetration can be regarded as a collision in which the outer electron is able to induce a transition in the core. The most simple property to characterize these relatively complicated atomic states is the statistical weight which approximately equals \( g(p) = 2g_p p^2 \) in which \( g_p \) is the number of states of the core. For a treatment of the multichannel qd theory we refer to [SEA 66] and [FAN 75].

Finally we have the so-called planetary atoms ([PER 77]) in which two electrons are simultaneously excited; this can be regarded as a generalization of the He atom. These planetary states are relatively scarce and autoionizing. Their influence in the excitation kinetics is not considered in this study. We confine ourselves to the first two classes of excited states which will be denoted by Rydberg states (cf. Table 3.2).

In a Rydberg state the outer electron moves in a field which can be regarded as a slightly modified Coulomb potential. The energy eigenvalues may be expressed in

\[
E_p = -\frac{Ry}{\varepsilon_p} \frac{a^2}{\varepsilon_p - \lambda^2}
\]

in which

\[
\varepsilon_p = \frac{p^2}{\varepsilon_p - \lambda^2}
\]

This is the energy variant of the famous empirical formula given by Rydberg in 1890.

The presence of the quantum defect (qd) \( \Delta \), expresses that the shielding of the nuclear field by the core electrons is not complete. The lower \( \Delta \), the more eccentric the orbit of the outer electron, the more it approaches or penetrates into the core and the greater the binding energy will be. As \( \Delta \) increases, the orbit becomes more circular, the qd decreases rapidly and the atom becomes more hydrogenic. The quantum defect \( \Delta \) scales roughly with \( \varepsilon_p^{-3} \) and is nearly independent of the excitation energy. This implies that for subsequent energy levels with the same \( \lambda \) value the effective quantum
number $p^*$, increases by integers along the series. Such a series is
called a Rydberg series. Atoms (ions and even molecules) which can be
-described in this way are Rydberg atoms (ions or molecules).

In the last decade a lot of activity concerning experimental research
of Rydberg states has become possible in laboratories due to the
advent of the tunable laser (cf. [Ins 83], [GAL 85] and [FAB 83]).
Since most Rydberg states are created by absorption of a photon by
ground state atoms a study of low $\lambda$ values has become possible by
these laboratory techniques. In astrophysics the study of highly
excited states has a longer history (cf. [MAR 60] and [HOG 60]). Here
it concerns larger $\lambda$ values ($\lambda=\infty$) found in recombination spectra
in the radio frequency range (typical $p=10$). Under these
circumstances the qd is not important (large $\lambda$ values) and the
differences between atomic species is only due to the difference in
the Rydberg energy, $\tilde{R}_Y$ (reduced mass dependent).

In our statistical study we have to realize that the number of states
in a given shell $\lambda$, for which $\Delta_n^2$ differs from zero becomes relatively
unimportant with increasing $p$-value. This is because $\Delta_n^2$ is $p$
independent, and scales with $\lambda^{-5}$ which implies that for relatively
small $p$-values the number of defect states remains constant whereas
the total number of states increases with $p^2$. So quantum deficiency
remains limited to the bottom of the system and even in complex
systems a hydrogenic description is possible provided $p$ is large
enough (cf. fig. 3.2). The precise transition to the hydrogenic
behaviour and its statistical implication deserves further study.
Hereafter we drop the asterisk and use in general the definition

$$p = \sqrt[\lambda]{\tilde{R}_Y|E_p|}. \quad (3.6)$$

For non-hydrogenics $p$ may have non integer values.

3.3 The correspondence principle

Approaching the ionization limit of an atomic energy scheme the
energy spacing between the levels will decrease, and the system
becomes more and more continuum-like. So it can be expected that a
classical description of the atom becomes increasingly better. This is
the idea behind Bohr's correspondence principle (CP). The applica-
bility of a classical theory will facilitate the task of finding a
description of the excitation kinetics of atomic systems. Therefore we
will discuss application and features of the CP. They will be
enumerated by CP1, CP2 etc.

In this study in which we are interested in statistical properties at
first, we start with the application of the CP on the statistical weight \( g(p) \) of hydrogenic states. From quantum mechanics we know that

\[
g(p) = 2p^2.
\]

To make a classical interpretation possible we transform \( g(p) \) to \( G_2^0(E) \), the number of states per energy interval. Realizing that

\[
G_2^0(E) \, dE = g(p) \, dp,
\]

and applying \( E = -\text{Ry} \, z^2 \, p^2 \) we find

\[
G_2^0(E) = \text{Ry}^{-1} \, z^2 \, p^5 = \text{Ry}^{3/2} \, z^3 \, |E|^{-5/2}.
\]

In classical mechanics it is not justified to distinguish between separate discrete states. Still it is possible to use the concept of "amount of space" which has to be applied in a continuous way to the phase space. The larger a volume \( d\Omega = d^3r \, d^3p \) of this phase space the larger "the amount of space" for a particle.

"CP1a" The "correspondence" between the classical "amount of space" and the number of quantum states is realized by the normalization \( d\Omega/\hbar^3 \).

In section (2.2.2) this counting of states was applied to a potential free space. In the presence of the Coulomb potential, the space coordinates are for a given energy \( E \) related to the momentum coordinates by

\[
H(z, p) - E = 0,
\]

in which \( H(z, p) \) represents the Hamiltonian. The phase space density with respect to energy can now be formulated with the help of the \( \delta \)-function as

\[
\frac{d\Omega}{d\varepsilon} = \int \delta(E - H) \, d\Omega.
\]

Applying the usual techniques for the \( \delta \)-function and the relations presented in table 3.1 it can be found [FER 75] that

\[
\frac{d\Omega}{d\varepsilon} = 1/2 \, \text{Ry}^{3/2} \, \hbar^3 \, z^3 \, |E|^{-5/2}.
\]

"CP1b" By multiplying eq. (3.11) with \( 2\hbar^{-3} \) (2 represents the number of electron spin states) we can derive the number of quantum states per energy interval. This gives the expression (3.8) derived from quantum mechanics.
In this way a correspondence is effectuated between all possible energy states of a given orbital quantum number \( \ell \) at one side and classical orbits with all kinds of eccentricity at the other side. Large \( \ell \) values correspond to circular orbits and small \( \ell \) values to highly eccentric orbits. The magnetic quantum number \( m \) corresponds with all the possible classical orientations of the orbital plane.

For non-hydrogenic systems the statistical weight is a factor \( g_{\ell} \) (the statistical weight of the core) larger than the hydrogenic value. Since the degeneracy is (partially) eliminated by the quantum deficiency, the spread out of the states over the energy is more gradual than in the hydrogenic case. So quantum deficiency makes the application of the CP better (cf. figs. 3.1 and 3.2).

Secondly we consider the correspondence between the classical orbital frequency and that of the radiation emitted in the transition from \( p \) to \( p-1 \). For the latter quantum mechanics predicts that

\[
v = (E_p - E_{p-1}) \hbar^{-1}.
\]

For high \( p \) values the energy difference can be approximated by

\[
\Delta E \approx 2 \hbar \omega Z^2 p^{-3}.
\]

Consequently, the radiation frequency

\[
v \approx 2 \hbar \omega Z^2 p^{-3} \hbar^{-1}
\]

has the same value as that of the classical revolution frequency (the inverse of the period \( T_p \), cf. table 3.1).

As a third example of the CP we discuss the paradox of the radiating stationary Rutherford atom. In this classical model the electron orbits around the nucleus. And as it is constantly accelerated it will emit a radiant power [JAC.75]

\[
\dot{E} = \frac{2}{3} \frac{e^2}{c} \mathbf{v}^2 \nabla^2 |\mathbf{v}|^2,
\]

with \( \mathbf{v}^2 = \frac{\epsilon}{4 \pi \epsilon_0} \), from a classical point of view the electron will lose energy and decay to a lower orbit. If the energy gap between initial and final orbits is \( \Delta E \), this decay takes place in a time

\[
\tau = \Delta E / \dot{E} \Rightarrow \text{which means that the decay frequency is given by}
\]

\[
A = \frac{\dot{E}}{\Delta E} = \frac{2}{3} \frac{e^2}{c} \mathbf{v}^2 \nabla^2 |\mathbf{v}|^2 \Delta E^{-1}.
\]

Suppose that the electron initially describes a circular orbit with energy \( E_p \), then the acceleration is constant and equal to \( \mathbf{v}^2 / c \). If we substitute the values listed in table 3.1 we get \( \tau = \frac{\mathbf{v}^2}{c} \omega_0^{-1} Z^2 p^{-3} \).

\[
A = \frac{\dot{E}}{\Delta E} = \frac{2}{3} \frac{e^2}{c} \mathbf{v}^2 \nabla^2 |\mathbf{v}|^2 \Delta E^{-1}.
\]
A sketch in which the quantum defected system of Ar I is compared with the hydrogen system. For increasing \( n \), the g.d. rapidly tends to zero (here \( \Delta g = 0 \)). The number of states is depicted. The number of states per energy interval around the level \( p = 3 \) is outlined by the dashed lines. We see that this is not affected by the g.d. The spread out over the energy range is more continuum like. It should be noted that the Ar I system has two different cores, one with \( g_x = 4 \), the other with \( g_y = 3 \) (cf. Fig. 10.7). There are consequently two ionization potentials. The energy scheme is presented in such a way that only the energy of the outer electron \( E_0 \) is reflected.

Fig. 3.2
The accumulated statistical weight,

\[ C_{\text{ass}}(p) = \frac{D}{2} g(p) \]

as a function of the (effective) principle quantum number for the Ar I and II system (\( * \)).

It can be seen that the differences with the II system are limited to the bottom of the Ar system, i.e., \( p^* < 4 \).
Consequently the radiant power will be

\[ \dot{E} = \frac{2}{3} \frac{e^2}{\alpha^3} \times 4 \times \alpha_{\odot}^{-2} z^6 p^{-5} \]  

(3.14a)

and the adjacent level \( p = 1 \), will be reached in a "decay time"

\[ \tau_p = \Delta E/\dot{E} = \frac{3}{2} \alpha_{\odot}^{-4} \times 1 \times 4 \times 2 \times 5 p^5 \]  

(3.14b)

If we compare this with the radiative life time as predicted by quantum mechanics (cf. Table 3.1) we see that eq. (3.14b) gives a too large value. But this cannot totally be described as a failure of the CP; it can also result from a deficiency of the circular approximation. By taking into account all possible elliptical orbits where accelerations will be larger and the 'decay time' smaller, it can be shown [RR 73] that the classical description is fairly good for large \( p \) values.

-CP3- In what is called the Strong Coupling Correspondence Principle [SCCP], a full classical Fourier transformation of all kinds of classical orbits is effectuated [RR 73] and the correspondence with quantum mechanics can be realized.

This relation between the quantum matrix elements and the classical Fourier components is Heisenberg's form of the correspondence principle and the success of the SCCP lies in the statistical approach of the decay phenomenon.

This last example shows that the transition from quantum to classical mechanics is in some cases very subtle [RR 73]. We emphasize this subtlety with referring to the phenomenon that although atoms of interstellar space can be as large as bacteria, they still generate a discrete spectrum. So in spite of the large linear dimensions a full classical description is not possible. Apparently "being large" is not a sufficient condition for a full classical approach.

In search of the validity of the CP we use the formal representation (cf. [RMS 64]) which states that in the limit of \( \hbar \) tending to zero, quantum mechanics tends to classical mechanics. To be practical this implies that we have to compare atomic properties of the dimension of action, \( A \) (energy \( \times \) time) with Planck's constant \( \hbar \). Since the energy of an atomic state scales with \( p^{-2} \) and the revolution time with \( p^3 \) (cf table 3.1), this means that action scales with \( p^3 \). This implies that for a classical description the demand of large actions can be traced back to the demand that \( p \gg 1 \). This is true as long as it concerns the description of stationary or statistical properties. For the latter we gave an example (the statistical weight, CP1), for the
former we can refer to the success of the WKS classical orbit description and example CP1. But in changes of atomic states the condition \( \Delta p \gg 1 \) is not sufficient. A necessary condition is that the change in action \( \Delta A \) is large compared to Planck's constant. This means that apart from \( \Delta p \gg 1 \), also \( \Delta p \gg 1 \) has to be satisfied in order to make a classical treatment possible.

To resume we may state that the CP is applicable
-CPA- for a stationary or statistical description provided \( \Delta p \gg 1 \)
-CPB- for transitions provided \( \Delta p \gg 1 \) and \( \Delta p \gg 1 \).

This means that it is useful to distinguish between step and jump transitions. Jump transitions for which \( \Delta p \gg \Delta p \) can be treated classically. Step transitions with \( \Delta p = 1 \) have to be handled with care; a classical description is in general not straightforward.

In the discussion of radiative and collisional transitions the features CPA and CPB will play an important role.

3.4 The oscillator strength; sum rules.

The oscillator strength is an important dimensionless quantity for both radiative and collisional transitions. For a transition from state \( |i\rangle \) to state \( |j\rangle \) the oscillator strength is defined as

\[
f_{ij} = 2m \hbar^2 |x_{ij}^t|^2 (E_j - E_i),
\]

in which \( x_{ij}^t \) is the \( x \) component of the dipole matrix element of the position vector \( x_{ij}^t = \langle j|\mathbf{x}|i\rangle \).

The quantum mechanical operator corresponding with \( \mathbf{x} \) is Hermitian with as a consequence that \( f_{ij} = -f_{ji} \). This is a formulation of the principle of microscopic reversibility (cf. sect. 2.2.1).

In the case in which the transition \( |i\rangle \rightarrow |j\rangle \) is an excitation (so \( E_j < E_i \)), the oscillator strength is positive and known as the absorption oscillator strength. In the opposite case the oscillator strength is negative and known as the emission oscillator strength [GRE.57].

For the transition between two degenerate levels \( p \rightarrow q \) the oscillator strength is defined as

\[
f_{pq} = \frac{1}{g(p)} \sum_{j \geq p} \sum_{j \geq q} f_{ij}.
\]

The sums are carried out over all sub-states \( |i\rangle \) of \( p \) and \( |j\rangle \) of \( q \).

The sum of all oscillator strengths with the same initial state \( |i\rangle \), equals one. This sum rule

\[
\sum_{j \neq i} f_{ij} = 1
\]

(3.17a)
known as the Thomas-Heike-Kuhn sum rule, is valid for hydrogenic systems. Using Eq.(3.16) this relation can also be applied to the oscillator strengths belonging to an energy level (or any group of sub-states), i.e.
\[ \sum_{\eta \neq \eta'} f_{pq} = 1. \]  
(3.17b)

If there are \( Z \) independent atomic electrons involved this rule predicts
\[ \sum_{\eta \neq \eta'} f_{pq} = Z. \]  
(3.17c)

For Rydberg states for which formulation (3.5) is valid, there is in fact one independent electron and we can apply (3.17c) with \( Z = 1 \) if the summation is carried out over all possible states of the outer electron with same core state.

Several other sum rules can be found in literature [KET 68]. In section 9.6 we will employ:
\[ \sum_{j \neq i} (E_j - E_i) f_{ij} = \frac{4}{3} (\epsilon_i - \langle v_i^2 \rangle), \]  
(3.18)

in which \( \langle v_i^2 \rangle \) represents the mean potential energy of the atom in state \( |i> \). For hydrogenic states the virial theorem states that the mean value of the potential energy equals twice the total energy and Eq. (3.18) can be written as
\[ \sum_{j \neq i} (E_j - E_i) f_{ij} = \frac{4}{3} \epsilon_i. \]  
(3.19)

For Rydberg states for which \( \Delta \epsilon \neq 0 \) Eq.(3.19) is only an approximation. It should however be noticed that in the upper part of the energy scheme only a relatively small part of an energy shell contains \( \Delta \epsilon \neq 0 \) - values. So Eq.(3.19) can be used provided we are high enough in the energy scheme.

3.5 Hydrogenic values of the oscillator strengths.

The results of quantum mechanical calculations, e.g. those carried out in [KREE 57], can be approximated analytically. For the oscillator strengths of transitions between hydrogenic levels for which the substates are statistically populated, Johnson [JOH 72] suggests
\[ f_{pq} = \frac{32}{(3/2)^3} \rho^{-5} q^{-3} (\rho^{-2} - q^{-2})^{-3} \times (\rho, q) , \]  
(3.20)
In which \( h(p, y) \) is a correction factor which depends on the principal quantum number \( p \) of the lower level and the ratio, \( y = \frac{E_\text{pq}}{E_\text{p}} \), of the transition- and the ionization-energies. This factor can be approximated by

\[
h(p, y) = h_0(p) + h_1(p) y^{-1} + h_2(p) y^{-2}.
\] (3.21)

The values of \( h_0, h_1 \) and \( h_2 \) can be found in table (3.3).

**Table 3.3 Gant Factor Coefficients (from [Görl 72])**

<table>
<thead>
<tr>
<th></th>
<th>( p - 1 )</th>
<th>( p - 2 )</th>
<th>( p \geq 3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( g_0(p) )</td>
<td>1.1330</td>
<td>1.0765</td>
<td>0.9935 + 0.2328 ( p^{-1} - 0.1296 p^{-2} )</td>
</tr>
<tr>
<td>( g_1(p) )</td>
<td>-0.4039</td>
<td>-0.2319</td>
<td>-1(0.6282 - 0.5598 ( p^{-1} + 0.5299 p^{-2} ))</td>
</tr>
<tr>
<td>( g_2(p) )</td>
<td>0.07014</td>
<td>0.02947</td>
<td>( p^{-2}(0.3887 - 1.181 p^{-2} + 1.470 p^{-2}) )</td>
</tr>
</tbody>
</table>

Above the ionization limit \( h(p, y) \) becomes the usual Gant factor for bound-free transitions. The oscillator strengths of Green et al [Görl 57] are reproduced within .5% by using eqs.(3.20-21) and table 3.3.

Further approximations can be deduced from the tables. For step processes, \( \Delta p/p \ll 1 \)

\[
f_{p\rightarrow c} = 1.52 \, p^{-5} \, q^{-3} \, (p^{-2} - q^{-2})^{-3}
\] (3.22)

can be obtained, which reproduces the tables of [Görl 57] within 3% for \( p > 1 \) and \( \Delta p = 1 \).

For jump processes, i.e., \( \Delta p/p \gg 1 \) we get the approximation

\[
f_{p\rightarrow c} = 1.95 \, p^{-5} \, q^{-3} \, (p^{-2} - q^{-2})^{-3}
\] (3.23)

which reproduces the tables within 12% for the transition \( p \rightarrow 2p \) and \( p > 3 \).

For increasing \( p \)-values, approximations (3.22) and (3.23) will become increasingly better. These approximations will be used in particular in the study of collisional processes, where it is useful to distinguish between step and jump processes.
Summary
The deviations from the hydrogenic system can be expressed by the quantum defect \( \Delta q \).
The \( \Delta q \) is only important for states which represent largely eccentric orbit, i.e. low \( l \)-values.
The number of defected states of an energy shell remains the same for increasing \( p \)-values. But relatively the defected part becomes progressively smaller since the statistical weight scales with \( p^2 \).
Su, any atomic system has a hydrogenic top. The lower boundary of the top depends on the atom in consideration and the accuracy desired.
In the top we deal with the classical limit of quantum mechanics where the correspondence principles (CP) manifests itself. The main features of the CP are that it is applicable to

-CPA- statistical and stationary properties provided that \( p > 1 \) and
-CPB- to transitions provided that \( \Delta p / p \geq 1 \) and \( p > 1 \).
It is useful to distinguish between step processes, i.e. \( \Delta p / p < 1 \) and jump processes \( \Delta p / p = 1 \). For step processes the CP is less trivial.
For hydrogenic states sum rules can be applied which provides a powerful tool in the statistical treatment of atomic transitions.
IV Radiative properties

4.1 Introduction and summary

In this chapter we deal with radiative properties of hydrogenic energy levels for which the sub-states are statistically distributed. In section 4.2 we compare classical and quantum mechanical results which each other; it is an extension of the application of the correspondence principle (CP) in section 3.3. In section 4.3 an analytical approximation of the total decay probability for opacity case A and case B (cf. sect. 2.6.3) will be given, while section 4.4 is devoted to the cascade contribution in FLTE. By the application of the CP in section 4.5, it turns out to be possible to relate capture (two-particle recombination) to (FLTE-)cascade. Both production rates can be put together in one (FLTE-)formula.

From a mathematical point of view the introduction (in sect. 4.6) of a boundary between radiative-hot (R-hot) and R-cold levels appears to be useful.
- levels for which $E_p > 1$ are said to be R-hot
- levels for which $E_p < 1$ are said to be R-cold.

Especially for hot levels the description of the radiative kinetics of the system (part) is easy. It turns out that the equilibrium value of the sum of the capture and cascade production rates is not much different from the equilibrium value of the number of decay processes. So, in the R-hot part of the system radiative processes are not very much equilibrated even in the absence of absorption. In section 4.7 we try to give a physical interpretation of the boundary between R-hot and R-cold levels.

4.2 The spontaneous decay probability.

In quantum mechanics, the spontaneous decay probability $A(j, i)$ from an upper state $j$, to a lower state $i$, is related to the square of the matrix element of the atomic $x$ component by

$$ A(j, i) = 4\pi^2 c^{-3} h^{-1} \omega^{-3} |x_{ji}|^2. \tag{4.1} $$

Comparing this with eq.(1.15) shows that $A(j, i)$ can be related to the oscillator strength $f_{ij}$. Taking degeneration into account this relation reads

$$ A(j, i) = (g(i)/g(j)) 4\pi^2 c^{-3} h^{-1} \omega^{-2} E_{ij} f_{ij}. \tag{4.2} $$
For hydrogenic levels the decay probability can now be calculated using eq. (3.20) provided that the sublevels are statistically distributed. We find for the decay from an upper level \( u \) to a lower level \( l \) the value:

\[
A(u,l) = 2\gamma \frac{2}{\hbar} \frac{Z^4}{\tilde{E}^3} (1 - u^2 - \tilde{w}^2)^{-1} h(l,y),
\]

(4.3)

with \( \gamma = 7.87 \times 10^9 \text{s}^{-1} \) as defined in table 3.1 and the the Gaunt factor \( h(l,y) \) as defined in the eqs. (3.20-21).

The correspondence with the results of classical mechanics can be studied if we rewrite eq. (4.1) as

\[
A(j,i) = \frac{4}{3} \frac{Z^4}{\hbar^2} \frac{2}{\Delta \tilde{E}^3} \frac{u^3}{\tilde{w}^4} |r_{ji}|^2.
\]

(4.1b)

Comparing this with eq. (3.13) we see that the correspondence can be traced back to the relation \( 2\omega^3 |r_{ji}|^2 = |\tilde{E}|^2 \), which differs a factor 2 from the classical circular relation \( \omega^3 = |\tilde{E}|^2 \).

More specifically we can compare the quantum mechanical value eq. (4.3) for hydrogenic systems with the classical value of \( A = \tilde{E}/\Delta \tilde{E} \) applied to circular orbits. For that purpose we have to substitute eq. (3.12) for the emission power \( \tilde{E} \) and \( \Delta \tilde{E} = Ry \tilde{E} (1 - u^2 - \tilde{w}^2) \) for the energy gap.

This gives

\[
A(u,l) = 2.77 \frac{Z^4}{\hbar^2} u^3 (1 - u^{-2})^{-1}.
\]

(4.4)

We see that for \( p >> 1 \) this classical circular approach gives an overestimation of a factor 1.74 for the decay \( p = p - 1 \) (the Gaunt factor equals .78 for the step transition) but for jump-like transitions with \( \Delta p > 0.17p \) and \( p >> 1 \), the quantum mechanical result will be larger due to the fact that \( l^{-3} \) is larger than \( u^{-3} \).

From this we develop the concept of radiation for large \( p \)-values which can be summarized as follows:

- In the decay \( p = p - 1 \) circular orbits \( \{ l = n - 1 \} \) are most important.
- The decay takes place in the way as described in section 3.3 (eq. (3.12-3.14)). The frequency of the emitted radiation is almost the same as that of the classical revolution frequency (cf. CP).
- Not all orbits with energy \( E \) are circular which implies that the quantum mechanical value for the \( p = p - 1 \) decay rate will be smaller than that predicted by the classical circular approach.
- In the jump-wise decay, where \( \Delta p > 1 \), elliptical orbits are most effective. Due to the eccentricity, the overlap \( |r_{ji}|^2 \) with lower
levels will be larger.

The presence of these elliptical orbits makes the radiative lifetime of the \( p \) level smaller than the value calculated by the classical circular value.

In sect. 4.5 we give another interpretation of the decay probability.

4.3 The total spontaneous decay frequency

The reciprocal of the natural lifetime of \( n \)-like level \( p \)

\[
T_p^{-1} = A(p) = \sum_{1 < l} A(p, l)
\]  

(4.5)

can now be calculated with the help of eq. (4.3). Two limiting cases of

opacity have to be distinguished (cf. sect. 2.6):

Case A: a plasma optically thin for all radiation

Case B: a plasma opaque for resonant (Lyman) radiation.

By inserting eq. (4.3) in eq. (4.5) and replacing the sum by an integral

we get the following approximations:

In case A

\[
A(p) = \sum_{1}^{n-1} A(p, l) \approx \int_{1}^{P-1} A(p, l) dl \approx \gamma Z^4 \rho^{-5} \ln(E_{l,p} / E_{l-1,p})
\]  

(4.5a)

and in case B

\[
A(p) = \sum_{2}^{n-1} A(p, l) \approx \int_{2}^{P-1} A(p, l) dl \approx \gamma Z^4 \rho^{-5} \ln(E_{l,p} / E_{l-1,p})
\]  

(4.5b)

For increasing \( p \) values the arguments of the logarithms tend to \( 1^3 \),

so that the main \( p \)-dependence of \( A(p) \) is described by \( \gamma Z^4 \rho^{-5} \ln p \).

By the introduction of an opacity dependent parameter \( \zeta \) we can

construct the analytical formula

\[
A(p) = \gamma Z^4 \rho^{-5} (3 \ln p - \zeta)
\]  

(4.6)

with \( \zeta = 0.25 \) for case A, and

\[
\zeta = 1.84 \quad \text{for case B.}
\]

These values of \( \zeta \) are adjusted in such a way that eqs. (4.6) reproduce

the numerically calculated values of \( A(p) \) as good as possible. In fig.

4.4 the analytical expressions (4.6) are compared with the numerical

calculations (found in [BIEA 59b]).

It appears that the analytical expressions reproduce the total

transition probability within 7\% for the lowest level (\( p=2 \) in case A

and 3 in case B) and within 3\% for higher levels. The higher the \( p \)
Fig. 4.1

Functional dependence of the total decay frequency $\nu_\pm(\sigma)$ expressed by

$$\nu_\pm = \gamma^{-1} \lambda_\pm \sigma_\pm A(\sigma)$$

$\sigma = \text{case A}, \lambda = \text{case B}$ according to [NEW 59b].

Solid curves: $1 \ln p - \xi$, with $\xi = 0.25$ (case A) and $\xi = 1.24$ (case B).

Dashed line: $2 p^{1/5}$

$$\begin{align*}
E & \quad F_p & \quad E_{p+1} \\
\gamma < 1 & \quad y = \frac{AE}{|E_p|} & \quad 0 \\
\gamma > 1 & \quad y = \frac{AE}{|E_p|} & \quad y = 1 \\
\epsilon & \quad \epsilon_{p+1} = \frac{|E|}{E_p} & \quad \epsilon_{p+1} = E_p
\end{align*}$$

$p = \alpha \sqrt{\sigma/|E_p|}$

Fig. 4.2: The relation between the location parameters in the energy scheme.
value the better the approximation.
A more crude approximation for case A is obtained by inserting $2 \sqrt{p}$ instead of $3 \ln p - 0.25$. This approximation

$$\alpha(p) = 2 \gamma \sqrt{p}^{-4.5}$$

(4.7)
is also depicted in Fig. 4.1 from which appears that it reproduces the correct $\alpha(p)$-values for case A within 1% for $p=3$ and within 6% for $4 \leq p \leq 25$.

4.4 The equilibrium value of the cascade contribution.
In the FITE part of the system we can calculate the cascade contribution to a level $p$ with

$$\sum_{u|p} n^u(u) \Delta(u,p)$$

(4.8)
in which $n^u(u)$ is the Saha density of a upper level. This summation runs over all excited levels for which $u|p$.
Inserting eq.(4.3) and changing the sum in an integral we get the approximation

$$\sum_{u|p} n^u(u) \Delta(u,p) = n^u(p) \gamma 2^4 p^{-5} \int_{\frac{E_p}{T_{p+i}}}^{|E_p|/kT} \exp \frac{E_p}{T_{p+i}} h(p,y)dy$$

(4.9)
in which the continuous variable $E=\Delta E/kT$ is a generalization of the energy gap normalized to the temperature

$$E_{pq} = \frac{E_p}{kT}$$

Furthermore we define $\xi_p \equiv \xi_p,ion = |E_p|/kT$. (4.10)

In Fig. 4.2 the relation between $\xi$, $\gamma$, and $E_{pq}$ is outlined.

It should be noted that the Jacobi factor $h(p,y)=h(p,E_{pq})$ is (weakly) $\xi$-dependent and can not be taken out of the integral. In section 4.6 we will give a further approximation of equation (4.9).
4.5 The equilibrium value of the capture contribution.

Apart from the decay of higher bound states, a level \( p \) can also be populated due to 'radiative decay' of free states. This population mechanism is known as two-particle recombination or capture process and can be represented by the reaction equation

\[
e + A^+ + A_p + h\nu.
\]

As we know that the bound states merge continuously into the free states, we suggest that it must be possible to see how cascade merges into capture. So we have to generalize the equilibrium value of the bound-bound population contribution \( n^B(u) A(u,p) \) in such a way that it can be lifted over the ionization limit and can be applied to combinations of ionic cores with free electrons. Such an \( u \) combination which is able to 'decay' to a bound state will be denoted by a 'quasi atom'. It is a situation in which an electron with \( E0 \) and an ionic core cohabit in the same atomic volume \( V_E \). The precise value of the volume \( V_E \) is unknown but we propose that in the generalization of \( n^B(u) A(u,p) \) the density of quasi atoms is proportional to \( V_E \), whereas \( A(u,p) \) is proportional to \( V_E^{-1} \). This implies that the product is \( V_E^{-1} \)-independent. These assumptions will be confirmed by the following derivation.

First we write the equilibrium number of atoms in upper state \( u \) in the generalized form \( n_u n_p V_E f^E(E) dE \), where \( f^E(E) dE \) represents the number of quasi atoms of energy between \( E \) and \( E + dE \). The Maxwell distribution function of free electrons is denoted by \( f^M(E) \). The number of quasi atoms can be rewritten as

\[
g_u n_p V_E \bar{f}_E(E) C_{E,V} dE.
\]

The quantities \( C_{E,V}(E) \) and \( \bar{f}_E(E) \) are defined in eqs. (2.20), (2.23) and (2.24).

To generalize \( A(u,p) \) we notice that the factor \( p^{-3}(p^{-2} - u^{-2})^{-1} \) (cf. eq. (4.3)) contains the ratio of the energy gap and the ionization potential \( \gamma = E_{pu}/[E_p] \). Thus we can replace \( p^{-3}(p^{-2} - u^{-2})^{-1} \) by \( p^{-1} \gamma^{-1} \). Values of \( \gamma \geq 1 \) correspond with free-bound transitions. In the factor \( u^2 \) we recognize the number of bound states per bound energy range in the atomic energy scheme; in eq. (3.8) we saw that \( u^2 \approx Z^2 \hbar \gamma (p, y)/(\hbar \gamma A_{E_p}(u)) \). So we can write in a general representation

\[
A(u,p) = 2\gamma Z^2 \hbar (p, y)/(\hbar \gamma A_{E_p}(u))
\]

and this can be transformed to the continuum replacing \( A_{E_p}(u) \) by \( C_{E_p,V} V_E \).
in which \( V_a \) is a volume of typical atomic dimensions and \( G_{E,V} \) is the distribution of free quantum states (cf. eq. (2.19)). In section 3.5 we have seen that this free quantum state distribution can also be described in a classical way, a correspondence denoted by CP. So the replacement of \( \sum G_{E,V}^m(u) \) by \( G_{E,V}^m V_a \) is justified by the CP and we get for free-bound transitions the 'decay probability'\

\[
A(E,p) = 2\gamma Z^2 h(p,\gamma)/(\gamma y G_{E,V}^m V_a). \tag{4.14}
\]

The expressions (4.13-14) show that the probability of leaving a location is inversely proportional to the state density at that location. So the less 'space' the less particles want to stay.

Combination of eqs. (4.13) and (4.14) makes it possible to lift \( n^o(u) A(u,p) \) across the ionization limit with a result that:

\[
n^o(u) A(u,p) = n_o^o \frac{h^3}{e^2} \frac{1}{(2\pi mkT)^3/2} h(p,\gamma) Z^2 \gamma^{-1} y^{-1} \exp^{-S/\kappa T} d\gamma. \tag{4.15}
\]

Integration of this equation over all possible positive electron energy values gives the total rate of capture processes in state \( p \).

Expressed in the usual form of \( n_o n_o A(p) \) we get for the recombination coefficient

\[
h(p) = \frac{h^3}{e^2} \frac{1}{(2\pi mkT)^3/2} \gamma Z^4 \Gamma^{-3} \exp \int_{\kappa p}^{\infty} \frac{\exp^{-\kappa p}}{\kappa} h(p,\gamma) d\gamma. \tag{4.16}
\]

This formula is the same as that obtained by regarding capture as the reverse process of photo ionization [89A39a]. The similarity between cascade and capture becomes more striking if we rewrite

\[
n_o n_o A(p) = n_o p \frac{1}{\Gamma} \int_{\kappa p}^{\infty} \frac{\exp^{-\kappa p}}{\kappa} h(p,\gamma) d\gamma. \tag{4.17}
\]

By comparing this with eq. (4.9) we see that capture is merely an extension of the equilibrium value of the cascade over the ionization limit. For the LTE top of the system the capture and cascade contribution can be put together in one formula by adding eqs. (4.9) and (4.17). This gives

\[
n_o n_o A(p) = \sum_{u,p} n^o(u) A(u,p) = n_o p \frac{1}{\Gamma} \int_{\kappa p}^{\infty} \frac{\exp^{-\kappa p}}{\kappa} h(p,\gamma) d\gamma. \tag{4.18}
\]

So by writing \( n^o(u) A(u,p) \) in an appropriate form it turns out to be possible to relate capture to cascade.

<CP> In fact this is a manifestation of the correspondence principle
and can be seen as an extension of CPI.

Bound and free states are not essentially different although the former group has to be described quantum mechanically while the latter can be treated classically. In this case the CF effectuates a relation between elliptic and parabolic orbits, a relation which is successful since it deals with a statistical approach (feature CPA, cf. section 3.3).

4.6 Temperature dependency

In search of the temperature dependence of the cascade and capture population rates we first notice that the electron temperature enters eq. (4.16) by the parameter $\frac{p_0}{\epsilon}$, high temperatures correspond with low $p_0$ values. Secondly we realise that via $\frac{p_0}{\epsilon}$ this T-dependence is mainly determined by the exponential integral [-$\text{Ei}$(-x)] $= x \int_0^\infty \exp(-x) dx$.

The T-dependence induced by the Gaunt factors is less important and will be neglected.

This well-known exponential integral has the following limiting values [JAH 66]

\[ [-\text{Ei}(-x)] = \ln x^{-1} \gamma_e \text{ for } x \ll 1 \]  
\[ (4.19a) \]

and

\[ [-\text{Ei}(-x)] = \frac{\epsilon p_0 - x}{x} \text{ for } x \gg 1 \]  
\[ (4.19b) \]

with $\gamma_e \approx 0.57$ is Euler's constant.

First we consider the case of high temperatures, such that $\frac{p_0}{\epsilon} \ll 1$

Using eq. (4.18) and the approximation $\frac{p_0}{\epsilon} \approx 2 \text{ Ry} \approx 2 \text{ Ry} kT$ we get

\[ n_{e^+}(p) = \int \frac{\pi}{u^3(p)} A(u,p) = n^3(p) \gamma^2 e^{-5} \left[ 3 \ln p - \ln(2^2 \text{ Ry}/kT) + c \right] \]  
\[ (4.20) \]

in which $c$ is a correction term to adjust eq. (4.20) to its actual value. Apart from Euler's constant and $\ln 2$ it also contains the influence of the Gaunt factor. It turns out that $c$ is level-dependent but close to one for large $p$ values.

The capture contribution can be found by applying eqs. (4.17) and (4.19a) which gives

\[ n_{e^-}(p) = n^3(p) \gamma^2 e^{-5} \left[ 2 \ln p - \ln(2^2 \text{ Ry}/kT) - \gamma_e \right] \]  
\[ (4.21) \]

So the cascade must be responsible for the contribution

\[ \int \frac{\pi}{u^3(p)} \text{ A(u,p)} = n^3(p) \gamma^2 e^{-5} \left[ \ln p + \gamma_e - c \right] \]  
\[ (4.22) \]
i.e. the difference between eqs. (4.20) and (4.21).

The following remarkable conclusions can be drawn:
- For the PLTE part of the system and relatively high temperature, i.e. $\epsilon_p \ll 1$, the capture and cascade contribution can be put together in

$$n_\text{eq} \frac{\alpha(p)}{\epsilon_p} + \sum_{\nu} n_{\nu}^\text{eq} A(\nu,p) = n^\text{eq}(p) \gamma Z^4 \rho^{-5} [3 \ln p - \xi(T)], \quad (4.23)$$

with

$$\xi = \ln \left( \frac{\text{Ry}}{kT} \right) + 1.0$$

for $p > 1$ and $\epsilon_p \ll 1$.

- Globally one third is due to cascade and two thirds is due to capture.

- The temperature dependence of $\xi$ is in first order due to the temperature dependence of the capture only. The cascade contribution from the PLTE part of the system is in first approximation temperature-independent.

- In PLTE the number of decay processes has a very similar form

$$n^\text{eq}(p) \sum_{\epsilon_p} A(p,1) = n^\text{eq}(p) \gamma Z^4 \rho^{-5} [3 \ln p - \xi] \quad (4.24)$$

so that if $|\xi - \xi|$ is not too large, there is not much difference between the equilibrium amount of population processes due to the cascade and capture at one side and decay at the other side.

We pay some more attention to this remarkable fact. In section 2.2.4 we have seen that the Saha density, which is the equilibrium density, results from the proper balance of collisional ionization and three particles recombination. This equilibrium will be established if the electron density $n_e$ is large enough. But here we see that ionization and three particles recombination are not much disturbed due to the presence of radiative processes. So even if the PLTE equilibrium maintaining processes are omitted e.g. in the case of a very low $n_e$ value and the system is left to radiative processes only, the equilibrium departure will be limited if $|\xi - \xi|$ is small. It is possible to find a electron temperature such that $|\xi - \xi| = 0$.

This striking fact already discussed in 1938 by Baker and Menzel in [BAK 38] will be treated in sect 8.3 where we deal with the Capture Radiative Cascade balance.
For low temperatures, i.e., \( \delta_p \gg 1 \), capture gets a different form (cf. eq. (4.19b)) and the proportion cascade:capture as 1:2 is no longer valid and cascade becomes relatively more important in the LTE top. Yet, however, the electron density is too small to maintain LTE, capture will be the leading process in populating the levels and severe deviations from the Saha density can be expected. Making use of eqs. (4.17) and (4.19b) we find that the number of capture processes to a level \( p \) with \( \delta_p \gg 1 \) is given by

\[
\eta_{c,p} \equiv \alpha(p) = n^0 p \gamma \frac{\exp(-\frac{\epsilon_p}{kT})}{\epsilon_p^3}.
\]  

(4.25)

4.7 The radiative hot/cold boundary. A physical interpretation.

The preceding makes clear that there is an important difference in the kinetics of capture and cascade between the levels for which \( \delta_p \ll 1 \) and the levels for which \( \delta_p \gg 1 \). For not too high temperatures this means that there is a boundary in the energy scheme which separates two domains. A lower domain for which \( \delta_p \ll 1 \), and an upper domain for which \( \delta_p \gg 1 \), in which \( \delta_p \) is close to unity. We choose \( \delta_p = 1 \).

- Levels for which \( \delta_p \ll 1 \) are said to be radiative cold whereas
- Levels for which \( \delta_p \gg 1 \) are said to be radiative hot.

We come to this boundary from a mathematical point of view. Two different limiting values of the functional dependence describe two situations different in kinetics. Faced with the challenge to give a physical interpretation of this boundary we go back to the picture of quasi atoms. Their number density is given by \( n_0 n_a V_a \) in which \( V_a \) has to be determined. With respect to the level \( p \) it is useful to consider the classical volume of the p-shell

\[
V_p = \frac{\delta V}{\delta p} = 2\pi a_0^3 p^2 z^{-3}
\]  

(4.26)

I.e. the volume of a sphere between the radii \( a_p = a_0 z^{-1} p^2 \) and \( a_{p+1} = a_0 z^{-2}(p+1)^2 \). Now we define

\[
n^0(p) = n_0 n_a V_p
\]  

(4.27)

as the number of quasi atoms in the p-shell and we suspect that \( n^0(p) \) provides an important supply in the population of the p-shell bound states. This is justified by eq. (4.1) in which we see that the overlap determines the decay probability and \( n^0(p) \) represents the number density of orbits in such an overlap. Now we compare \( n^0(p) \) with \( n^a(p) \).
First we realize that both bound and quasi atoms in the p-shell experience the same force and acceleration due to the ionic core. Second we note that the energy gap in the free-bound transition will generally be larger than that of decay processes from bound p-states to lower states. So in the classical picture in which $A = \Delta E/\Delta t$ (cf. 4.3) we may expect that the number of capture processes will remain below the equilibrium value of the decay processes, if there are less quasi atoms than the equilibrium number of bound states in the p shell. So when

$$n^0(p) < n^8(p).$$

(4.28)

Applying eqs. (4.26), (4.27) and (2.33) we find that this happens if

$$\frac{1}{\beta p} < \epsilon^{3/2}_p \exp \epsilon_p$$

(4.29)

which determines a boundary in the energy scheme very close to that of cold and hot levels.

Another interesting fact becomes manifest if we rewrite eq. (4.28) as

$$\frac{V_p}{p^2} < \frac{\hbar^3}{(2m_em^2_e)^{3/2}} \exp \epsilon_p.$$  

(4.30)

At the rhs we meet apart from the exponential factor the spatial volume of a free quantum state. At the lhs the spatial volume of the bound states in the p-shell can be found. Again we are faced with a boundary in the energy scheme not far away from that between hot and cold levels. And we arrive at the statement that

- if the volume of the free states is larger than that of a state in the p shell, it is not attractive for electrons to be in the p state,

- the number of quasi atoms in the p-shell is less than the Saha density and the capture processes are not able to maintain the equilibrium value of the number of decay processes.
Chapter V  Electron collisions

5.1 Introduction

There is a large variety of collision theories in literature and in the literature of cross sections, sometimes presented in graphs or tables and in other cases by semi-empirical formulae. To break a way through this wilderness we make the following approach. First we confine ourselves (mainly) to collision theories dealing with transitions between excited states. In contrast with the ground state excitation, these transitions deal with relatively small energy gaps and we expect that a classical approach must be possible. In addition, we can assume that the atom (or ion) can be regarded as composed of one core and one outer electron and that this latter effectuates the transition. Secondly we distinguish between cold and hot collisions. Cold collisions are collisions in which the (mean) velocity of the incident electron is much smaller than that of the bound electron, i.e. $kT_e << |E_p|$. The collision is essentially a three particle event and in most cases the total kinetic energy of the electron which leaves the atom is increased. For hot collisions the contrary applies; $kT_e >> |E_p|$ and the incident electron is the leading particle in the collision which in most cases results in an energy loss of the incident electron. Since for increasing values of the principal quantum number $p$ the ionization energy $|E_p|$ approaches zero, the top of the atomic system is always determined by hot collisions and that is why they are of large interest. We start the study with an analysis of these hot collisions and follow the line of increasing complexity. First we consider the energy transfer from a fast electron to a free electron initially at rest treated in the classical way of Rutherford. By increasing the complexity more and more we approach the actual situation of the electron-atom collision but we try to keep sight on the simple situation of the binary, two electron approach. In this comparison of electron-electron with electron-atom collision we are guided by applications and features of the correspondence principle (CP) and we will come to the conclusion that there is no substantial difference between the energy transfer from a free to a bound electron on one hand and the energy transfer between two free electrons on the other hand. In section 5.10 attention is paid to the classical approach of cold collisions. And in section 5.11 we discuss semi-empirical collision theories which try to get cold and hot collisions together in one formula. In section 5.12 a formula for the total collisional destruction rate will be constructed.
5.2 Energy transfer to a free electron, initially at rest

5.2.1 The classical treatment

The differential cross section for the scattering of a particle with mass \( m \), charge \( e \) and velocity \( v \), by a fixed Coulomb potential \( V = \frac{Ze^2}{r} \) is according to the classical Rutherford formula given by

\[
\frac{d\sigma}{d\sigma^*} = \frac{e^2}{2\mu} \left( \frac{\hat{e}^2}{\hat{v}^2} \right) \frac{\sin \hat{\sigma}^*}{\sin \hat{\sigma}^*}.
\]

(5.1)

where \( \hat{\sigma}^* \) is the scattering angle and \( \hat{e}^2 = \frac{e^2}{4\pi\epsilon_0} \).

Applied to the collision between two electrons eq. (5.1) gives the differential cross section in the centre of mass system.

If we consider in the laboratory system an electron \( 1 \), with initial velocity \( \vec{v}_1 \), and kinetic energy \( E_1 = \frac{1}{2} m v_1^2 \), which impinges on electron 2 initially at rest (cf. fig. 5.1), we can use eq. (5.1) after a transformation from the centre of mass to the laboratory system. This results in

\[
\frac{d\sigma}{d\sigma^*} = \frac{2n^2}{\mu} \frac{\cos \hat{\theta}}{\sin^2 \hat{\theta}}.
\]

(5.2)

Since \( m_1 = m_2 \) conservation of momentum and kinetic energy predicts that the final velocities \( \vec{v}_1^* \) and \( \vec{v}_2^* \) are perpendicular to each other and the fixed relation

\[
\Delta E = E \sin^2 \hat{\theta}
\]

(5.3)

holds between the deflection angle \( \hat{\theta} \), and the energy transfer \( \Delta E \).

Fig. 5.1

\[
\begin{array}{c}
\begin{array}{c}
1 \\
\text{Initial}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
2 \\
\text{Final}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\vec{v} \\
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
\vec{v}_1^* = 0 \\
\end{array}
\end{array}
\end{array}
\]

Combination of eqs. (5.2) and (5.3) gives the relation between the effective cross section \( d\sigma E \), and the corresponding energy transfer between \( \Delta E \) and \( \Delta \hat{\sigma} = d\sigma E \)

\[
\frac{d\sigma}{d\hat{\sigma}^*} = \frac{\mu^2}{\hat{e}^2} \frac{1}{\Delta \hat{\sigma}^*}.
\]

(5.4)

It is useful to relate the energy transfer \( \Delta E \) to the impact parameter \( R \). If we apply \( d\sigma^* = 4\pi R^2 \) and integrate eq. (5.4) we get the relation
\[ \Delta E = \frac{\mu}{R_n} \cdot \frac{1}{R^2 + R_n^2} \]  

(5.5)

In which \( R_n \) corresponds with the smallest distance between the two electrons and the maximum value of the energy transfer. For large \( E \) values or distant encounters, \( R_n \) is negligible and eq. (5.5) gets the simple form

\[ \Delta E = \frac{\mu}{R^2} \]  

(5.6)

We emphasize the fact that both eqs. (5.5) and (5.6) show that there is a one-to-one relation between impact parameter and energy transfer. A close collision (small \( R \) values) implies a large energy transfer.

5.2.2 Quantum mechanical results

The quantum mechanical (QM) treatment of Rutherford scattering gives the same result as long as it concerns a collision between non-identical particles. For collisions between identical particles there are differences between the classical and quantum results.

The relation between cross section and energy transfer from an electron with energy \( E \) to an electron initially at rest, as given by quantum mechanics (cf. [LAN 65]), is given by

\[ \frac{d\sigma}{d\Delta E} = \pi \mu^2 \frac{1}{E^2} \left[ 1 - \frac{1}{(E/\Delta E-1)^2 + (E/\Delta E-1)^2} \right] \]  

(5.7)

The expression between the square brackets represents the difference between the QM and CL results. This difference increases if \( E/\Delta E \) approaches unity. This is caused by the fact that from the quantum mechanical point of view identical particles are indistinguishable. In the comparison between electron-atom and electron-electron collisions, this \( \Delta E \approx E \)-region of e-e collisions corresponds with the threshold region in ionization and excitation processes for e-a collisions (cf. sect. 2.4.3).

Concluding, we establish the following application of the CP:

-CP5- Apart from the threshold region, the classical and quantum mechanical approach of the energy transfer from an incident electron to an electron initially at rest give the same result. So if an electron-atom collision can be regarded as a binary collision between a free and a bound electron, and the energy transfer is much less than the kinetic energy of the incident electron, the correspondence principle must be applicable for the electron-atom collision.
5.3 The binary encounter approximation.

If a swift electron gives into an atom and a close encounter with a bound electron takes place, the latter will forget its binding force and behaves as if it were free.

It is of interest to search for a 'correspondence' between this kind of collisions and that of classical collisions between two free electrons. Suppose the interaction results in the transition \( p \rightarrow q \) in which \( p \) and \( q \) are principal quantum numbers. In the case of a hydrogenic atom both \( p \) and \( q \) are sharply determined in energy, which implies that the energy difference \( E_{pq} \) is also determined sharply. In the classical analogon the possible states in the \( q \) shell are continuously distributed over an energy band of value \( E_q \), centered around \( E_q \). It is plausible that if the correspondence principle (CP) is applicable, it should relate the quantal transition \( p \rightarrow q \) with the continuous range of classical collisions where energy between \( E_{pq} \) and \( E_{pq} \) is transferred. Under the assumption that the atomic electron is initially at rest we can apply eq. (5.4). Together with \( \Delta E_{pq} = \frac{\hbar}{\pi \sqrt{2 q + 1}} \) (for large \( q \)-values), which results in the cross section

\[
\sigma_{pq} = \frac{n_E}{E_p} \frac{\hbar}{\pi \sqrt{2 q + 1}} \quad \text{(5.8)}
\]

The cross section for ionization can be obtained by integration of eq. (5.4) over the energy band \( (E_p, E) \), which gives

\[
\sigma_{ion,p}(E) = \frac{\pi E_p^2}{E} \left( \frac{1}{|E_p|} - \frac{1}{E} \right) \quad \text{(5.9)}
\]

This ionization cross section is comparable to that given by Thomson [THO 12].

So far it was assumed that the atomic electron was initially at rest which is not true in the reference frame of the atomic nucleus. It is possible to take the velocity distribution of the atomic electron into account in a classical way by comparing the excitation process with that of the passage of a swift electron through a gas of free electrons, which are supposed to have the same velocity distribution as that of the atomic electron. The differential cross section with respect to energy transfer is in this case found to be [PER 75]

\[
\frac{d\sigma}{d\Delta E} = \frac{\pi E_p^2}{E} \frac{1}{\Delta E^2} \left( 1 + \frac{\Delta E}{E_p} \right) \quad \text{(5.10a)}
\]

A more general representation can be obtained by employing \( y = \Delta E/|E_p| \) this gives
\[
\frac{dc}{dy} = \frac{2\hbar^4}{E_{pq}} \gamma^{-2} \left( 1 + \frac{4}{3} \gamma^{-1} \right) \quad .
\] (5.10b)

Substitution of \( \Delta E = \frac{\hbar}{p} \) and \( \Delta \gamma = 2\hbar \gamma q^{-3} \) in eq. (5.10a) results in
\[
c_{pq} = \frac{2\hbar^4}{E_{pq}} \gamma \gamma^{-3} \left( 1 + \frac{4}{3} \frac{\gamma^{-1}}{\gamma^{-1}} \right) .
\] (5.11a)

The second term between brackets reflects the initial velocity distribution of the atomic electron with mean kinetic energy, \( E = \left| E_p \right| \).

This formula has a remarkable history. First presented by Thomas in 1927, it was largely forgotten when the burst of activity after the publication of Gryzinski [Gry 59] led to a comparable result. The validity of eq. (5.11) as presented by the various authors is discussed in [PER 75]. The theory is known as the classical impulse or the binary encounter approximation (BEA) and can be seen as an application of the correspondence principle.

-CPA- The correspondence between the quantal transition on one hand and the classical differential cross section with the energy gap \( E_{pq} \) on the other hand, is denoted by the density-of-states correspondence principle (cf. [PER 75]).

This BEA cannot be applied to step processes i.e. transitions of the kind \( \Delta p = 1 \). There are several reasons for this.

First, we note that a basic assumption of the BEA is that the encounter of the two electrons is so close that the core of the atom has no influence on the collision. Since a step process involves a small energy transfer which implies a large impact parameter (cf. eqs. (5.5) and 5.6), this basic assumption is violated.

Second, one of the main features of the correspondence principle (CPA cf. section 3.3) is that the CP can only be applied to transitions for which the change in section \( \Delta A \) is large compared to Planck's constant, \( \hbar \). Since \( A \) scales with \( p \), this implies that the BEA is only applicable to so-called jump processes, i.e. transitions for which \( \Delta p = q-p \gg 1 \).

Third, the determination of the cross section with the help of the classical differential cross section with respect to energy can only be realized without ambiguity if this differential cross section is more or less constant over the energy gap \( E_{pq} \), and this is certainly not the case for the transition \( p \rightarrow p+1 \). This is illustrated by fig. 5.2, where the transition \( p \rightarrow q \) corresponds with the area under the curve. For jump processes where \( E_{pq} \ll CE \), there is not much variation in the differential cross section over the energy range \( E_{pq} \) and the approximation...
FIG. 3.2

The differential cross section $\frac{d\sigma}{dy}$ as a function of $y = \frac{\Delta E / k_p}{E}$, the ratio of transition to ionization energy. The two lower axes give the application in the calculations of the cross sections of the transitions with start-level $p = 5$ and $p = 10$. The hatched areas correspond to the transition $10 \to 14$ and $5 \to 8$.

\[ \sigma_{pq} = \frac{d\sigma}{dE} = 2Ry^2 \frac{q^{-3}}{e^{-3}}, \]  

(5.11b)

is expected to be justified. But for the step processes the area is not easy to define and the BEA is not valid. Moreover it should be realized (cf. table 3.1) that the approximation $E_{pq} \approx 2Ry^2 q^{-3}$ gives an over-estimation. For the level $p = 5$ this is more than 30%. Nowadays it is generally assumed that Gryzinski's BEA cross sections give too large values for step processes (cf. fig. 5.6), [Ske 62], [Sro 64], [Joh 72] and [Def 79]).

- Resuming, for small values of the impact parameter, the collision of a fast electron with an atom can be regarded as a binary encounter of the two electrons. Since small impact parameters involve large energy transfers, this means that the BEA can be applied to jump processes. The correspondence principle gives a relation (CP6) between the quantal transition $p \to q$ on one hand and the differential cross section $\frac{d\sigma}{dE}$ with respect to energy transfer and the energy gap $E_{pq}$ on the other hand. For step processes for which large values of the impact are involved, the CP is not applicable in this form. But the classical theory is not appropriate either. A theory in which the shielding influence of the core is taken into account has to be consulted. This will be done in the next section where we study the classical theory of energy transfer to a harmonically bound particle.
5.4 Energy transfer to a harmonically bound charge

In the previous section attention was paid to atomic transitions caused by a swift electron "diving" into an atom. Now we consider the situation where the electron stays outside the atomic region. The electron is said to be "bypassing" instead of "diving" and the BBA is no longer supposed to give a good description. Better results can be expected from the dipole approximation (DA). We follow Jackson ([JAC 75]) who gives a comprehensive description of early theories like that given by Bohr (1913).

In the DA the following assumptions are made:
- initial and final amplitudes, \( a_p \) and \( a_p' \), of the oscillating electron are small compared to the impact parameter \( R \).
- Consequently, \( R \) can be measured from the origin \( O \) of the binding force and the variation in the position of the bound electron can be neglected with respect to \( R \) (cf. fig. 5.3).

\[ \text{(5.12a)} \]

![FIG. 5.3 The dipole approximation.](image)

- Then only the electric field \( \mathcal{E}(t) \), caused by the projectile, needs to be included in the force equation

\[ \mathcal{F} + \mathcal{F}(t) + \omega_p^2 N = \frac{e}{m} \mathcal{E}(t) \]

of the electron which, in the absence of the external force, oscillates with a characteristic frequency \( \omega_p / 2\pi \). This results in an energy transfer given by

\[ \Delta E = \frac{\pi \hbar^2}{n} |\mathcal{E}(\omega_p)|^2 \]

in which \( \mathcal{E}(\omega_p) \) is the Fourier amplitude ([JAC 75]) of the electric field caused by the bypassing particle and \( m \) is the mass of the bound electron.
- The incoming particle is only slightly deflected by the energy transfer. So its path can be approximated by a straight line and the electric field induced by this rectilinear orbit at the origin of the oscillator is known as a function of time, velocity, impact parameter, and the charge of the bypassing particle. Fourier transformation of this electric field can be effectuated and eq. (5.12b) gets the form

$$\Delta E(R) = \frac{2k^2}{m v^2} \frac{1}{R^2} \left[ R^2 k_0^2 (\tilde{R}) + R^2 k_1^2 (\tilde{R}) \right] .$$

(5.13)

The modified Bessel functions $k_0$ and $k_1$ correspond to the longitudinal and transverse electric fields respectively as caused by the bypassing particle at the origin of the binding force. The argument of the Bessel functions is given by

$$\tilde{R} = \omega_p R / v .$$

(5.14)

The expression in the square brackets in eq. (5.14) has the limiting values

$$[ \ ] = \begin{cases} 1 & \text{for } \tilde{R} \ll 1 \\ \frac{\pi}{2} \frac{a^2}{2R} & \text{for } \tilde{R} \gg 1 \end{cases}$$

(5.15a, 5.15b)

The factor multiplying the square brackets is just the approximate result given by eq. (5.6).

The parameter $\tilde{R}$ is sometimes called the adiabaticity parameter. It compares the collision time, $R/v$, with the oscillation period $2\pi p$. For $\tilde{R} \ll 1$, the collision is sudden. It takes place during a time which is short compared to the oscillation period. In that case (cf. eq. (5.15a)) the energy gain has the same value as that given by the simple formula eq. (5.6). Apparently the bound electron behaves as if it were free. In the opposite limiting case where $\tilde{R} \gg 1$, the collision is adiabatic. The collision time is long compared to the oscillator period. The bound electron will make many cycles of motion during the passage of the incident particle and adapts adiabatically to the slowly varying electric field strength. As a consequence, only a small amount of energy will be transferred which is manifested by the exponent in eq. (5.15b).

Thus far, impact parameters less energy is transferred than predicted by the binary eqs. (5.5) and (5.6). The presence of the binding force can be regarded as providing a shielding against bypassing particles. In fig. (5.6) an impact parameter analysis is
presented. It shows how the BEA region merges in the DA region for increasing $k$-values.

**FIG. 5.4**

Energy transfer as a function of the impact parameter for a given energy $E$. The minimum value $R_{\text{min}}$ is comparable with the amplitude of the oscillator $a_0$. The maximum value corresponds with $R_{\text{max}} = u_0 R/\nu = 1$.

The BEA concerns large energy transfer and low $k$-values. The DA is applicable for $R > a_0$. For too large $k$-values, in the adiabatic region, energy transfer is reduced with respect to the simple classical formula eq. (5.6) represented by the dashed line.

The DA has several interesting features. For instance, it turns out that for a given value of $R$, the electric field created by the bypassing particle is only dependent on its charge and velocity but not on its mass. The mass in eq. (5.13) is that of the bound particle. Thus the DA can be applied to all kind of bypassing particles, (if relevant eq. (5.13) should be multiplied by the charge number $Z$ of the projectile) and a large variety of targets. In cases where the target is charged, the rectilinear orbit of the projectile will change into a parabolic. However, this will not change the results of the sudden region. In the most general case we can apply eq. (5.12b) to all kinds of non-relativistic oscillators embedded in an electro-magnetic radiation field, irrespective of the origin of the radiation.

**Conclusion**

The dipole approximation (DA) provides a good classical description of the electron-atom interactions for collisions with large impact parameters, i.e., small energy transfer. The effect of the binding core can be regarded as a shielding of the electron against bypassing particles. This shielding is effective for adiabatic collisions.

In the next section we will look for a corresponding quantum mechanical treatment and the conditions for the application of the CP will be discussed.
5.5 Time dependent perturbation theory

In quantum mechanics time dependent perturbation theories (TDPT) applied to dipole transitions give results very similar to eq. (5.14). The main difference between the classical and quantum mechanical results can be understood by taking into account the probabilistic nature of quantum mechanics. A bound electron in state $p$ is not performing just one particular oscillation but participates simultaneously in an (infinite) number of oscillations, each belonging to a transition $p \rightarrow q$. The distribution over the various oscillations is given by the oscillator strength $f_{pq}$. In this way it is evident that the sum rule $\sum_{q \neq p} f_{pq} = 1$ (cf. sect. 3.41) should be satisfied.

The QM analogon of eq. (5.13) for an electron-atom collision is

$$\sum_{p} f_{pq} = \frac{1}{E} \sum_{p} \frac{1}{R^2} \sum_{q \neq p} f_{pq} \left[ k_{pq} \left( \frac{R}{R_{pq}} \right) \right]$$

in which $f_{pq}$ is the probability for the transition $p \rightarrow q$. The corresponding energy transfer is $k_{pq}$. We see that we have lost the fixed relation between impact parameter and energy transfer as presented in the classical description. But let us consider the mean energy transfer in the collision with impact parameter $R$ and initial state $p$. To achieve this we sum eq. (5.16) over all possible transitions, which gives

$$\langle \Delta E \rangle = \frac{1}{E} \sum_{p} f_{pq} \left[ \sum_{q \neq p} f_{pq} \left[ k_{pq} \left( \frac{R}{R_{pq}} \right) \right] \right].$$

Each term of this summation contains the expression between brackets, and is a function of the adiabaticity parameter $\tilde{R}_p$. But this parameter has different values for all the possible excitations of the $p$ level, which implies that in general the square brackets cannot be taken out of the summation. However, a glance at the limiting values (eq. 5.15) points out that the brackets expression equals one for $\tilde{R}_p \ll 1$. So, for the maximum of all $R_{pq}$ related to ionization, the relation

$$\tilde{R}_p = \sqrt{E_p / v_p} = \sqrt{E_p / (\text{MeV})} \ll 1$$

holds, the square brackets in eq. (5.17) can be replaced by one, the sum rule can be applied, and we get

$$\langle \Delta E \rangle = \frac{1}{E} \sum_{p} \frac{1}{R^2}$$

This is the same as the classical formula (5.6) and the sudden dipole
approximation (eqs. (5.14) and (5.15a)). And we may conclude that,

-CP- the QM result for mean nut energy transfer to the bound electron
due to all possible down- and upward transitions in the sudden
collisions of swift charged particles with atoms, is the same
as the classical binary result.

This manifestation of the correspondence principle was found by
Williams in 1931 [NPL 31] and it can be seen as a consequence of the
feature CPA (sect. 3.3), i.e. that the CP is applicable to statistical
properties.

The difference with the binary approach is manifest in the adiabatic
region. A difference which can also be understood classically (cf.
sect. 5.5): the atomic core provides a shielding for the bound electron
against bypassing particles. This shielding can be compared with the
Debye shielding in the interaction between free electrons. However,
the atomic shielding length is much smaller than the Debye length.

The basic idea of the time dependent perturbation theory was initially
given by Bohr in 1913. It was applied to nuclear problems by Alder
[ALD 56]. In 1962 Seaton followed this method to study electron-atom
collisions [SRA 62].

For the transition $p \rightarrow q$ the cross section can be calculated using
eq (5.16) in the following way:

$$
\sigma_{pq} = \int_{R_{\text{min}}}^{\infty} 2\pi R_{\text{pq}}^2 \, dR = \frac{2\pi \hbar^4}{E} \int_{R_{\text{pq}}}^{\infty} \frac{[\text{ }]}{R_{\text{pq}}^4} \, dR.
$$

(5.19)

The integral in eq. (5.19) can be approximated as follows. First we
realize that due to the exponential decay we can neglect the square
bracket form, i.e. $[\ ] = 0$ for $R \gg 1$ (cf. eq. (5.15b)) so that the
upper boundary of the integral can, in a first order approximation, be
replaced by one. Furthermore we apply for the square bracket function
the approximation $[\ ] = 1$ for $R < 1$ and we obtain

$$
\sigma_{pq} = \frac{2\pi \hbar^4}{E} f_{pq} R_{\text{pq}}^{-4} \ln(R_{\text{pq}}^{-1})
$$

(5.20)

So the calculation of $\sigma_{pq}$ is closely related to the determination
of the minimum value of the adiabaticity parameter. Since the step
process $p \rightarrow p+1$ is the most dominant one (the $f_{pq}$ decreases with $\Delta \bar{R}^{-3}$)
we make an approximation for $R_{\text{pq}} = 1$. This is done by
using the atomic radius $R_{\text{pq}} = \frac{\omega_{pq}}{v}$ for the minimum value of the impact
distance and realizing that the product of the circular frequency and
radius gives the velocity of the bound electron, i.e. $\omega_{pq} R_{\text{pq}} = v_{p}$
(cf. table 3.1) so we find that
\[ G_{pq} = \frac{2\pi a^4}{E} f_{pq} E^{-1} \ln \left( \frac{v_p}{v_q} \right) = \frac{2\pi a^4}{E} f_{pq} E^{-1} \ln \left( \frac{E_p}{E_q} \right) \]  

(5.21)

for \( q \approx p \). This shows the well-known \( E^{-1} \ln E \) dependence typical for dipole transitions.

Due to the fact that the rectilinear assumption of the DA is certainly not true for incident electrons with small \( E \)-values, fundamental laws like conservation of energy and the principle of DB are violated. Violations which are more serious when \( E \) is lower. In what is called the impact parameter method [SZA 62], this DA is refined in such a way that extrapolations to lower \( E \)-values can be effected.

Saraph [SAR 64] employed this method to calculate the cross sections for step processes \( \Delta p = 1 \). In the literature these results are considered as accurate for the cross section of dipole step transitions for energy values down to 1 ev. It is stated in [NGI 68] that they are preferable to the results of the first Born approximation. In the limit of high kinetic energy \( E \) the cross sections presented in [SAR 64] get the limiting form

\[ G_{pq} = \frac{2\pi a^4}{E} f_{pq} E^{-1} \ln(0.88 \frac{p^2 E}{Ry}) \]  

(5.22)

which is almost the same as the approximation eq.(5.21). Expression (5.22) is believed to be accurate for \( E \geq 4 \) and \( p > 4 \).

Concluding we may state that

the CP can be applied to step processes. By this application (CP) the correspondence is effectuated between the classical DA and the quantum mechanical TDPT, focused on the mean net energy transfer. The relation between QM and CI theory can in this case be ascribed to the feature CPA (cf. sect.3.3), which states that the CP is applicable to statistical properties.

In contrast with the jump processes the classical approach of individual step processes is not possible.

The determination of the cross section as effectuated by the TDPT, is closely related to the determination of the minimum value of the adiabaticity parameter i.e. the minimum value of the impact parameter. Below this minimum value jump processes are more dominant and the BKA is applicable.

So far we confined ourselves to the stepwise transitions with dipole character and did not regard non-dipole step processes. It is in principle possible to apply the TDPT to optically forbidden transitions (cf.[STA 65] and [PUL 66]) and the results can be
discussed in terms of the minimum R-value. However, we will not follow this line but discuss the combination of dipole and non-dipole transitions between hydrogenic energy levels, making use of the results of a time independent perturbation theory (the Born approximation).

5.6 The results of the Born approximation

The most simple time dependent perturbation theory is the first Born approximation (BA). It is based on the assumption that the interaction between the target atom and the incident electron is so weak that the scattering potential only gives a small perturbation on the kinetic energy of the electron. It is possible to expand the Born cross section in negative powers of the kinetic energy of the electron. Retaining the first two terms of this expansion the cross section can be written as

\[
\sigma_{pq} = 2\pi a_0^2 \frac{R_y}{p_{pq}} \left( A_{pq} \ln(E/2R_yZ^2) + B_{pq} \right),
\]

(5.23)
in which \( A_{pq} \) and \( B_{pq} \) are dimensionless coefficients. They are not to be confused with the Einstein coefficients \( A(p,q) \) and \( B(p,q) \) for radiative decay, stimulated emission and absorption. In the case of ionization, \( A_{pq} \) and \( B_{pq} \) are replaced by \( A_p \) and \( B_p \). This will be discussed in the section 5.8.

The quantity \( A_{pq} \) is related to the oscillator strength

\[
A_{pq} = \frac{2A_y}{p_{pq}} \frac{E_{pq}}{R_y},
\]

(5.24)
and \( B_{pq} \) is given by

\[
B_{pq} = 4\pi a_0^2 \frac{2}{q_{pq}^2} \frac{E_{pq}}{E_y} \left( 1 + \frac{6}{E_{pq}} \frac{E_y}{E_{pq}} \right).
\]

(5.25)

The cross section as given by the eqs. (5.23-25) includes contributions of dipole as well as non-dipole transitions from the energy level \( p \) to \( q \). It is obvious that the first term in eq.(5.23) with \( \frac{1}{E_{pq}} \ln E \)-dependence and the \( \frac{1}{E_{pq}} \) factor describes the dipole character of the transition. In the first two parts \( B_{pq,1} \) and \( B_{pq,2} \) of the \( B \) -term we recognize the RPA processes. The first part \( B_{pq,1} \) corresponds to the approximation in which the atomic electron is
supposed to be initially at rest (cf. 5.8). The second term takes account of the mean value of the kinetic energy \( |\mathbf{p}| \) of the bound electron (cf. eqs. (5.10)–(5.11)).

We have seen in section 2.4 that for step processes the BEA is not applicable. Therefore, this adjustment of the \( B \) term to the BEA results seems to be somewhat forced for step processes \( \Delta p = \lambda \). The third term \( B_{pq,3} \) has to correct this. By means of the factor \( b_p \) it is adjusted in such a way that eq. (5.23) agrees with results of Born calculations at high impact energy. Results of Born calculations carried out in [KIN 66] and [OMI 69] deliver values of \( b_p \). According to Vriens and Smets [VER 80] these \( b_p \)-values can be approximated by an analytical expression

\[
b_p = 1.4 \ln p - 0.7 - 0.51 p^{-1} + 1.16 p^{-2} - 0.55 p^{-3} .
\]  

(5.26)

In the next section we examine the step character of the asymptotic Born expression. Section 5.8 is devoted to the jump character.

The results of Born calculations as presented in the literature concern in most cases the hydrogen atom. We will generalize to hydrogenic ions, i.e. we include cases for which the charge number of the core is larger than unity, i.e. \( Z \rangle \). This implies that the argument of the logarithm contains the factor \( z^{-2} \), while \( A_{pq} \) and \( B_{pq} \) scale with \( z^{-4} \).

5.7 Step processes.

The step behaviour of \( A \) can be found by the power expansion

\[
z^2 A_{pq} = 0.19 (p^4 \Delta p^{-4} + 3 p^3 \Delta p^{-3} + 2.5 p^2 \Delta p^{-2} + \ldots) .
\]  

(5.27)

In this power expansion, valid for \( \Delta p / p \ll 1 \), we employed eq. (3.22) for \( f_{pq} \) and the relation \( E_{pq} = R_y z^2 (p^2 - q^2) \).

In the same way we find for the \( B \)-terms

\[
z^2 B_{pq,1} = p^3 \Delta p^{-2} - 1/4 p + \ldots .
\]  

(5.28a)

\[
z^2 B_{pq,2} = 2 p^4 \Delta p^{-3} + p^3 \Delta p^{-2} - 1/6 p + \ldots .
\]  

(5.28b)

\[
z^2 B_{pq,3} = p^3 (p^4 \Delta p^{-4} + 3 p^3 \Delta p^{-3} + 2.5 p^2 \Delta p^{-2} + \ldots) .
\]  

(5.28c)
From this analysis the following conclusions can be drawn:

Apart from the slowly imp-like varying $B_p$ factor, the $B_{pq,3}$ term has the same step-behaviour as $\Delta p_{pq}$ which suggests that it has a dipole character. This idea is strengthened if we inspect the pure dipole formula as found with the time-dependent perturbation theory (cf. eq. (5.22) in which also a $\ln p$ dependence is present.

But there is more: addition of $B_{pq,1}$ and $B_{pq,2}$ gives

$$Z^2 \left( B_{pq,1} + B_{pq,2} \right) = \frac{2}{3} \Delta p \left( p^4 \Delta p^{-4} + 3 p^3 \Delta p^{-3} + \ldots \right). \quad (5.29)$$

This equation shows that $B_{pq,1} + B_{pq,2}$ also has a step character comparable with the dipole part $\Delta p_{pq}$. Although the additional $\Delta p$ factor shows that its decrease as a function of $p$ is less rapid than that of $\Delta p_{pq}$. It was already noted, that this particular way of writing $B_{pq}$ as expressed by eq. (5.25) with $B_{pq,3}$ as correction term is inspired by the jump-like BAA results. For the description of step processes, for which the BAA fails, it would be better to calibrate the $B_{pq}$ to the dipole processes. This is in principle possible due to the step character of the $B_{pq}$ terms as expressed in eqs. (5.28).

We suggest to apply the formulation

$$\sigma_{pq} = 2n_0^2 \rho Y E^{-1} A_{pq} \left( \ln(3.5 p^2 E/(Z^2 Ry)) + F_{pq} \right), \quad (5.30)$$

in which

$$F_{pq} = \frac{B_{pq}}{A_{pq}} - \frac{\ln(7 p^2)}{p} \approx \frac{2.75 \Delta p}{\ln(p) - \ln(7 p^2)}. \quad (5.31)$$

The value 1.5 in the argument of the logarithm is chosen such that $F_{pq} = 0$ for the transition $3^+$. As a consequence the second term in eq. (5.31) is less than 6% of the first one for $p > 3 \text{ if } T > 1 \text{ eV.}$ The first term in eq. (5.30) is active for local processes while the second term reflects the jump processes and is almost zero for $\Delta p = 1$. So it turns out to be possible to write the BAA results as a sum of step and jump processes. This split up procedure is outlined in table 5.1.

5.6 Jump processes.

In order to study collisional jump processes we return to the representation as given in eq. (5.23) of the results of the BAA. These results are expected to be comparable with those obtained from the BAA where the cross section for excitation $p + q$ was supposed to correspond to the classical differential cross section for energy
Table 6.1
Energy transfer $\Delta E$ from a free electron with kinetic energy $E >> \Delta E$
to a bound electron with kinetic energy $|E_p| << E$.

<table>
<thead>
<tr>
<th>Large $R$ values</th>
<th>Small $R$ values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>$\frac{d\sigma}{d\Delta E} = \frac{\pi}{2} (1 + \frac{2</td>
</tr>
<tr>
<td>$C_1$ $D_{AE}$</td>
<td></td>
</tr>
<tr>
<td>$\Delta E = \frac{6}{E} R^2$</td>
<td></td>
</tr>
<tr>
<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
<td>p</td>
</tr>
<tr>
<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
<td>p</td>
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<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
<td>p</td>
</tr>
<tr>
<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
<td>p</td>
</tr>
<tr>
<td>Born</td>
<td></td>
</tr>
<tr>
<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
<td>p</td>
</tr>
<tr>
<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
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<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
<td>p</td>
</tr>
<tr>
<td>$\sigma_{pq} = \frac{\pi}{2} \frac{\langle p \rangle}{pq} \ln\left(\frac{E_{pq}}{</td>
<td>p</td>
</tr>
<tr>
<td>$K(p,q,T) \approx \text{Rate}(T) \alpha_{pq} \ln(2\gamma_{pq}) (5.49)$</td>
<td></td>
</tr>
<tr>
<td>$S(p) \approx \text{Rate}(T) \beta_{pq} (5.49)$</td>
<td></td>
</tr>
</tbody>
</table>

Rates for $\gamma = 0$

| $K(p,q,T) \approx k_p Z^{-2} \frac{|p|}{p} \Delta p^{-4}$ | $S(p) \approx s_p Z^{-2} \frac{2}{p}$ (5.52) |

local leap
transfer, \( \frac{d\sigma}{d\Omega} \), and the energy gap \( E_{q,q+1} \), such that

\[
\sigma_{pq} = \frac{d\sigma}{d\Omega} \bigg|_{E_{q,q+1}}.
\]  

(5.32)

We start with the \( B \) coefficient (eq. (5.23)) in which we recognize the energy difference \( E_{q,q+1} = 2Ry \cdot z^{-3} \). Apparently \( B \) can be considered as obtained from a differential quotient by

\[
\frac{dE}{dy} = \frac{dE}{d\Delta E} \bigg|_{E_{q,q+1}}.
\]  

(5.33)

We follow Johnson [Joh 72] and apply the parameter \( y = \Delta E/\Delta \) (cf. the sections 3.5 and 4.4 and fig. 4.2) which becomes continuous-like for increasing values of \( \Delta \). Realizing that \( \frac{d\sigma}{d\Omega} = \frac{dE}{dy} \bigg|_{E_{q,q+1}} \) we find

\[
\frac{dE}{dy} = 2Ry \left| \frac{E_p}{p} \right|^{-1} y^{-2} \left( 1 + \frac{4}{3} \frac{1}{y} + \frac{8}{3} \frac{1}{y^2} \right).
\]  

(5.34)

The first two terms are just the same as those obtained in the BEA cf. eq. (5.10b).

In the same way we can tackle \( B \) which results in

\[
\frac{d\sigma}{d\Omega} = \frac{2Ry}{p} \left| \frac{E_p}{p} \right|^{-4}.
\]  

(5.35)

In which eqs. (5.24) and (3.23) are employed.

The cross section of a jump transition \( p \to q \) can be obtained by using eq. (5.23) in which \( A \) and \( B \) are obtained by multiplying the eqs. (5.34) and (5.35) with \( \left| E_{q,q+1}/p \right| \). Another cross section of interest is what we call the level from level \( p \). It is the collective result of all jump processes which excite level \( p \) to much higher levels. The cross section for the level from \( p \) can be obtained integrating eqs. (5.34) and (5.35) from some lower value \( y^* \) to infinity. This gives

\[
A_p = \int_{y^*}^{\infty} \frac{d\sigma}{dy} \ dy = \frac{2}{3} \frac{Ry}{p} y^{-3}
\]  

(5.36)

and

\[
B_p = \int_{y^*}^{\infty} \frac{dE}{dy} \ dy = \frac{2}{3} \frac{Ry}{p} \left( y^{-1} + \frac{2}{3} y^{-2} + \frac{b}{3} y^{-3} \right).
\]  

(5.37)

The value of \( y^* \) can be chosen. The values of eqs. (5.36) and (5.37) for \( y^* = 1 \) correspond with the cross section for ionization of the \( p \) level.
The following conclusions can be drawn:
- Again we see that $A_{pq}$ has the same character as the third term of $B_{pq}$. Since they both have a $p^{-1}$-dependence they are negligible with respect to the first two terms of $B$ for high $p$ values and $\gamma^*$ close to one.
- For $\gamma^* = 1$ the integrals consist of all possible jump processes across the ionization potential. As stated before, this corresponds with ionization. Indeed the first two terms of (5.37) are those of the ionization cross section (cf. [PER 78]).
- With the help of eq. (5.37) it is possible to extend the ionization cross section from the continuum to the upper part of the energy scheme. This can be done by applying an appropriate value of $\gamma^*$ less than one.

In this and the preceding section we have seen that it is possible to recognize the dipole- and REA part in the cross section as obtained by the Born approximation. In section 5.3 we have seen that, as an application of the correspondence principle, the cross section can be treated classically as long as it concerns the mean energy transfer resulting from all possible step processes. Thus all step processes can be taken together to describe what happens with the mean energy transfer to the atomic energy scheme at location $p$. This is what we call the local aspect of the excitation processes. In section 5.3 we studied the correspondence for jump processes and it appears that jump processes can also be taken together in what we call the leap from level $p$. This split up of processes in local and leap provides a powerful technique which makes it possible the simplify collisional radiative models to a rather limited lower part of the energy scheme (cf. section 6.5).

The relation between the different cross section theories is outlined in table 5.1.

5.9 Rate coefficients in the limit of $\gamma_p \rightarrow 0$.

The rate coefficients for excitation $K(p,q)$ and ionization $N(p)$ are determined by the average over the electron velocity distribution of the product of velocity and cross section. (cf. sect. 2.4.1). Once these rates of forward processes are determined, the rates for the backward processes of recombination and deexcitation can be obtained by the application of the principle of DB. In this section we will focus our attention to rates of endoergic processes for small threshold transitions. If $k_e |E_p|/kT \ll 1$, the high energy part of $\sigma(E)$ is dominant, threshold behaviour is not important, and the functional
dependences as given by eqs. (5.39) and (5.51) can be extrapolated to the threshold. This is illustrated in Fig. (5.5) where the $\sigma(E)$ can be

FIG. 5.5
The Maxwell distribution function $F(E)$ and the cross section $\sigma(E)$ as functions of energy. For a small threshold transition, i.e. $E_{\text{th}} < 1$, the Born cross section of eq. (5.23) can be extrapolated to the threshold (dashed line).

The error in this approximation decreases if $\epsilon p_{\text{th}} / kT_e$ decreases.

described by eq. (5.39) over the whole energy range $E > E_{pq}$. Multiplying $\Phi(p,q)$ with the velocity $v$ and integrating over a Maxwell distribution function yields

\[ K(p,q,T) = \frac{3 \pi a_o^2}{2} \left( \frac{2 \pi m k T_e}{\epsilon} \right)^{0.5} A_{pq} \exp(-\epsilon_{pq}) \times \]

\[ \left[ \ln \left( \frac{E_{pq}}{\epsilon_{pq}} \right) + \int_{\epsilon_{pq}}^{\infty} \exp(-\epsilon + \epsilon_{pq}) d\epsilon + \frac{1}{\epsilon_{pq}} \right] \epsilon_{pq} \]

(5.38)

in which $\epsilon_{pq} = (E_{pq} / kT_e)$. If $\epsilon_{pq} = (E_{pq} / kT_e)$ tends to zero, $\epsilon_{pq}$ will approach zero even faster, the exponential integral in eq. (5.52) can be replaced by $-\ln \epsilon_{pq}^{-\gamma e}$, cf. eq. (4.19a), and we get

\[ K(p,q,T) = \text{Rate}(T_e) A_{pq} \psi_k(p,q,T) \]  

(5.39)

in which

\[ \text{Rate}(T_e) = \frac{3 \pi a_0^2}{2} \left( \frac{2 \pi m k T_e}{\epsilon} \right)^{0.5} \]

\[ = \frac{1.60 \times 10^{-13}}{T_e} \]  

(5.40)

and

\[ \psi_k(p,q,T_e) = \ln \left( \frac{0.28 kT_e / Z^2}{\text{Ry}} + \frac{8 p_{pq}}{A_{pq}} \right) \]

(5.41)
Following the technique given in sect. 5.10 this rate can be written as a sum of a local and leap part, i.e.,
\[ \psi_{\text{c=0}}(p, q, T_e) = \psi_{\text{c=0}}(p, q, T_e) + \psi_{\text{c=0}}(p, q, T) \] (5.42)
in which
\[ \psi_{\text{c=0}}(p, q, T_e) = \ln \left( \frac{2c}{p} \right) \] (5.43)
reflects the local part. Note that \( \psi_{\text{c=0}} \) depends on \( c_p \) and not on \( c_p^{-1} \).

For large \( c_p \)-values for which the asymptotical approximation is not justified we can write
\[ K(p, q, T_e) = \psi_{\text{c=0}} \frac{A_{pq}}{p} \psi_{\text{c=0}}(p, q, T) \exp \left( - \frac{c}{p} \right) \] (5.44)
in which \( \psi_{\text{c=0}}(p, q, T) \) is the threshold dependent shape factor. Section 5.11 is devoted to the semi-empirical approximations of those shape factors to which we may put the demand that they approach the asymptotical \( \psi_{\text{c=0}} \) value for \( c_p \) tends to zero.

If we employ eq. (5.24) we can write for the general \( c_p \) case
\[ K(p, q, T_e) = \psi_{\text{c=0}} \frac{A_{pq}}{p} \psi(p, q, T_e) \] (5.45)
in which
\[ \psi(p, q, T_e) = 2 \psi_{\text{c=0}}(T_e) \psi_{\text{c=0}}(p, q, T_e) \]
\[ = 4.35 \times 10^{-12} \frac{e^3}{m} 0.5 \psi_{\text{c=0}}(p, q, T_e) \text{ (eV m}^3\text{ s}^{-1}) \] (5.46).

In this equation \( T_e \) is the electron temperature in eV.

In order to study the p-dependence of \( K(p, q) \) we employ the step-approximation of \( A_{pq} \). Eq. (5.27) giving for \( p \gg 1 \) and \( \psi_p \ll 1 \).
\[ K(p, q, T_e) = k_p z^{-2} p^\mu dp^{-4} \] (5.47)
in which
\[ k_p = 3.0 \times 10^{-14} \frac{e^{-0.3}}{m} \psi(p, q, T_e) \text{ (m}^3\text{ s}^{-1}) \] (5.48).

This formulation shows that
- the \( p^{-2} \) \( z^{-2} \)-dependence, typical for the geometrical cross section (cf. Table 3.2) is present,
the p-dependence of \( k_p \) can be neglected in comparison with that of \( p^4 \).

- due to the \( \Delta p^{-4} \)-dependence (valid for large p-values, cf. eq.(5.27)) the excitation process is a typically local event.

In an analogous way we find the \( c_p = 0 \)-limit value of the rate coefficient of ionization to be

\[
S(p) \approx \text{Rate}(T_e) \cdot B_p \cdot \psi_p(p) \quad (5.49)
\]

in which

\[
\psi_p(p) = 1 + \frac{\Lambda}{B_p} \ln \left( 0.28 \frac{kT}{e^2} \chi \right). \quad (5.50)
\]

This \( c_p = 0 \) value will approach unity for increasing p-values and is consequently independent of \( c_p \). Applying eq.(5.37) for \( y^n = 1 \) we can give eq.(5.49) the simple representation

\[
S(p) = \frac{s_p \pi}{p^2} \quad (5.51)
\]

with

\[
s_p = 5.3 \times 10^{-13} \frac{\psi_p(p)}{B_p} \quad (5.52)
\]

again \( \psi_p(p) \) can be adjusted to the shape of the ionization cross section.

A comparison of the excitation- with the ionization rate leaves that

- they have the same (direct) \( T_e \)- and \( Z \)-dependence,
- the indirect \( T_e \)- and \( Z \)-dependence introduced by the shape factors is very weak and that
- the excitation cross section increases more rapidly as function of \( p \).

The quotient \( s/k \) will be an important parameter in the description of the shape of the distribution function. We denote it with the name "competition parameter" and according to eqs.(5.48) and (5.52) it equals

\[
\frac{s_p}{k_p} = 17.7 \frac{\psi_p(p)}{\psi_k}. \quad (5.53)
\]

Another parameter of interest is the rate of energy transfer by collisional step processes to atoms with energy level \( E_p \). Making use
of the technique discussed in sect. 5.7 which results in the subdivision of \( \psi_k \) according to eq. (5.42), we can calculate this rate of excitation energy transfer in the \( E_p = 0 \) limit. By employing the sum rule eq. (3.17) this results in:

\[
< \varepsilon > = \sum_k (p,q) P_{pq} = \Xi_p
\]

(5.54)

in which

\[
\Xi_p = 16\pi a_0^2 \alpha \gamma^3 \left( \frac{2\pi n_k T_e}{\hbar} \right)^{-0.5} \ln(2e^{-1}) .
\]

(5.55)

The summation runs over all levels \( \neq p \) and it is assumed that de-excitation can be treated in the same way as excitation.

5.10 Cold collisions

All collision theories treated in the preceding sections are based on the assumption that the kinetic energy of the incident electron is large compared to that of the bound electron. Close encounters can be regarded as binary processes, whereas for large impact parameters the description of energy transfer to an oscillator turns out to be successful. If the kinetic energy of the incident electron is small with respect to that of the bound electron, these relatively simple descriptions are no longer valid and threshold phenomena will be important. The collision is essentially a three-body event, which takes more time than the period of the bound electron. The impact of an electron with a neutral can be regarded as a formation of a negative ion followed by a detachment. In table 5.2 (at the end of this chapter) we give a comparison of the two limiting energy regions.

Although quantum mechanics should give the proper description of these low energy interactions, it turns out to be not very successful. A full analytical description is not possible, while especially for high \( p \)-values even the numerical representation of wave functions is a problem.

Results are much easier to be obtained from a classical three-body theory using Monte Carlo trajectory calculations. Here we reproduce the results of Mansbach and Keck [MAN 69]. They are not presented in the form of cross sections but expressed in analytical formulae for \( \Delta \mathcal{E} \) in which \( k(T_e) \) is the rate for the energy transfer from the Maxwellian electron gas to an atom and \( \varepsilon = E/kT_e \) is the energy transfer expressed in \( kT_e \).
For endoergic processes (supply of energy to the atoms i.e., $\varepsilon > 0$) leading to excitation or ionization of atoms with initial energy level $E_p$, they give

$$\frac{d\varepsilon}{d\varepsilon} = \Phi(\varepsilon, T_e) \exp -\varepsilon,$$  \hspace{1cm} (5.56)

with

$$\Phi(\varepsilon, T_e) = \frac{2.56 \times 10^{-12}}{1.5 \times 2.33} = 2.18 \times 10^{-14} \frac{0.83}{T_e^{4.66}} \text{ m}^3 \text{ s}^{-1}.$$ \hspace{1cm} (5.57)

while for exoergic processes ($\varepsilon < 0$)

$$\frac{d\varepsilon}{d\varepsilon} = \Phi(\varepsilon, T_e) \frac{4.83}{(e - \varepsilon)^{4.83}}.$$ \hspace{1cm} (5.58)

The equations (5.56) and (5.58) are related to each other by the principle of DB and valid in the limit of large $p$-values.

With these formulae, rates for ionization and the total rates for deexcitation, excitation, and destruction can be calculated. It can be found that,

$$K(p) = \int_0^\infty \frac{d\varepsilon}{d\varepsilon} = \Phi(\varepsilon, T_e) \exp -\varepsilon,$$  \hspace{1cm} (5.59)

for the ionization rate,

$$\int \frac{K(p, q)}{q_p} = \int_0^\infty \frac{d\varepsilon}{d\varepsilon} \exp (\varepsilon - q) \Phi(\varepsilon, T_e)(1 - \exp (\varepsilon / p)),$$  \hspace{1cm} (5.60)

for the total excitation rate and

$$\int \frac{K(p, q)}{q_p} = \int_0^\infty \frac{d\varepsilon}{d\varepsilon} = \Phi(\varepsilon, T_e) \varepsilon / 3.83,$$  \hspace{1cm} (5.61)

for the total deexcitation rate.

Addition of eqs. (5.59), (5.60) and (5.61) gives

$$K(p) = \int_0^\infty \frac{d\varepsilon}{d\varepsilon} = \Phi(\varepsilon, T_e)(1 + \varepsilon / 3.83),$$  \hspace{1cm} (5.62)

for the total rate for destruction.

From these results it appears that
- step processes are no longer dominant over jump processes and that
- for $\varepsilon > 3.83$ the total deexcitation exceeds the sum of excitation
and ionization which implies that the exoergic processes are in favour.

Experimental results for rate coefficients of cold collisions were obtained by Davoš, Boulmer and Belpoche, [DEV 79], using time resolved transition-selective fluorescence techniques in a low temperature He after glow. In fig.5.6 their results of total destruction $K(p)$, are compared with the theoretical values of [Joh 72], [Man 69] and [Gry 65]. In the same figure we presented the values of $\sigma_g \psi$ the in which $v = \sqrt{\frac{3kT}{m}}$ is the m.s. velocity and $\sigma_g$ the geometrical Bohr cross section (cf. table 3.1).

![Graph showing comparison of experimental and theoretical values of total destruction rate coefficient $K(p)$ vs. $p$.]

**FIG. 5.6**
The total collisional destruction rate coefficient $K(p)$ as a function of $p$ presented in a double log plot. Note the $p^4$ dependence of the geometrical cross section $\sigma_g = m v^2 p^4$.

Comparison shows that:
- the geometrical $p^4$-dependence is present, which suggests that the results can be interpreted as a 'hard sphere' collision in which any passage of an electron within the distance $a_p$ from the bound electron, i.e., a distant $2 a_p$ from the core, affects the bound state, (cf. fig. 5.7).
- the BEA values of Gryzinski are much too large especially for high $p$ values and that
- the total destruction rates as given by [Joh 72] and [Man 69] do not differ much from each other. In both cases the theory gives values which are 50 to 60% larger than those found in the experiment.
But it is stated in [DEV 79] that if the total destruction rate is decomposed in the various transitions, the experimental results are in favour of the three-body calculations presented in [MAN 69], i.e. step processes are no longer dominant over jump processes.

**FIG. 5.7**

If a slow electron approaches an atom it will be hit by the bound electron. The bound electron loses energy if the smallest distance between the two electrons is smaller than or comparable with the atomic radius $R_0$. This simple hard sphere model predicts a total destruction rate coefficient of $K(p) = 4\pi a_p^2 \lambda_p^* / \rho h_0$ (the radius of the hard sphere is $R_0$).

Figure 5.8 shows the dependency of the measured values of $K(p)$ as a function of $T_e$. The decreasing dependency $T_e^{-0.5}$ in the case of hot collisions is replaced by an increasing dependency (roughly with $T_e^{0.7}$). Note that again the interpretation of a 'hard sphere' collision scaling with $T_e^{0.5}$ is not so bad.

**FIG. 5.8**

The rate coefficient for total collisional destruction as a function of the electron temperature. The dots refer to the experimental values found in [DEV 79]. Theoretical values of [Joh 72] and [MAN 69] are also shown. The hard sphere model of Fig. 5.7 provides the rate coefficient for the...
5.1 Semi empirical approximations

In literature several attempts can be found to connect the theoretical well-known high energy Born tail with the threshold part as predicted by the three particles Monte Carlo calculations for high p-values or as deduced from empirical results for ground state excitation. These approximations are known as semi-empirical (SE) approximations. We will discuss some of them and focus our attention to the rates for Maxwellian electrons.

Drewin and Xiao [DRA 77] suggest for the excitation rate coefficient

$$\gamma_{pq}(p,q,T) = \pi \frac{\hbar N(T)}{e^{pq}} \exp(-pq^2) \hat{\psi}^d,$$

(cf. eq. (5.44)) and their shape function is given by

$$\hat{\psi}^d = [\hat{\psi}(e_{pq}, \beta_{pq}^d) - 0.1 \hat{\psi}_{pq}] \hat{\psi}^d$$

in which \( \hat{\psi} \) is a tabulated function and \( \hat{\psi}_{pq} \) and \( \beta_{pq}^d \) adjustable parameters in order of unity. For the definition of \( \hat{\psi}_{pq} \) and \( \hat{\psi}(e_{pq}, \beta_{pq}^d) \) we refer to eqs. (5.24) and (5.40). In section 9.2, fig. 9.2 the function \( \hat{\psi}^d \) will be discussed. The representation of eq. (5.63) is based on a dipole description for which we have seen that it is justified for step processes (cf. sect. 5.9). In the \( \varepsilon_{pq} = 0 \) limit the shape function can be approximated by

$$\lim_{\varepsilon_{pq} \rightarrow 0} \hat{\psi}^d = \ln (0.7 \varepsilon_{pq}^{-1} \beta_{pq}^d)$$

in which \( \beta_{pq}^d \) can be adjusted to the transition in question. After a proper adjustment rate coefficients of this structure can give good approximations for excitation processes originating from the ground state. For a comparison of their SE approximations with experimental results we refer to [DRA 77] in which it is stated that the SE cross sections reproduce experimental results within the error bars. Figure 5.9 compares the SE results as presented in [DRA 77] and [VRI 80] with close coupling calculation carried out by van de Ree [REE 82]. It shows a reasonable agreement. For transitions between highly excited levels for which \( \beta_{pq}^d \) is put equal to unity in [DRA 77], there are differences with our \( \varepsilon_{pq} = 0 \) limit value. The argument of the logarithm in eq. (5.64) contains \( \varepsilon_{pq}^{-1} \) instead of \( \varepsilon_{pq}^{-1} \) (cf. eq. (5.44)). Since for step processes the relation \( \varepsilon_{pq}^{-1} = \frac{1}{2} \varepsilon_{pq}^{-1} \) holds, the rate coefficient of Drewin will be too large for large p-values. However this discrepancy will be diminished by the logarithm.
FIG. 5.9
A comparison between the results of close coupling calculations of cross section in the electron-hydrogen collision as a function of energy as presented in [R65 82] with the semi-empirical approximations as presented in [DRA 77] and [FRI 80]. In 1-3 we denote the transition from $p=1$ to $p=3$, including all sublevels.

For ionization the cross section of Drawin is based on the classical value of Thomson (eq. 5.99), which, in order to take dipole transitions into account, was multiplied with $f_{\text{p}}^{d} \ln \frac{1.25}{p^{d} \text{ Ry}}$, where $f_{\text{p}}^{d}$ is a quantity which in [DRA 77] is called the oscillator strength for the bound-free transition. But since they take $f_{\text{p}}^{d} = 1$ for $p=3$ while the bound-free oscillator strength scales with $2/p$ (cf. [GRE 57]), this is not correct. In this way Drawin and Board obtained for the ionization cross section

$$
\sigma_{\text{p}, \text{ion}}(E) = 4\pi\alpha^{2} \text{ Ry} \left( \frac{1}{p^{2}} - \frac{1}{E} \right) \frac{d}{p} \ln \left( 1.25 \frac{a^{d}}{p} \frac{E}{p} \right).
$$

The idea of combining classical BNA results with the dipole calculations is an appropriate one, but as we saw in Sect. 5.8 the Born approximation predicts that this combination is rather an addition than a multiplication. The rate coefficient for ionization as obtained in [DRA 77] can be written as

$$
S(p) = 2 \pi \alpha \tau \left( \frac{E}{p} \right)^{-1} \frac{d}{p} \psi_{p} \left( \frac{E}{p} \right) \exp \left( -\frac{E}{p} \right).
$$

The $n=0$ limiting value of the tabulated function (cf. Fig. 9.2) is
\[
\lim \varphi (c_p, c_p^d) = \ln(0.7 c_p^{-1}) \quad \text{(5.67)}
\]

Comparing this with the present \( c=0 \) values shows that for high
\( p \)-values (for which \( A_{pq} \) and \( B_{pq} \) can be neglected cf. (5.36) and (5.37))
the relation
\[
\begin{align*}
\varphi_{c=0}^{(p)} & = \frac{2}{3} \ln(0.7 c_p^{-1}) \varphi_{c=0}^{(p)} \\
& \quad \text{(5.68)}
\end{align*}
\]
holds. This means that the \( c=0 \) limit value of the ionization rate
given in [DRA 77] is not correct. But again the cross sections are
reasonable for lower lying levels.

Resuming
- The rate coefficients for excitation as given in [DRA 77] are mainly
  based on the dipole description. The BEA part of the cross section
  is not treated properly.
- The rate coefficient for ionization is a product of an incomplete
  BEA formula and a quasi oscillator strength.
- They are well applicable in the bottom of the CR models (cf.
  fig.5.9) and simple in structure. The SE cross section can easily be
  adjusted to experimental results if available.
- In the top the \( c=0 \) values for both ionization and excitation are
  not in agreement with the results of the Born calculations.

The rate coefficients from Vriens and Smeets [VRI 80] were obtained
by connecting the high energy Born tail with the low energy values
obtained from Hansbach and Reck (cf sect.5.10). The results can be
written as
\[
K^V(p,q,T) = \text{Rate}(T_e) A_{pq} \exp(-\gamma_{pq} \rho_e) \psi^V_L(p,q,T_e) \quad \text{(3.69a)}
\]
in which
\[
\psi^V_L(p,q,T) = \left(1 + \frac{\Gamma_{pq}}{p_T} \right)^{-1} \left\{ \ln(0.3 \frac{kT_e}{\text{Ry}} + \Delta_{pq}) + \frac{\pi_{pq}}{p_T} \right\} \quad \text{(5.69b)}
\]
with
\[
\Delta_{pq} = \exp(-\frac{a_{pq}}{c_{pq}}) - \frac{0.06}{q} (\frac{p_T}{p})^2 \quad \text{(5.69c)}
\]
and
\[
\Gamma_{pq} = \text{Ry} \ln(1 + p^3 \frac{kT_e}{\text{Ry}}) \left\{ 3 + 11 \left(\frac{\Delta_{pq}}{p_T}\right)^2 \right\} \times
(6 + 1.6 \rho_{pq} + 0.3 \Delta_{pq}^{-2} + 0.8 \frac{q}{(\Delta_{pq})^{0.5}} (\Delta_{pq} - 0.6)^{-1}) \quad \text{(5.69d)}
\]
From these formulas it appears that they give the same limit value as that given in sect. 5.5.

For the ionisation they give

\[ \psi^{(V)} = \text{RHS of } T_\nu \left( \psi^{(V)} (\xi_r) \right) \]

with

\[ \psi^{(V)} (\xi_r) = (0.76 \xi_r^{1.33} + 3.32 \xi_r^{0.72} + 1)^{-1} \exp(-\xi_r) \]

which approaches unity for \( \xi_r \to 0 \). Thus the \( \xi_r \to 0 \)-limit-value is the same as that given in section 5.9. As stated before the high energy tail of the cross section of Vriens and Sneets are based on analytical expressions of Sa results as presented in [Joh 72]. It is interesting to note that a full classical treatment of this high energy tail based on the Strong Coupling Correspondence Principle (cf. sect. 2.4) gives similar results. For a comparison between this full classical treatment as given in [Gee 76] and the SE approximation we refer to [Vri 80]. In fig. 5.10 we reproduce one of the figures as presented in [Vri 80].

**Fig. 5.10**
Electron impact cross sections for atomic hydrogen (p-5) according to [Gee 76] and [Vri 80].

- Concluding we may state that the results of the SE approximations of Vriens and Sneets give the proper functional dependence in the \( \xi_r \to 0 \) limit. However the analytical structure is rather complicated and for groundstate excitation processes the results of [Dra 77] are good alternatives.
5.12 The total rate of collisional destruction

An important quantity which qualifies the excitation kinetics is given by the total destruction rate $n_k p A(p)$ of the level $p$. The radiative part, $A(p)$, which equals the inverse of the radiative lifetime, was already discussed in section 4.3. Here we construct a general form for the total rate of collisional destruction $K(p)$. It is based on the following considerations.

- In the limit of small $c$ values an important role is played by the stepwise excitation process (cf. eqs. (5.42) and (5.47)) for which

\[ K(p,p+1) = 3 \times 10^{-14} \rho^{-2} \frac{Z^2}{T_e^{1/2}} \rho^{-0.5} \ln(2c^{-1}) , \]

(5.71)

with its typical $\rho^{-2} p^{-4/3} T_e^{-1/2}$ dependency. Since for higher levels the stepwise deexcitation has almost the same rate, we suggest that

\[ K(p) \approx 2 K(p,p+1) . \]

(5.72)

For lower levels the relation $K(p,p-1) \approx K(p,p+1)$ is certainly not

![Graphs showing the rate for total collisional destruction for the level $p=10$ as a function of temperature (left) and $K(p)$ as a function of $p$ for $T_e = 400K$. Dots [DEL 75]; dotted curve [YRI 80]; dash/dot [MAN 89] and full curve Eq. (5.71).](image)

Figs. 5.11 and 5.12
true but for these levels the $\Delta pf$ I processes are of more importance (cf. eqs. (5.27-28)).

- As we have seen in the figs. 5.6 and 5.8 the collisions are comparable with a hard sphere collision, with the typical $T^2$ dependency, in the intermediate range of $E_p$.
- For high $E_p$ values, $K(p)$ should approach values which are comparable with the experimental results in [DEV 79] and the theoretical values of [HAN 69]. In the latter an important role is played by the factor $(1 + e_p/3.63)$, cf. eq. (5.60).

So we suggest

$$K(p) = 6.10^{-14} Z^{-2} p^4 \times \frac{e_p^{0.5}}{e_c^{0.5}} \ln(2/e_p) + 1.3)\left(1 + e_p/4\right). \quad (5.73)$$

In the figs. 5.11 and 5.12 a comparison is effectuated between these analytical destruction rates and experimental, theoretical and semi empirical results.

Table 5.2
A comparison between cold and hot collisions.
$E$ is the energy of the free electron; $|E_p|$ the kinetic energy of the bound electron.

<table>
<thead>
<tr>
<th>Cold</th>
<th>Hot</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E \ll</td>
<td>E_p</td>
</tr>
</tbody>
</table>
| a three body problem | for $R \ll a_p$ binary encounter
| exchange and spin interaction important | for $R \gg a_p$ dipole approximation
| all collisions adiabatic | exchange and spin interaction not important
| exoergic in favour | endoergic in favour |
Chapter VI  Collisional radiative models: The general set up

6.1 Introduction

The aim of this thesis is to classify plasmas with the help of the distribution function of excited states. Since these distribution functions result from the excitation kinetics, i.e. the activity of microscopic processes in which excited states are involved, they will give a good image of the plasma.

In Chapter II we studied elementary processes and it was found that in a large variety of plasmas the excitation kinetic is determined by the electrons only. This class of plasma to which we confine ourselves is denoted by the name electron-excitation-kinetic plasmas, shortly EEK-plasmas. The study of the distribution functions in EEK-plasmas is essentially the study of how bound electron behave themselves in the competition of two types of interactions: the interaction with the nucleus or core and the interaction with the free electron gas. Thus in EEK-plasmas we only deal with the elementary processes of radiative decay and that of electron-atom collisions.

In this chapter we will study the technique frequently used to calculate the distribution function, i.e. that of the collisional radiative (CR) model. The name indicates that the population density of excited levels is determined by collisional and radiative processes only. Other processes like transport can be neglected and the determination of the number densities of the excited states is simplified to that of the solution of a set of linear equations. This method is called the Quasi Steady State Solution (QSSS) and cannot be applied to the ground- and ion state. The densities of ground- and ion states, \( n_0 \) and \( n_+ \), are input parameters of the set of the linear equations which describe the populations of the excited levels. As a result these populations can be regarded as a superposition of two contributions, one originating from the ground state and one originating from the ion state.

In section 6.2 the continuity equation will be presented in its most general form. By the assumption discussed in section 6.3 and 6.4 the continuity equation will be simplified and by the cut-off procedures in section 6.5 the number of equations can be reduced. The solution of the set of linear equations will be presented in sections 6.6. In section 6.7 the distribution function will be discussed in relation with its equilibrium value and section 6.8 deals with the coefficients for total ionization and recombination.
6.2 The continuity equation

In the absence of equilibrium, the density of atoms in state \( p \) has to be determined by solution of the continuity equation. In this equation, the zeroth moment of the Boltzmann equation (eq. (6.1)), spatial and temporal relaxations are related to atomic production- and destruction processes.

With the processes discussed in chapter II we get

\[
\frac{\partial}{\partial t} n(p) + \nabla \cdot (n(p)v(p)) = \sum_{q \neq p} n_e n(q) K(q,p) - n(p) n_e \sum_{q \neq p} K(p,q)
\]

*temporal + spatial relaxation*

\[
\text{coll. production} \quad \text{coll. destruction}
\]

\[+ \sum_{q \neq p} n(q) \left( A(q,p) + B(q,p) \right) \rho_q - n(p) \sum_{q \neq p} B(p,q) \rho_q,
\]

*3 part rec.*

\[\text{coll. ion}
\]

\[+ \sum_{q \neq p} n(q) \left( A(q,p) + B(q,p) \right) \rho_q - n(p) \sum_{q \neq p} B(p,q) \rho_q,
\]

*casc. (spont.+ stim.)

\[\text{photo excitation}
\]

\[+ \sum_{q \neq p} n(q) \left( A(q,p) + B(q,p) \right) \rho_q - n(p) \sum_{q \neq p} B(p,q) \rho_q,
\]

*absorption*

\[\text{emission (spont.+ stim.)}
\]

\[+ n_e n_e (n(p) + B(p) \rho_p) - n(p) B(p,+) \rho_p,
\]

*rad. rec. (spont.+ stim.)*

\[\text{photo ion.}
\]

(6.1)

The elementary processes in eq. (6.1) are grouped together in forward and corresponding backward processes.

Equation (6.1) has the structure

\[
\frac{\partial}{\partial t} n(p) + \nabla \cdot (n(p)v(p)) = P(p) - n(p)D(p)
\]

(6.2)

in which \( P(p) \) is the so-called production term and \( D(p) \) the so-called destruction factor of the level \( p \).
It is obvious that in this general formulation the determination of the number density $n(p)$ is not a simple task. There are serious difficulties:

i) Due to the radiative terms like $n(q)B(q,p)\gamma_q$, the determination of the level density is coupled with radiation transfer which, on its turn, is determined by the number of $q$ state atoms locally and elsewhere in the plasma. For the solution of $n(p)$ at a certain location we have to take into account all other plasma parts. Therefore a purely local treatment is not possible. The equation (6.1) is an integral equation.

ii) The equation (6.1) is also differential in space and time. The spatial relaxation term $\gamma n(p)\gamma(p)$ reflects the transport phenomena of the plasma. By means of higher order moments of the Boltzmann equation this transport term is related to gradients and forces. Consequently restriction to the continuity equation is not allowed in the most general case.

iii) In the relatively simple case of hydrogen, the rate coefficients $K(p,q)$ and $S(p)$ are not fully known.

iv) The density of level $p$ is determined by the level densities of an infinite number of other levels. In fact we have to solve an infinite number of integro differential equations.

6.3 Simplifications and limitations

To tackle these problems we have to make simplifications such that the determination of the distribution function is manageable for a large variety of plasmas. Therefore the following assumptions are often made in the framework of CR models:

1) In a large variety of cases it is justified to omit stimulated emission from eq. (6.1). In some other situations stimulated emission is only important for a few transitions in the presence of irradiation by an external source, e.g. a laser in the case of laboratory plasmas and strongly radiating stellar objects in the case of astrophysical plasmas (cf. case C and D in sect. 2.6.3). In these cases the problem can be approached by the introduction of the intensity of the external source as independent parameter.

Trapping is important only for resonant radiation (sect. 2.6.3) and in many cases it can be treated by introducing the escape factor $\theta$ and the effective probability $\theta A(p,1)$. (cf. 2.6.2). This makes a local treatment of eq. (6.1) possible. In this way eq. (6.1) is reduced from an integro-differential to a differential equation.

II) Elimination of the differential part of eq. (6.1) is in many cases justified for excited states. This so-called Quasi Steady State
Solution (QSSS) which is treated in section 6.4, has a large range of applicability but e.g. rapid transient plasmas, for which the decay- or growth time are in the order of atomic lifetimes, cannot be described by the QSSS method.

II) In the EEC-plasmas molecular formation or destruction is of importance with respect to the atomic excitation (cf. section 2.4.6). Moreover heavy particle collisions are not effective for (de)excitation or ionization/recombination (cf. sects. 2.4.6 and 2.5.1) but only significant in retaining a statistical distribution between sub levels. This implies that heavy particle collisions can be omitted from eq.(6.1). Only transitions due to electronic collisions or radiative decay are important.

Examples of CR models for plasmas in which heavy particle collisions are important are found in [GOU 84].

For the cross sections of the electron-induced transitions we can use SR approximations (cf. section 5.1)). In this approach it is useful to distinguish between the bottom and top of the atomic system.

In the EEC-plasmas we assume that at least the bulk of the electron distribution is Maxwellian. This means that the calculation of rate coefficients for transitions between excited states is straightforward (cf eq.2.6) and that rate coefficients of forward and backward processes are related to each other by the principle of DR (eq.2.12).

IV) There are several techniques to reduce the number of levels. In section 6.5 we will discuss the technique presented in [BAT 62] and we will introduce a more rigorous cut-off procedure.

6.4 The quasi steady state solution

The basic idea of the QSSS is that the ground- and ion states can be considered as two large particle reservoirs which are filled or drained on a relatively large time scale, i.e. the time scale for the plasma- growth or decay. From these large reservoirs a small amount is distributed over the system of excited levels. This distribution happens on the small time scale of atomic processes. Thus the two basic assumptions to be made for the QSSS are that

- the diffusion- or plasma decay time must be much longer than the lifetime of the atomic excited states,
- the total number of atoms in excited states must be much smaller than the number of groundstate atoms or ions.

The QSSS was first introduced in [BAT 62]. Conditions for the QSSS were discussed in [WHI 63] and [CUC 76].

In the framework of the QSSS the continuity equation of excited levels can be simplified by omitting the temporal and spatial
relaxation terms which are small with respect to the production and destruction terms. As a consequence the continuity equation can be written as

\[ n(p) D(p) = P(p) \quad (6.3) \]

For the ground- and ion states the temporal and spatial relaxation terms have to be retained. With the basic assumptions of section 6.3 the continuity equation of groundstate atoms can be written as

\[ \nabla \cdot n_1 \mathbf{v}_1 - \frac{\partial n_1}{\partial t} = \sum_{q>1} n(q) \left( n_e K(q,1) + \Theta q \right) A(q,1) \]

\[ + n_{e=1} (n_e K_e(1) + \alpha(1)) \]

\[ - n_{e=1} \sum_{q>1} K(1,q) = n_{e=1} S(1) \quad (6.4a) \]

for the ions of a singly ionized system this continuity equation reads

\[ \nabla \cdot n_e \mathbf{v}_e + \frac{\partial n_e}{\partial t} = n_e \sum_{q>1} n(q) S(q) + n_{e=1} S(1) \]

\[ - n_{e=1} \left( \sum_{q>1} n_e K_e(q) + \alpha(q) \right) \]

\[ - n_{e=1} (n_e K_e(1) + \alpha(1)) \quad (6.4b) \]

It is not the aim of the CR model to solve these equations but it is possible to get a more compact formulation (cf eq. 6.40). The ground- and ion state density are input parameters for the production/destruction balances of type (6.3). The rhs of equation of eq.(6.3), the production term, can be seen as the sum of three terms. The first term indicates the production of p state atoms directly from the ground state; the second reflects the production directly from ion state, and the third represents the production originating from other excited states. So we can write

\[ n(p) D(p) = P(p) = C^1(p) + C^e(p) + C^q(p) \quad (6.5) \]

with

\[ C^1(p) = n_1 D_{1p} \]

\[ D_{1p} = n_e K(1,p) \quad (6.6a) \]

\[ C^e(p) = n_e n_p D_{ep} \]

\[ D_{ep} = n_e K_e(p) + \alpha(p) \quad (6.6b) \]

\[ C^q(p) = \sum_{q \neq p} n(q) D_{qp} \]

\[ D_{qp} = n_e K(q,p) + A(q,p) \quad (6.6c) \]
This notation clarifies that the depopulation of \( q \) in favour of \( p \), 
\( n(q) D_{qp} \), is a production of \( p \) at the expense of \( q \). In general \( D_{qp} \) 
consists of a \( n \)-dependent (collisional) and a \( n \)-independent 
(radiative) part. By convention \( A(p,q) = 0 \) if \( q > p \).

The destruction factor is given by

\[
D(p) = \eta_q K(p) + A(p)
\]  

(6.7a)

where

\[
K(p) = \sum_{1 \leq q < p} K(p,q) + \Delta(p)
\]  

(6.7b)

and

\[
A(p) = \sum_{1 \leq q < p} A(p,q) + \delta_q^p A(p,1)
\]  

(6.7c)

The equations of type (6.5) are coupled to each other by the mutual 
contributions \( C(p) \). But the densities of the other excited states are 
finally also originating from ground- and ion states, which are the 
only sources in the QSSS. So it must be possible to split up these 
mutual contributions and to show how \( n(p) \) is composed of ground state 
and ion state contributions only (cf Fig. 6.1). This technique is 
given in section 6.6.

\[
n(p) D(p) = C^*(p) + C^1(p) + C^2(p) = F^*(p) + F^1(p)
\]

(6.7d)

\[
\begin{array}{c}
\text{Fig. 6.1} \\
\text{The production/destruction balance of a level} \ p. \text{ The right part of the} \\
\text{figure clarifies that the contribution from other levels is nothing} \\
\text{but a contribution from ground and ion state via other levels.}
\end{array}
\]
6.5 Cut-off procedures

We discuss two different cut-off procedures. The first one, introduced by Bates, Kingston and McWhitter in [BKT 62], deals with the connection between lower levels and PLTE. The second, introduced by this study, deals with the connection of lower levels with the collisionally dominated hot part of the system, i.e., the levels for which \( E_p = E_p / KT << 1 \) and \( n_e K(p) >> \Lambda(p) \).

1) The cut-off, as discussed in [BKT 62], is based on the assumption that there is a level \( N \) such that the levels \( u > N \) are in PLTE, i.e., \( n(u) = n_e^*(u) \) or \( b(u) = 1 \). Denoting this group of upper levels by \( U \) and introducing

\[
X_{U}(p) = \sum_{u \in U} \frac{n^g(u)/\langle n_e n_e \rangle}{A(u,p)}
\]

and

\[
\alpha_{U}(p) = \sum_{u \in U} \frac{n^g(u)/\langle n_e n_e \rangle}{A(u,p)}
\]

eq. (6.5) can be rewritten as

\[
n(p) \Omega(p) = \sum_{1 < q < p < N} n(q) D_q = n_e n_e \sum_{1 < q < p < N} \left( E^{K_e^*(q)} \right) \left( E^{\alpha^*(q)} \right) \left( E^{1} \right)
\]

In which

\[
K_e^*(p) = K_e(p) + K_U(p)
\]

and

\[
\alpha^*(p) = \alpha(p) + \alpha_U(p)
\]

are extended coefficients for three-particle- and two-particle recombination (capture).

With the help of the analytical approximations discussed in chapter IV and V we can investigate if the calculations of \( \alpha^* \) and \( K^* \) are possible. In section 4.5 we have seen that capture and cascade can be put together in one formula. A generalization of eq. (4.18) gives:

\[
n_e n_e \alpha^*(p) = n_e^p (p) \gamma^2 p^{-5} \int_{E_p,N+1} \frac{exp[-C]}{C} dc
\]

which for radiative hot levels can be approximated by

\[
n_e n_e \alpha^*(p) = \gamma^2 p^{-5} \left( \ln(p^{-2} - (N+1)^{-2})^{-1} - \ln(\frac{Ry}{E_p} - \gamma_e) \right)
\]

So the determination of \( \alpha^* \) is not cumbersome and due to the \( p^{-5} \)
dependence unimportant for large p-values. The determination of $K^*$ is not so simple. If we apply the principle of DB we can write

$$U_u \ n_u \ K_u^*(p) = \eta_u \ n^g_u(p) \ S(p) + \eta_u \ n^g_u(p) \ \int_{u \mu} K(p, u) \, du \ . \quad (6.13)$$

We note that for jump processes, $K(p, u)$ is relatively small. In section 5.6 it was shown that the sum of all jump processes has a $p^2$ dependency, i.e. the same dependency as the ionization rate. Ionization processes can be regarded as jump processes over the ionization limit and it is possible to put jump and ionization processes together in

$$S^p(p) = S(p) + \int_{u^*}^a K(p, u) \, du \quad (6.14)$$

in which $u^* \gg p$ and $u \in U$. For step processes $K(p, p+1)$ is large and scales with $p^4$. This means that small departures from the Saha density can still create a considerable step flow over the levels and problems can be expected if this flow is utilized due to the cut-off procedure. A method to avoid this problem is to take much more levels into account than the number of non-PLTE levels, i.e. to go far in the PLTE.

1) A more elegant technique is the following cut-off procedure based on the properties of stepwise processes. It can be executed in the domain of hot collisions, i.e. $kT_e \gg |\Delta E_e|$ and $\eta_u K(p) \gg A(p)$.
The stepflow across an intersection between the level N and the level N+1 is given by (cf. fig. 6.2)

$$J(N, N+1) = \eta_u \ n(N) \ K(N, N+1) - \eta_u \ n(N+1) \ K(N+1, N) \ . \quad (6.15)$$

If we employ the principle of DB and the factor $b(N) = n(N)/n^g(N)$ this can be written as

$$J(N, N+1) = \eta_u \ n^g(N) \ K(N, N+1) \ (b(N) - b(N+1)) \ . \quad (6.16)$$

With the cut-off procedure the stepflow will be affected in such a way that it becomes

$$J^{cut}(N) = \eta_u \ n^g(N) \ K(N, N+1) \ (b(N) - 1) \quad (6.17)$$

since the level N+1 is artificially put in equilibrium. To get the actual value for the stepflow, one should multiply $J^{cut}(N)$ with the
A comparison between two cut off procedures.

In procedure I the flow over the levels is mutilated, in procedure II the flow is not affected.

\[
\begin{align*}
J(n) &= n(N)K(N, N+1) = b(n)\rho_0/(\kappa(N, N+1)) \\
&\quad - n(N+1)K(N, N+1)b(n+1)\rho_0/(\kappa(N+1, N)) \\
(b(n) - b(n+1))n^2(N)K(N, N+1) &= a(n)
\end{align*}
\]

This equation is justified since we know from analytical, numerical and experimental results that \(5b(N) \approx b(N) - 1 \ll N^{-6}\).

So to be practical and to avoid that the stepflow will be mutilated we should adjust the destruction factor of the cut-off level which becomes

\[
E^*(N) = b_e \left( \sum_{q < N} K(N, q) + E^*(N) + S^*(N) \right)
\]
\[ K^*(N) = K(N, N+1) \left(1 - N^6(N+1)^{-6}\right). \]  

(6.20)

For the extended capture rate of the cut-off level we employ (cf. eq. (4.23))

\[ \eta_{\ast} n^\ast(N) = n^8(N) \gamma Z^4 N^{-5} \left[3 \ln N - \xi(\Upsilon)\right]. \]  

(6.21)

So the recipe of the cut-off procedure II is:

- determine the boundary \( P_{\text{cr}} \) between radiative and collisional levels (cf. eq. (7.18)) and hot and cold levels \( P_{\text{h}} \) (eq. (7.19)),
- choose a cut-off level \( N > \max \left(P_{\text{cr}}; P_{\text{h}}\right) \),
- use eqs. (6.12) and (6.14) for the lower levels \( p < N \),
- and eqs. (6.14), (6.19) and (6.20) for the boundary level \( N \).

With this cut-off technique it is possible to lower the boundary value as long as we stay in the upper region of the energy scheme where we deal with collisional dominated hot levels. This means that the number of levels can be reduced drastically if this analytical topping is used.

6.6 The solution of the numerical model

In both case I and II we can proceed in the way as given in [RAT 82]. The coupled linear equations of the \( N-1 \) lower levels (cf. eq. (6.9)) can be put in the vector representation

\[ \mathbf{N} = \mathbf{P}^* + \mathbf{P}^1. \]  

(6.22)

in which \( \mathbf{N} \) is an \( N-1 \) dimensional vector whose components are the \( n(p) \) values. The vector \( \mathbf{P}^* \) gives the population contribution for the levels \( p \) originating from the outermost part of the system and the continuum. The components are

\[ \Pi^*_p = \gamma_p n_p, \quad \Pi^*_p = n_p \left[\eta_{\ast} K^*(p) + u^*(p)\right]. \]  

(6.23)

The vector \( \mathbf{P}^1 \) gives the population contribution from the groundstate. The components are

\[ \Pi^1_p = \gamma_p n_1 K(1,p). \]  

(6.24)
The matrix \( \mathbf{Y} \) has components

\[
\mathbf{Y}_{pq} = -\mathbf{D}_{qp} = -n_{e}K(q,p) = \mathbf{A}(q,p) \quad (6.25a)
\]

for \( q \neq p \) and

\[
\mathbf{D}_{pp} = \mathbf{D}(p) = n_{e}K(p) + \mathbf{A}(p) \quad (6.25b)
\]

in which \( \mathbf{D}(p) \) is the destruction factor of level \( p \). For the cut-off level in procedure II one should apply eq.(6.19)

The solution of the system (6.22) can be written as

\[
n(p) = n_{+}(p) + n_{-}(p) \quad (6.26)
\]

with

\[
n_{+}(p) = (\mathbf{Y}^{-1} \mathbf{n}_{+}) = \left( \sum_{q \neq p} n_{+}^{*}(q) \mathbf{D}_{qp} + n_{e}n_{e}^{*} \mathbf{D}_{pp} \right) / \mathbf{D}(p) \quad (6.27a)
\]

and

\[
n_{-}(p) = (\mathbf{Y}^{-1} \mathbf{n}_{-}) = \left( \sum_{q \neq p} n_{-}^{*}(q) \mathbf{D}_{qp} + n_{e} \mathbf{D}_{pp} \right) / \mathbf{D}(p) . \quad (6.27b)
\]

With \( \mathbf{Y}^{-1} \) the inverse matrix of \( \mathbf{Y} \) is denoted. The contribution, \( n_{e}n_{e}^{*} \mathbf{D}_{pp} \), is defined by eq. (6.23). The last equality in eq.(6.27a) is obtained if we insert the \( n_{+}^{*}(q) \)-values in eq.(6.9) where \( n_{e}n_{l}K(l,p) \) is omitted. The last equality in eq.(6.27b) is obtained in an analogous way.

Comparing these equations with (6.5) we see that the population in \( \mathbf{Y}_{pp} \) contributions from other excited levels \( C(p) \) is decomposed in \( C_{+}^{0}(p) \) and \( C_{-}^{0}(p) \) value, determined by ion- and ground states respectively (cf. Fig. 6.1) and that eq.(6.5) can apparently be written as

\[
n(p) D(p) = P_{+}(p) + P_{-}(p) \quad (6.28)
\]

with \( P_{\pm}(p) \) determined by the ion state

\[
P_{\pm}(p) = C_{\pm}^{0}(p) + C^{*}(p) + \sum_{\mathbf{U}} n_{\mathbf{U}}^{*}(u) \mathbf{D}_{u \mathbf{U}} \quad (6.29a)
\]

and \( P_{\pm}(p) \) determined by the ground state

\[
P_{\pm}(p) = C_{\pm}^{0}(p) + C^{*}(p) . \quad (6.29b)
\]
So in the QSSS the population density of a level can be regarded as a superposition of two contributions, one from the ion state and one from the ground state (cf. fig. 6.3).

\[ n(p) = n^+(p) + n^-(p). \]  

(6.26)

The \( n^+(p) \) values are related to the ion state and related to each other, while the \( n^-(p) \) values are related to the ground state and related to each other. In the mathematical framework of CR models there is no relation between \( n^+(p) \) at one side and \( n^-(p) \) at the other side. Naturally in each real plasma a relation between \( n^+ \) and \( n^- \) exists which implies that there is also a relation between the \( n^+(p) \) and \( n^-(p) \) values. This relation however is not determined by CR models but must be evaluated with a plasma model including transport phenomena.

**Fig. 6.1**

A comparison between the superposition of contributions to levels with a system of communicating vessels.

- Contribution from the "ground state"
- Contribution from the "ion state"
- Superposition

The combination of top and hole refers to transport phenomena in plasmas.
6.7 The distribution function and the population coefficients.
In search for the properties of the excited states distribution function we applied the quasi state solution and found that the population density of a level \( n(p) \) can be regarded as a superposition of two contributions. One \( n^*(p) \) from the ion state, and one \( n^1(p) \) from the ground state.

It is useful to relate these contributions to the equilibrium value of the population density which can be done on several ways.

A) First we can relate the ion state contribution \( n^*(p) \) to the Saha density, and \( n^1(p) \) to the Boltzmann density. This leads to the expression

\[
\tilde{n}(p) = r^*(p) \, n^*(p) + r^1(p) \, n^1(p)
\]

in which \( r^*(p) = n^*(p)/\tilde{n}(p) \) and \( r^1(p) = n^1(p)/\tilde{n}(p) \) are the so-called population coefficients. By this definitions and the properties of \( n^*(p) \) and \( n^1(p) \) as expressed in the eqs. (6.23) and (6.24) it is obvious that \( r^*(p) \) is independent of \( n^1 \) while \( r^1(p) \) is independent of \( n^1 \). In the notation of eq.(6.30) the two particles reservoirs of ground- and ion states are treated in an equivalent way.

B) But there are large differences between these two fundamental states. In contrast to the ion state the ground state is separated from the rest of the system by a large energy gap. Since this means that most levels will be determined by the ion state rather than by the ground state it is instructive to use a notation in which the ion state is the leading state. This can be done by dividing eq.(6.30) by \( n^*(p) \) which results in

\[
b(p) = r^*(p) + r^1(p) \, b_1 \, ,
\]

This expresses that the equilibrium departure \( b(p) \) of a level \( p \) depends linear on the equilibrium departure of the ground state \( b_1 \). In the absence of ground state atoms the equilibrium departure is given by \( r^*(p) \) which is determined by the ion state only.

A essential feature of the derivation of the superposition is that we found \( n^*(p) \) if \( n_1 \) was put equal to zero while \( n^1(p) \) was obtained if \( n^1 = 0 \). In fact we impose a non-equilibrium situation on the system in order to get information from it. For instance by putting \( n_1 = 0 \) the ionization will not be compensated by any particle recombination and this creates a sink in the upper side of the system. The influence of
this sink will be propagated to lower parts of the system in the sense that an excitation flow will be generated to supply this ionization sink.

In an analogous way we create a downward flow in the system by putting \( n_{\text{e}} = 0 \) in order to obtain \( n_{\text{e}}^* \) (or \( r^\dagger(p) \)).

So \( r^* \) and \( r^\dagger \) reflect non-equilibrium densities and the statement that the population density is a superposition of \( n_{\text{e}}^* \) and \( r^\dagger \) part is equivalent to the statement that an actual plasma can be regarded as a superposition of a purely recombining and a purely ionizing plasma (cf. [PU 79a]). In this way \( r^* \) reflects the purely recombining and \( r^\dagger \) the purely ionizing plasma.

C) In the limit of \( n_{\text{e}} \rightarrow \infty \), collisions are dominant over radiation and the whole system tends to equilibrium if \( b_\downarrow = 1 \). This means that \( b(p) = r^*(p) - r^\dagger(p) \rightarrow 1 \) for \( n_{\text{e}} \rightarrow \infty \). So it is instructive to regard the plasma as a superposition of a plasma in equilibrium and a purely ionizing (or recombining) plasma if \( n_{\text{e}} \) is large.

For that purpose the relative overpopulation \( \delta b(p) = b(p) - 1 \) is a useful parameter and a convenient representation of the distribution function is

\[
\delta b(p) = \delta^*(p) + \delta_b^\dagger(r^\dagger(p))
\]  

(6.32)

where

\[
\delta^*(p) = r^*(p) - r^\dagger(p) - 1
\]  

(6.33)

provides an alternative parameter to describe the equilibrium departure.

For a further study of the distribution function we have to investigate the \( r \)-coefficients and the functional behaviour of \( \delta b(p) \). By employing eqs (6.27a) and (6.27b) and the principle of DB, we get the following expressions for the population coefficients:

\[
r^*(p) = \frac{\int \lambda_{\text{n}}(q) n_{\text{e}}(p, q) + \lambda(q, p)}{n_{\text{e}}(p) + \lambda(p)}
\]  

(6.34a)

and

\[
r^\dagger(p) = \frac{\int \lambda_{\text{n}}(q) n_{\text{e}}(p, q) + \lambda(q, p)}{n_{\text{e}}(p) + \lambda(p)}
\]  

(6.34b)

in which
\( \tilde{\lambda}(q,p) = \pi^\infty(q) A(q,p)/n^S(p) \) \hspace{1cm} (6.35)

and

\( \tilde{\alpha}(p) = \alpha(p)/n^S(p) \). \hspace{1cm} (6.36)

In principle the summations in the equations (6.34) extend over an infinite number of levels. It is possible to effectuate the cut-off procedure I or II in the same way as discussed in section 6.5. The precise value of \( \tau^+(p) \) and \( \tau^-(p) \) can only be given by inserting the \( K \) and \( A \) coefficients. But general features of the population coefficients can already be deduced from this formula. This will be done in section 7.4.

By employing eqs. (6.31) and (6.34) we relate the overpopulations of levels to each other by

\[
\tilde{\alpha}(p) = \frac{\int \tilde{\alpha}(q,p) n_e K(p,q) + \tilde{\lambda}(q,p) + n_e K(p,1) + \tilde{\lambda}(p) - A(p)}{\int n_e K(p) + A(p)}
\]

in which

\( \tilde{\lambda}(p) = \sum_{q} \tilde{\lambda}(q,p) \). \hspace{1cm} (6.38)

The \( \rho^\ast \) coefficients are related to each other by

\[
\tilde{\rho}^+(p) = \frac{\int \tilde{\rho}^+(q) n_e K(p,q) + \tilde{\lambda}(q,p) + \tilde{\lambda}(p) - A(p)}{\int n_e K(p) + A(p)}
\]

(6.39)

The eqs. (6.37) and (6.39) clarify that there are two independent sources of equilibrium deviation: the leak of radiation or the overpopulation of the ground state. The first term relates the equilibrium deviation of excited levels to each other. In the \( n_e^{-\infty} \) limit the \( \rho^+ \) coefficient will tend to zero. This is a consequence of the fact that \( \tau^+(p) + \tau^*(p) = 1 \) in the \( n_e^{-\infty} \) limit.

6.8 The coefficients for total ionization and recombination

It is now possible to give eqs. (6.4) the simple structure

\[
\frac{\partial}{\partial t} n_1 = \frac{\pi}{\dot{\gamma}} n_e n_1^S_{cr} - n_e n_1^S cr \hspace{1cm} (4.40a)
\]

\[
\frac{\partial}{\partial t} n_1 = \frac{\pi}{\dot{\gamma}} n_e n_1^S_{cr} - n_e n_1^S cr \hspace{1cm} (4.40b)
\]
in which $n_{cr}$ and $S_{cr}$ are respectively the coefficients for total recombination and ionization. Substitution of eq. (6.31) in eq. (6.4a) gives

$$ n_{cr} = n_e K_e(1) \cdot \sigma_1(1) + \Sigma \sigma_e(p) n_e(p) / (n_e n_e) \cdot (n_e K_e(p) + \theta_p A(p)) $$  \hspace{1cm} (6.41a)

$$ S_{cr} = S(1) + \Sigma \sigma_e(p) \cdot n_e(p) \cdot (n_e n_e) \cdot (n_e K_e(p) + \theta_p A(p)) \cdot . $$ \hspace{1cm} (6.41b)

Equation (6.41a) explains that the total rate of recombination processes $n_e n_e \cdot n_{cr}$ equals the direct recombination to the groundstate plus deexcitation of that part of the excited levels population which originated from the ionstate.

The second equation (6.41b) shows that from the total groundstate evacuation $n_e n_e \cdot S_{cr}$ a part comes back by deexcitation processes. This part originated from the groundstate.

We can also substitute eq. (6.31) in (6.4b), which gives

$$ n_{cr} = n_e K_e(1) \cdot \sigma_1(1) + \Sigma \sigma_e(p) n_e(p) \cdot \Sigma \xi_e(p) S(p) \cdot n_e(p) / n_e $$ \hspace{1cm} (6.42a)

$$ S_{cr} = S(1) + \Sigma \xi_e(p) \cdot n_e(p) / n_e(1) \cdot S(p) \cdot . $$ \hspace{1cm} (6.42b)

Both eqs. (6.41) and (6.42) clarify that the recombination is coupled to the $\xi^e$ coefficients while the total ionization is coupled to the $\xi^1$ coefficients. Evidently, eqs. (6.41) and (6.42) must be the same. This can be proved by adding up eqs. (6.5) over the system of excited levels. A splitting up in $n_e$ and $n_e$ dependent terms gives:

$$ n_e \cdot \Sigma D_{1p} = \Sigma n_1(p) \cdot (D_{pl} + D_{p}) $$ \hspace{1cm} (6.43a)

$$ n_e \cdot \Sigma D_{p0} = \Sigma n^+_e(p) \cdot (D_{pl} + D_{p}) \cdot . $$ \hspace{1cm} (6.43b)

These equations express the fact that the total influx to the system must be the same as the total outflux and that there are two independent influxes, one originating from the groundstate and one originating from the ionstate. These facts are essential for the OSS solution, in which the only two sources for the excitation space are independent.
6.9 Analytical versus numerical models

This chapter was mainly devoted to the numerical set up of collisional radiative models. For each level a continuity equation was constructed, and after some simplifications it was possible to solve the set of coupled linear equations in terms of the densities of the ground and ion states. It is useful to face the question if it is possible to construct just one equation valid for all excited states in which collisional and radiative processes are given as analytical functions of the population or the energy E. In that case it is possible to obtain the distribution function by solving that general equation.

In the next chapter we will see that the excitation kinetics in the atomic energy scheme can be classified in 5 balances. And in chapter VIII and IX we will study the relation between the distribution function and the underlying balances. This study proceeds along analytical lines and turns out to be very successful, partly because the results are in most cases comparable to or better than those obtained by the numerical approach and partly because the analytical structure is much more transparent. However in chapter X we will see that not every system can be treated analytically and that levels have to be treated separately, i.e. one balance equation per level. In particular this is the case if the system is largely quantum defected and capricious of structure. In chapter III we have seen that for higher levels this quantum deficiency is relatively unimportant. A good approach of these systems is to apply a numerical model for the bottom and an analytical model for the top of the system. In this sense the cut-off procedure as introduced in section 6.5 is a powerful tool.

We may conclude that the title of this section is somewhat misleading. There are a lot of cases in which the combination of the two: numerical and analytical, provides the proper approach.
Chapter VII  Classification of domains in atomic systems.

7.1 Introduction

If a distribution function of excited states deviates from its equilibrium value, this originates from the fact that elementary processes are not balanced in the proper way, i.e. production and destruction of a level population are not each other's inverse processes. We say that the level is dominated by an improper balance. The part of the system in which a balance dominates is the so-called balance domain.

In this chapter a classification will be given of the main features of the distribution function in relation with the underlying improper balances for which appears that there are only four different types. In chapter VI we have seen that the distribution function of excited levels can be written in departure factors and reads

\[ b(p) = r^+(p) + b_1 r^1(p) \]

the \( r^+ \) reflects to the ion state contribution (the recombinating part), and \( r^1 \) to the groundstate contribution (the ionizing part). The relative importance of these parts of the distribution function with respect to each other is determined by the equilibrium departure of the groundstate \( b_1 \) which on its turn is related to the ionizing state of the system and the transport properties of the plasma. As discussed in section 7.3 we can distinguish between:

1) Ionizing systems,
2) Recombining systems and
3) Systems in ionization/recombination equilibrium.

In section 7.4 we discuss properties of the \( r^+ \) and \( r^1 \) coefficients by which appears that four improper balances are of importance. Besides it turns out that \( r^+ \) and \( r^1 \) have important properties in common which are due to the common depopulation factor \( D(p) = \frac{\delta}{\sigma} \), \( K(p) \), and \( \Lambda(p) \). The fact that \( D(p) \) has a \( \eta_\text{e} \)-dependent and a \( \eta_\text{n} \)-independent part reflects a competition between collisional and radiative processes. For intermediate values of \( \eta_\text{e} \) there will be a boundary in the system which separates lower (radiative) from higher (collisional) levels. Apart from this there is also a hot/cold boundary.

The domain plane presented in section 7.6 shows how this classification of levels in hot/cold and collisional/radiative results in a classification of improper balances and corresponding parts of distribution functions.
7.2 The Excitation Space

In the study of the relation between the ionizing state and the transport properties of a plasma, the excitation space is a useful concept. It is a generalization of the atomic energy scheme which gives insight in how transport phenomena are related to atomic processes.

The excitation space is defined as a one-dimensional space in which four different metric or location parameters can be used (cf. fig.4.2). Most frequently we use the (negative) energy \( E \) of the bound electrons and the principal quantum number \( (pqn) p \), which is related to \( E \) according to

\[
p = \sqrt{\text{q}^2 + \frac{\text{q}}{\text{r}}}.
\]  

(7.1)

The particles in the excitation space are the bound electrons. The population density \( n(p) \) at location \( p \) equals the number density of bound electrons (or atomic states) with label \( p \).

Due to atomic processes like radiative decay and electronic (de)excitation, flows, sinks and sources are induced in the excitation space. These flows, sinks and sources are closely related to transport phenomena in configuration space. For example, in an ionizing plasma in steady state a net ionization has to be balanced with outward diffusion of electrons.

In this way the excitation space can be regarded as an extension of the configuration space of the plasma, where electrons with positive energy are free, to the negative energy values where electrons are bound.

The two "spaces" are linked up by transport of electrons.

7.3 Classification of the Ionizing State of Systems.

Ionizing systems are characterized by the relation

\[
\Gamma^{\text{eff}} = n_o n_e \sigma \epsilon^r - n_o n_e \sigma \epsilon^r > 0
\]  

(7.2)

which means that there is a net flow \( \Gamma^{\text{eff}} \) in the excitation space in upward direction. In the case of a single ionized and stationary plasma we can apply eqs. (6.40), which together with eq. (7.2) result in

\[
-\text{\text{q}}. n_{p=1} = \nabla.n_{e=+} = \Gamma^{\text{eff}} > 0.
\]  

(7.3)
This reflects an inward transport of ground state atoms and outward transport of ions, supported by a flow in excitation space (cf. Fig. 7.1a). In Fig. 7.1b a sketch of a distribution function typical for ionizing plasma is given in a semi-log plot. The slope is not constant and a determination of the electron temperature $T_e$ with the help of the Boltzmann factor $\exp(-E/kT_e)$ is not possible, at least not with the densities of the lower excited levels. These are overpopulated with respect to the Saha-values; this overpopulation originates from the ground state. In Fig. 7.1c the distribution function is given in a log $b(p)$ versus $E$ plot. It shows how the overpopulation is spread out over the system, i.e. lower levels are largely overpopulated, higher levels are less, while for the highest levels the overpopulation is small compared to the equilibrium value of the population density.

Fig. 7.1

An ionizing system

a) Inward transport of ground state atoms and outward transport of ions, supported by a flow in the excitation space.

b) A distribution function typical for ionizing systems $n(p) \propto \nu(p)/\nu(p)$ the number density per statistical weight.

c) The distribution function in the $b(p) = n(p)/n^\mathrm{eq}(p)$ representation.
This distribution of the overpopulation can be understood qualitatively by the following: First we have to realize that the distribution function cannot be the equilibrium one. This would violate the principle of DB which predicts that in equilibrium there is no net activity of collisional processes and consequently no excitation flow.

Secondly we have to note that radiative processes can only cause a flow in downward direction (if absorption is negligible). So for the existence of an upward flow an overpopulation is a demand, i.e. b(p) > b(q) for pq. The more important radiative decay processes are, the more profound the overpopulation must be in order to enable collisional processes to overcome the downward radiative processes.

The fact that the overpopulation tends to zero for increasing p-values can be understood by realizing that high in the spectrum the departure from equilibrium must vanish. The levels are so close to the continuum that the excitation flow is small compared to the activity of ionizing and recombing processes.

In the limiting case for which downward processes can be neglected, the flow in the excitation space is given by

\[ \dot{\mathbf{I}}^\text{eff} = \mathbf{n}_\text{e} \cdot \mathbf{S}^c \]  
(7.4)

In this case the distribution function of lower excited levels is determined by the \( r^c \) coefficient only. It should be emphasized that the upper part of the system should be in equilibrium with the continuum, i.e. that \( r^c(p) \) should approach zero for increasing p-values.

Examples of ionizing systems can be found in several types of current carrying discharges such as arcs, positive columns, gas lasers, active parts of flames and so on.

Recombing systems are characterized by the relation

\[ \dot{\mathbf{I}}^\text{eff} = \mathbf{n}_\text{e} \cdot \mathbf{S}^c - \mathbf{n}_\text{e} \cdot \mathbf{n} \cdot \mathbf{a}^c < 0 \]  
(7.5)

which means that there is a net flow \( \dot{\mathbf{I}}^\text{eff} \) pointed in the downward direction of the excitation space.

We can deduce from eqs. (6.40) that in the case of a stationary single ionized plasma

\[ \nabla \cdot \mathbf{I}_I = -\nabla \cdot \mathbf{J}_I = \dot{\mathbf{I}}^\text{eff} < 0 \]  
(7.6)
holds. This implies that there is an inward transport of ions and outward transport of ground state atoms supported by a downward flow in excitation space (fig. 7.2a). In fig. 7.2b an example of a distribution function for a recombining plasma is sketched in a semi log plot. Again, the slope is not constant and the determination of $T_e$ in the conventional way is not possible with the densities of the lower excited states. These are underpopulated. In fig. 7.2c the distribution function is given in a log b(p) versus E representation.

Fig. 7.2
A recombining system with inward transport of charged particles.

Fig. 7.3
A radiatively pumped system.
The situation in which the lower states are underpopulated is merely an example of a recombinining system. In fact the underpopulation of lower levels is not a demand for the downward recombination flow. Contrary to the ionizing case the recombination flow can be radiative instead of collisional. And the number of decay processes depends on the population and not on the overpopulation. As long as absorption can be neglected radiative processes always tend in the downward direction of the energy scheme.

In the limiting case of a purely recombinining plasma, the flow in the excitation space is given by

\[ \Gamma_{\text{eff}} = \frac{n_0 n_i}{\alpha_{\text{cr}}} \]  

(7.7)

In this case the distribution function can be described by the \( \Gamma^*(p) \) only. In contrast with the properties of the \( \Gamma^0 \) coefficient there are situations in which the description of the distribution function for the whole energy scheme with the \( \Gamma^* \) coefficient only, is very well possible. This asymmetry between \( \Gamma^0 \) and \( \Gamma^* \) is closely related to the different character of ground- and ion states (cf. section 2.5.2); in contrast with the ion state the ground state is separated from the rest of the system by a large energy gap.

A second example of a downward flow in an atomic system is given by the figures 7.3a-7.3c. This situation can be found in irradiated plasmas in which photon ionization realizes a direct ionization channel separate from the system. By recombination processes through the system a balance is given for this radiative pump process. It depends on the electron temperature whether the excitation space is over- or underpopulated (cf. section 8.3).

Examples of recombinining systems can be found in many types of non-current carrying plasmas such as after-glow, the non active part of plasma torches, outer regions of flames and so on. Examples of radiative pumped systems can be found in the outer part of stellar atmospheres, planetary nebulae and \( \text{H}^\text{II} \) regions.

A system in ionization/recombination equilibrium can be regarded as a superposition of a purely ionizing and a purely recombinining system such that

\[ \Gamma_{\text{eff}} = \frac{n_0 n_i}{\alpha_{\text{cr}}}, \frac{n_0 n_i}{\alpha_{\text{cr}}} = 0 \] 

(7.8)
There is no net flow in the excitation space. In a steady state this means that
\[ V \cdot n_e \mathbf{w}_e = V \cdot n_I \mathbf{w}_I = 0 \] (7.9)

Equation (7.8) provides a relation between ground state and ion state densities, i.e.
\[ n_I / n_e = \frac{\alpha_{\text{cr}}}{S_{\text{cr}}} \] (7.10)

For hydrogen plasmas with \( n_e > 10^{23} \text{m}^{-3} \), the relation expressed by eq. (7.10) approaches the Saha relation. This is shown in fig. 7.4. But for lower \( n_e \) values the ratio given in eq. (7.10) is larger than that given by Saha. This can be understood by realizing that as \( n_e \) decreases the relative importance of radiative processes increases. In the absence of absorption, this means a preference for downward directed processes, i.e. the recombination flow. To realize an offset of this flow, the ionization processes have to be enhanced which is only possible if \( n_I \) is enhanced. So \( n_I \) must exceed the Saha value.

Examples of systems in ionization/recombination equilibrium can be found in the transition region between ionizing and recombinating part of plasmas.

Fig. 7.4
The ratio \( n_I / n_e \) as a function of the electron density for a hydrogen system in ionization/recombination equilibrium; \( T_e = 1.2 \times 10^6 \text{K} \); straight line: optically thin; broken line: optically thick with escape factors \( \beta_1 = 10^{-9}, \beta_2 = 10^{-1} \). From [BBK 77].
7.4 Properties of $r^*(p)$ and $r^1(p)$

In the preceding we studied qualitatively the influence of the ionizing state and transport properties on the shape of the distribution function. For instance, an ionizing system needs an overpopulated lower part of the atomic energy scheme in order to generate an ionization flow. This information however is still very global and further study is needed. A better understanding of the distribution function requires knowledge of its components $r^*(p)$ and $r^1(p)$ which on their turn are determined by collisional and radiative rate coefficients.

But we can already trace remarkable properties of $r^*(p)$ and $r^1(p)$ by making use of the general feature of eqs. (4.14) which for this purpose are reproduced here

\[
r^*(p) = \frac{\int_1^\infty r^*(q)\left(\frac{n_eK(q,p) + \lambda(q,p)}{n_eK(p) + A(p)}\right) dq}{\int_1^\infty \frac{n_eK(p) + A(p)}{n_eK(p) + A(p)}} \quad (7.1a)
\]

\[
r^1(p) = \frac{\int_1^\infty r^1(q)\left(\frac{n_eK(q,p) + \lambda(q,p)}{n_eK(p) + A(p)}\right) dq}{\int_1^\infty \frac{n_eK(p) + A(p)}{n_eK(p) + A(p)}} \quad (7.1b)
\]

We distinguish between three kinds of properties of the population coefficients, namely: radiative, complimentary and common properties.

\section*{1 Radiative properties}

We focus our attention on the low $n_e$-value of eq. (7.1b). In the denominator which reflects the destruction processes, the collisional term $n_eK(p)$ will disappear and the $n_e$-independent $A(p)$ will be dominant. In the numerator $n_eK(p)$, which reflects the population direct from the ground state, will be dominant and is proportional to $n_e$. The $r^1(q)\lambda(q,p)$ reflects the population processes coming from the ground state via higher levels (cascade) and is consequently also proportional to $n_e$. This implies that the $r^1(p)$ coefficients are proportional to $n_e$ for low $n_e$-values (cf., fig. 7.5).

The preceding clarifies that the $r^1(p)$ part of the distribution function is dominated by one type of balance if $n_e$ is small enough. The balance is the so-called corona balance and it is marked by the adjacent vignette.

The population density of a corona level results from the $\downarrow$ production due to excitation of groundstate atoms balanced with the destruction due to radiative decay.
The lower part of the energy scheme dominated by the corona balance is the so called corona (balance) domain. Its upper boundary is determined by the equality \( n_e k(p) = A(p) \) which will be discussed in section 7.5. The features of the corona domain will be discussed in section 9.2.

**Fig. 7.5**

The \( r'(p) \) coefficient for an optically thin hydrogen plasma [\( DRA/\lambda \)] as a function of \( n_e \),

\[ T_e = 1.2 \ (\text{eV}) \, \text{K}. \]

Note that \( r'(p) \) is proportional to \( n_e \) for small \( n_e \)-values and independent of \( n_e \) for large \( n_e \)-values.

**Fig. 7.6**

The \( r'(p) \) coefficient for an optically thin, low temperature hydrogen plasma at

\[ T_e = 4.16 \, \text{K} \]

according to [\( DRA/\lambda \)]. Note that \( r'(p) \) is independent of \( n_e \) for both small and large \( n_e \)-values.

The \( r' \) has different radiative properties which can be deduced from eq. (7.14a). If \( n_e \) decreases the numerator as well as the denominator become independent of \( n_e \). So below a certain critical \( n_e \)-value the \( r'(p) \) will remain constant (cf. fig 7.6).
The \( r^+(p) \) function for low \( \eta \) values is equivalent to

the distribution function of the Capture Radiative Cascade (CRC) balance. This balance is marked by the adjacent vignette. The production of the level population consists of capture and cascade \((r^+(q)\lambda(q,p)+\lambda(p))\), the destruction is realized by radiative decay \( \lambda(p) \).

More specific features of the domain of the CRC are given in the sections 8.2-8.4. The upper boundary of this domain is just as in the case of corona determined by the equality \( \eta \frac{\lambda(p)}{\lambda(p)} = A(p) \).

If Complementary properties.

Much can be learned from the equilibrium situation in the case that \( \eta \) is sufficiently large.

a) It can be proved (cf. [FUJI 73]) that for this equilibrium the relations \( b_1 = 1 \) and \( r^+(p) + r^-(p) = 1 \) hold (\( r^+(p) \) is \( r^-(p) \) in the \( \eta \rightarrow \infty \) limit). So \( r^+ \) and \( r^- \) are complementary and knowledge of one provides information about the other.

b) Moreover, in the limit of \( \eta \rightarrow \infty \), \( r^+ \) and \( r^- \) are independent of \( \eta \), which follows from eqs. (7.11) and is shown by the figs. 7.5 and 7.6. So we can write

\[
\begin{align*}
\lambda^+(p) &= f(p, T_e) \\
\lambda^-(p) &= 1 - f(p, T_e)
\end{align*}
\]  

(7.12)

which states that the population coefficients are only dependent of \( p \) and \( T_e \). Fig. 7.7 shows the \( \lambda^+(p) \) and \( \lambda^-(p) \) as function of the reduced temperature as obtained by Fujimoto. It can be seen that the increase of \( \lambda^+(p) \) as a function of \( T_e/\xi^2 \) is accompanied with a decrease of \( \lambda^-(p) \). This is a demand of the complementary property.

![Fig. 7.7 The \( \eta \) and \( \xi \) limit values of \( \lambda^+(p) \) and \( \lambda^-(p) \) as functions of \( T_e/\xi^2 \).](image-url)
c) If $p$ increases the energy distance between the level and the ion state $p$ decreases; consequently the level becomes more and more ion state-determined so that $I^u_e(p)$ has to approach zero for increasing $p$-values. A criterion can be formulated in terms of the ratio between the ionization potential of the level $p$ and the temperature. If $e_p = \frac{E_p}{kT_e}$ is small, which implies that $\frac{e_p}{2} < \omega \frac{kT_e}{Z^2}$, the rates of the excitation and ionization are more or less $T_e$-independent. The deexcitation rates are already very weak functions of the temperature. So all rate coefficients which appear in $I^u$ and $I^r$ (eqs. (7.11)) approach values which are nearly $T_e$-independent if $p = \infty$. This implies that

$$I^r_e(p) = \frac{\partial f}{\partial \nu}$$

with $\frac{\partial f}{\partial \nu} = 0 \Rightarrow \frac{\partial f}{\partial \nu} = 0$ for $e_p = 0$, \hspace{1cm} (7.13)

$$I^u_e(p) = 1 - I^r_e(p)$$

and is supported by fig. 7.7.

Resuming we may state that in the limit of high $T_e$ and $n_e$ values the population coefficients are $\nu_e$ and $T_e$ independent and the function $f(p)$ is decreasing for $p = \infty$ (cf. fig. 7.6 and 7.7).

These complementary properties can be used to describe any plasma with sufficient large $\nu_e$-value even if $b_1 \neq 1$. All we have to do in order to find the distribution function is to adjust the part of the distribution function which originates from the groundstate by inserting the actual value of $b_1$ in $b(p) = b_e(p) + b_1 r^u_e(p)$. The $r^u_e$ and $r^r_e$ values are known.

The $r^r_e(p)$ coefficient for large $\nu_e$-values is determined by electron collisions only. Moreover it describes a plasma for which the ion density is put equal to zero, i.e. $n_i = 0$. So the ionization processes will not be balanced by the three particles recombination and the sink created by putting $n_i = 0$ will create an excitation flow over the levels in upward direction.

The population density of a level will be the results of an improper balance, the so-called excitation saturation balance $ESB$ marked by the adjacent vignette.

In the same way the $r^u_e(p)$ coefficients describe the distribution function of a purely recombining plasma in which due to $n_i = 0$ a downward flow is created. This improper balance is marked by the adjacent balance.
III. The common properties of \( \tau^+ \) and \( \tau^- \) are mainly generated by the de-population factor which appears in the denominator of both coefficients. This factor

\[
D(p) = n_{e} \kappa(p) + A(p),
\]

(7.14)

expresses the competition between two terms: a collisional and a radiative term. The collisional term depends on \( n_{e} \) and \( T_{e} \), i.e., properties of the electron gas, while \( A(p) \) reflects typical atomic events like radiative decay and is consequently independent of \( n_{e} \) and \( T_{e} \). The total decay probability is related to the radiative lifetime by \( A(p) = \tau_{p}^{-1} \). There is a dependency of \( A(p) \) on the groundstate density. This dependency is related to the opacity and of decreasing importance for increasing \( \pi \)-values (cf. eqs. (4.6)).

For the description of the competition between electron collisions and the atomic properties of the atom with \( \pi \)-value \( p \), we use two parameters:

\[
\tilde{e}_{e}(p) = n_{e} \kappa(p)/A(p),
\]

(7.15)

\[
\tilde{T}_{e}(p) = kT_{e} n_{e}/[ \pi_{p} ],
\]

(7.16)

in which \( \pi_{p} \) is an adjustable parameter. The first one expresses the number of collisions in a radiative lifetime. We say that for \( \tilde{e}_{e}(p) > 1 \) the level is collisional, while for \( \tilde{e}_{e}(p) < 1 \) the level is radiative.

The second parameter relates the kinetic energy of the mean free electron to that of the bound electron. We say that for \( \tilde{T}_{e}(p) > 1 \) the level is hot, while for \( \tilde{T}_{e}(p) < 1 \) the level is cold.

In a collision between a free electron and an electron in a hot level, the free electron is the leading partner and most transitions are endoergic. In a collision in which a cold level is involved most transitions are exoergic (the free electron is 'heated').

7.3 The boundary criteria.

For a low \( n_{e} \)-value the parameter \( \tilde{e}_{e} \) will effectuate a split up in the energy scheme. Lower levels are radiative while upper levels are collisional. The \( \pi_{p} \) of the boundary level is denoted by \( \pi_{cr} \) and is determined by

\[
\tilde{e}_{e}(p) = 1 = n_{e} \kappa(\pi_{cr})/A(\pi_{cr}),
\]

(7.17)
which employing eqs. (4.6) and (5.72) results in

\[
\frac{9}{\rho_{cr}} = \frac{1.32 \times 10^3}{n_e} \left( \frac{Z}{\rho_e} \right)^{0.5} + \frac{2}{3} \ln p - \frac{C}{\ln(2/e_p + 1.3) [1 + \epsilon_p]}.
\]

This reflects a weak function of \( n_e \) and \( T_e \). For a given \( p \)-value the boundary relation \( n_e = n_e(p) \) determines a critical density \( n_{e,c}(p) \) such that for \( n_{e,cr}(p) > n_e \), the levels are collisional (cf. section 2.4.4).

A special role is played by the first excited level \( p=2 \). For \( n_{e,cr}(2) > n_e \), all levels are collisional. We say that the system is collisional. It can be seen from the \( p \)-dependence in eq. (7.18) that for a multi-electron atom, i.e. \( A \neq X \), the situation can exist in which the first system \( A1 \) is collisional while the second system \( A11 \) of that element is not collisional.

This collisional/radiative boundary was introduced by Griem in [GRI 63] as a boundary between the corona balance (CB) and partial local thermal equilibrium (PLTE) such that \( n_{e,cr}(p) = 10A(p) \). Nowadays we know that for ionising plasmas CB and PLTE are not next to each other but separated by the excitation saturation balance (ESB). The Griem criterion can be applied to the boundary between ESB and PLTE.

Fig. 7.8
The critical densities as functions of \( T_e \) for the levels \( p = 2, 3 \) and 4 of hydrogen.

- - - - - - [GRI 63]
- - - - - - [LMA 69]
- - - - - - [BIB 79]
- - - - - - present study

In fig. 7.8 we compare the present value of the critical densities with the values obtained in [GRI 63], [DRA 69] and [BIB 79]. The...
The difference between the present value and those obtained in [BIR 79] originates from the fact they consider the competition \( n_k(p, p+1) = A(p+1, p) \). The difference between our values and those obtained in [DRA 69] originates from the erroneous approximation for the oscillator strength used in [DRA 69]. There is a good agreement between our values and those presented in [BER 68] especially for large \( T_e \) values for which the difference in collision theories is limited.

For low \( T_e \) values the parameter \( T_e \) will split up the energy scheme in a lower cold part and an upper hot part. The phon of the boundary is given by

\[
P_{bc} = \frac{Z^2 \text{Ry}}{(kT_e)}
\]

For a given \( p \)-value, this equation determines a critical temperature \( T_e^c(p) \). For \( T_e > T_e^c(p) \) all levels with \( p \) are hot.

Here again a special role is played by the first excited level. If \( T_e > T_e^c(2) \) we say that the system is hot. And again for an atom \( A \neq H \) it may be possible that \( A \) is hot while \( A \) is not. All or higher systems contain cold levels.

The precise value of the hot/cold boundary is in discussion. First introduced in [BIR 62] the thought behind it was that somewhere in the atomic system there is a minimum in the equilibrium value of the rate of excitation processes \( n_{e}^{p}(p)K(p, p+1) \).

This can be understood realizing that \( n_{e}^{p}(p) \) scales with \( p^2 \exp\left(\frac{2Z^2 \text{Ry}}{p^2 kT_e}\right) \) while \( K(p, p+1) \) scales roughly with \( p^4 \). So the product has a minimum value if

\[
\frac{d}{dp} \left(p^6 \exp\left(\frac{2Z^2 \text{Ry}}{p^2 kT_e}\right)\right) = 0.
\]

This occurs for \( Z^2 \text{Ry}/p^2 kT_e = 3 \) which corresponds with \( T_e^c = 3 \).

Another formulation of the criterion can be deduced by comparing the excitation and deexcitation processes starting from the same level. The fact that the statistical weight increases in the upward, excitation, direction is in favour of the excitation processes. But a disadvantage for excitation processes is that they need a supply of energy from the electron gas. A supply which is less effective when the electron temperature is lower. A critical situation for the level \( p \) is that for which the rate of the excitation step process
equals that of deexcitation step process, i.e.

\[ n^e(p,p-1) = \frac{n^e(p) n^e(p-1) X(p-1,p)}{n^e(p)} \]  \hspace{1cm} (7.21a)

The last equality is derived from the principle of detailed balancing.

If we write eq. (7.21) in the form

\[ n^e(q) X(p,p+1) = n^e(p) X(p,p-1) \]  \hspace{1cm} (7.21b)

we see that this holds under the same conditions as that given in eq. (7.20).

For decreasing temperature the assumption that step-wise processes are dominant is no longer valid. If we use the results of Mauk and Keck as reproduced in eqs. (5.50-52) we see that the total rate of deexcitation processes exceeds that of the excitation processes of

\[ \alpha > 3.83 \] or \[ \delta^e > 3.83 \]

Still another criterion is given by Bierman as a result of a Pokker Planck treatment of the excitation kinetics. The boundary value given in [BIB 79] equals

\[ \delta^e = 1.5 \]

The level with \( \tilde{p} = 1 \) is sometimes called the bottleneck (cf. [BIB 79]). Levels below the bottleneck are more or less in equilibrium with the groundstate and the levels above this bottleneck are more or less in equilibrium with the ion state. There is not much activity of processes crossing this bottleneck which follows from the above discussion (cf. fig. 7.9).

Finally we remind of the temperature dependence of the capture mechanism (cf. sect. 4.4). It appeared to be useful to distinguish between radiative hot and radiative cold levels where the boundary was found to be

\[ \delta^e = 1 \]

A difference between the R-horpeboundary and the boundary discussed here, is that the former concerns a population and the latter a depopulation phenomenon. However, apart from the precise numerical value the boundary has the same functional dependence and comparable value.

Hereafter we use \( \delta^e = 5 \) in the determination of \( \tilde{p}^e(p) \).
Fig. 7.9
The level $\tilde{\epsilon}_h$ with $\tilde{\Delta}[\tilde{\epsilon}_h] = 1$, i.e. the boundary between the hot and cold domain, represents a bottleneck in the system. There is not much activity of processes crossing the bottleneck.

a) The bottleneck in an ionizing system

b) The bottleneck in a recombining system

With the capitals $B$ and $S$ we refer to the proper balances of Boltzmann and Saha.

7.6 The Domain plane
In the preceding we have seen that the excitation kinetics in EEE-plasmas is determined by the competition between collisional and radiative (CR) processes. For bound electrons this competition can be regarded as one between internal and external influences. Since the parameters $\tilde{\epsilon}_h$ and $\tilde{T}_e$ as defined in the eqs. (7.15) and (7.16) are successful in the description of this competition, we introduce a $\tilde{\epsilon}_h - \tilde{T}_e$ plane (cf. fig. 7.10). The vertical axis is the $\tilde{\epsilon}_h$ axis while the horizontal axis is the $\tilde{T}_e$ axis. A certain level with proper $p$ in a particular EEE-plasma characterized by a $\tilde{\epsilon}_h$ and $\tilde{T}_e$ -value is represented by a particular position in this plane.

We have also seen that the population density of excited states in an EEE-plasma is the result of population and destruction balances of CR processes only. There are five balances of importance, one proper balance (the FLYE balance) and four improper balances. A particular balance is dominant in a particular part of the atomic energy scheme, the so-called balance domain (cf. fig. 1.1 and table 1.3).

Such a balance domain corresponds with a area in the $\tilde{\epsilon}_h - \tilde{T}_e$ plane. And that is why we call this plane the domain plane.

We give a brief discussion of the four quadrants which are separated by the $\tilde{\epsilon}_h$ and $\tilde{T}_e$ axis (cf. fig. 7.10).
In the first quadrant we find collisional hot levels. It follows from the definition of $N_e$ and $T_e$ (cf. eqs. (7.14-15)) that for increasing $p$-values we have to reach this first quadrant. So the top of any atomic system has to end in this right upper corner. The balances in the first quadrant are the excitation saturation balance, the ESB, and the balance of PTE.

In the left upper corner we meet with collisional cold levels. These levels are subjected to frequent interactions with cold electrons and deexcitation will be dominant over excitation. The balance in this quadrant is the cold ESB. For 'ionizing' systems the Boltzmann balance can be found in this quadrant.

In the left lower corner we find radiative cold levels. In the case of a recombining plasma the cold capture radiative cascade balance (CRCB) can be found here. In ionizing plasma we meet in this quadrant with the corona balance CB.

In the right lower corner we find the radiative hot levels. The balances are in this case the hot CRCB and the CB.
In chapter VIII and IX specific features of the balances will be discussed. But some general remarks have to be made.

- A particular atomic level occupies one position in the domain which depends on $n_e$ and $T_e$ only.
- The distribution function is represented by a curve in the domain plane. It follows from eqs. (7.18) and (7.19) that $n_e$ scales roughly with $T_e^{-3.5}$ along the curve (cf. fig. 7.10).
- The domain curve is pointed towards the right upper direction, i.e., towards quadrant I where it has to end in PLTE.
- By the position of level $\nu = 2$ the domain curve is determined.
- At crossing one of the axes the domain curve enters a new balance domain and a substantial change takes place in the excitation kinetics of a level. This means that also the distribution function will change structurally. It has a so-called knee point which connects two different parts of the function (fig. 7.11).

**Fig. 7.11** Distribution functions and domain curves.

a) An optically thin $H$ plasma

$n_i = 10^{16} \text{m}^{-3}$, $n_e = 10^{20} \text{m}^{-3}$

and $T_e = 5.2 \times 10^6 \text{K}$.

b) An optically thin $H$ plasma

$n_i = 10^{16} \text{m}^{-3}$, $n_e = 10^{20} \text{m}^{-3}$

and $T_e = 3.2 \times 10^5 \text{K}$.

c) The corresponding domain curves of the figs. a, b and c.
- The domain plane is based on the common depopulation factor of the \( r^* \) and \( r^1 \) coefficients. It is not possible to express which of the two \( r^* \) or \( r^1 \) is the dominant part of the distribution function. As we have seen already this is determined by the Saha departure factor of the ground state \( b_1 \) which on its turn is related to transport phenomena.

- This means that a whole family of distribution functions are projected on the same domain curve (cf. figs. 7.12 and 7.13). Each member of the family has a knee point at the same level.

- Strictly speaking, it is not useful to distinguish between hot and cold levels in the lower halfplane. This is because the radiative destruction processes (decay) are not temperature dependent. However, it is useful to retain this division for recombining plasmas since there is a change in the radiative production as function of \( T_e \). For ionizing plasma this division makes no sense. There is no substantial difference between hot and cold corona. But as we will see in section 9.2 there is a substantial difference between transparent and opaque corona.

![Fig. 7.12](image)

A family of case A distribution functions projected on the same domain curve. Each member of the family has a knee point at the same level. Differences are related to different \( b_1 \) values, i.e. the ionizing state of the system. The knee point precludes the advent of new domain.

![Fig. 7.13](image)

A family of distribution functions with \( \phi_0 \) at the same position. Differences between the members are caused by different values of \( b_1 \), i.e. the ionizing state of the system.
Chapter VIII  Recombining plasmas

8.1 Introduction

This chapter is devoted to the distribution function of purely recombining plasmas and deals with the properties of the \( r'(p) \) coefficient.

Features of the distribution function will be studied in relation with underlying balances.

The domains of the balances are shown in the adjacent figure. The study will proceed along the clockwise curve as indicated in the adjacent domain plane where section numbers and keywords are shown.

8.2 The Capture Radiative Cascade balance

The quadrants III and IV are dominated by the Capture Radiative Cascade (CRC) balance. Models for this CRC balance are the earliest (collisional) radiative models and were already presented in the thirties by astrophysicists like Baker and Haensch [BAK 78].

In 1959 an new impulse was given by the group of Searle [SEA 59b]. In an extensive series of studies special attention was paid to the transition from the CRC to the PLTE domain of the system. Nowadays the CRC balance and its boundary with PLTE is of great interest in the study of stimulated emission as found in H\(^+\) regions (cf. [SHA 75] and [SH 79]).

Both the production and destruction of the levels in the CRC domain are radiative of character. In the QSS solution there will be a balance between capture and radiative cascade at one side and radiative decay at the other side (cf. adjacent fig.).

Thus the production/destruction balance of a level in the CRC domain reads

\[
\dot{n}(p) \sum_{i} \dot{\phi}(i, p) A(p, i) = n_{0} \varepsilon(p) + \sum_{u>p} n(u) \Lambda(u, p) . \tag{8.1}
\]
As discussed in (4.6) the kinetic of the capture and cascade processes will change as function of $e_p = \frac{E_p}{kT_e}$, i.e., the kinetic energy of the bound electron expressed in the free electron temperature. Therefore it is useful to distinguish between a hot CRC found in quadrant IV and a cold CRC found in quadrant III. We first treat the hot CRC.

8.2 The hot CRC

To get insight in the production and destruction processes in the hot CRC domain we refer to Fig. 8.1 which is obtained from [PUI 80a]. This figure shows that 70% of the population production originates from capture and 30% from cascade.

Fig. 8.1

The contributions of the various processes in percentages to the a) production and b) destruction of the levels $p = 5$ as functions of $n_e$. The hatched areas correspond to radiative transitions. $c$, $d$, $e$, and $f$ denote capture, three body recombination and ionization, respectively. A result of model calculations for a plasma $r = 1.28 \times 10^5 K$ is also presented in [PUI 80a].

Chapter IV was completely devoted to the study of radiative processes. Here we reproduce the results as far as they are needed in the study of the hot CRC domain.

The total number of decay processes of a level $p$ (i.e., the l.h.s. of eq. (4.1)) can be written as (cf. eq. (4.6))
\[ a(p) \Theta_{p1} A(p,1) = a(p) \gamma Z^5 p^{-5} (3 \ln p - \zeta) \]  \hspace{1cm} (8.2)

in which
\[ \zeta = 0.23 \] for case A and
\[ \zeta = 1.84 \] for case B.

The equilibrium amount of the cascade contribution for hot levels can be put together with the amount of capture processes in one formula

\[ n_e A_e a(p) + \int_{u_p} a^e(u) A(u,p) du = a^e(p) \gamma Z^5 p^{-5} (3 \ln p - \zeta(T_e)) \]

with
\[ \zeta(T_e) = \ln(By/kT_e) + 1.0 \] \hspace{1cm} (8.3)

in which \( a^e(p) \) is the equilibrium number density of level \( p \) according to Saha (cf. eq. 2.33). In section 4.6 we have seen that the cascade contribution in equation 8.3 is about 30%. This is in agreement with the results of extensive CR calculations of Fujimoto (cf. fig. 8.1).

If we assume that the actual value of cascade contribution is not far removed from the equilibrium value we obtain

\[ b(p) = \frac{n_e A_e a(p)}{n_e^e a^e(p)} = \frac{3 \ln p - \zeta(T_e)}{3 \ln p - \zeta} \] \hspace{1cm} (8.4)

as an approximate result from the production/destruction balance eq. (8.1). The corresponding value of the relative overpopulation equals

\[ \delta b(p) = b(p) - 1 = \frac{\zeta - \zeta(T_e)}{3 \ln p - \zeta} \] \hspace{1cm} (8.5)

More general is the result directly obtained from the \( \delta b(p) \) as obtained in eq. (6.37) which in the \( n_e = 0 \) limit reads

\[ \delta b(p) = \int_{q^2 p} \delta b(q) A(q,p) A(p) \frac{\zeta - \zeta(T_e)}{3 \ln p - \zeta} \] \hspace{1cm} (8.6)

The difference between eqs. (8.5) and (8.6), i.e. the first term of the above equation, reflects the influence of the equilibrium departure of higher levels.

In what we call the quasi LTE approach, this first term will be neglected. This will give reasonable results for the description of global properties of the hot CRC domain since - the cascade contribution is only 30% of the total production. The
rest comes from capture and this retains its equilibrium value as long as the free electrons are distributed according to Maxwell.

Due to the fact that $T_e$ appears in the logarithm the difference $|z-e|$ will be small for a large $T_e$ range. So the first order approximation eq. (8.5) predicts $\delta b$-values close to zero and the correction obtained by the first term in eq. (8.6) is limited.

From the analytical expression (8.5) the following conclusions can be drawn:

1) For low temperatures the equilibrium departures for opacity case A are more severe than for case B. This is a consequence of the fact that opacity reduces the effective decay.

2) In the limit of high $p$ values $\delta b$ approaches zero. This means that the Saha density is established without the presence of ionization and three particle recombination. This is remarkable since these latter processes are responsible for the maintenance of the proper LTE balance which retains the Saha density. And equilibrium of radiative processes can only be expected if absorption is present as the inverse process of emission, which is not the case in the CRC domain.

3) The equilibrium departure $\delta b$ is a weak function of $p$. The value $\delta b_{hi}$ for a certain level $p_{hi}$ is reduced with a factor $\frac{1}{2}$ at the level $p_{lo} = p_{hi} \exp(-c/\lambda)$. For the case A we obtain approximately $p_{lo} \approx \frac{1}{2} p_{hi}$ which reflects a weaker $p$-dependence than for case B where $p_{lo} \approx \frac{1}{4} p_{hi}$.

In fig. 8.2a and 8.2b the function $b(p) = \delta b + 1$ is sketched for two different temperatures. Fig 8.2a deals with case A and fig 8.2b with case B. The weak variations of $b(p)$ as a function of $p$ are shown in these figures.

Fig. 8.2a

The departure function $b(p)$ as a function of the parameter $p$ in the quasi LTE approach (eq. 8.5) at case A. The slope of $p^{-0.5}$ as predicted in [FUG280a] is shown. This approximation is limited to low $p$ and high $T_e$ values.
4) The sign of $5C - 5X$ is determined by the electron temperature and it appears that hot CRC systems can be divided into two subclasses: medium hot and very hot CRC systems. The boundary between these subclasses is related to $5C - 5X = 0$. Bakor and Mentes denote this boundary by "Pseudo Thermodynamic Equilibrium". It is remarkable that in this case an improper balance gives proper results and that although the inverse absorption processes are not (fully) present, levels are still populated as if the system were in equilibrium.

Applying eqs. (8.2) and (8.3) we find there is pseudo TE in case A at $T_e = 3.3 \times 10^4$ K and in case B at $T_e = 6.8 \times 10^4$ K. So this temperature boundary depends on the opacity. In Fig. (8.3) values from [Bak 3] and [Bak 38] are displayed for several temperatures. Both authors deal with a hydrogen system in case A. It can be seen that $\delta_b = 0$ is realized for temperatures between $2.0 \times 10^3$ K and $3.2 \times 10^3$ K. Since the curves in Fig. (8.3) are rather flat this means that pseudo TE occurs for each level at the same temperature.

Fig. 8.3

The relative overpopulation $\delta_b(p)$ as a function of $p$ for different temperatures:

1 [Dra 77] $T_e = 10^4$ K $\eta_e = 10^{10}$ m⁻³
2 [Dra 77] $5 \times 10^4$ K $\eta_e = 10^{10}$ m⁻³
3 [Dra 77] $2 \times 10^5$ K $\eta_e = 0$
4 [Bak 38] $3.2 \times 10^5$ K $\eta_e = 0$
5 [Bak 38] $1.6 \times 10^5$ K $\eta_e = 0$

$\delta_b$ refers to the collisional/radiative boundary level for $n_e = 10^{18}$ m⁻³
It should be noted that the model calculations from [DRA 77] in Fig 8.3 are carried out for the electron density value $n_e = 10^{16} \text{m}^{-3}$. So only the levels $p<7$ are in the CRC domain. The tendency of $b = 1$ for $p>7$ is due to the collisional processes and is not a CRC matter. The pure CRC values of [BAK 38] do not show this rapid approach to PLTE. The influence of electron collisions was neglected, which corresponds to $n_e = 0$.

In Fig. 8.4 the equilibrium departure of level $p=30$ is presented as a function of $T_e$. The values were obtained from [BAK 38] and [SEA 59b]. In both cases we deal with pure CRC calculations. For case A the values of [BAK 38] and [SEA 59b] are in agreement with each other within 5%. In case B the differences are about 10%. The values of [SEA 59b] had to be extrapolated to obtain the $8b = 0$-crossing. From Fig. 8.4 we deduce that pseudo TE occurs at about $2.3 \times 10^5 \text{K}$ in case A and at $8.7 \times 10^5 \text{K}$ in case B, which shows that the results of our quasi PLTE approach fits reasonably well with the results of extensive model calculations.

Fig 8.4
The relative overpopulation of level $p=30$ as a function of electron temperature, triangles: [BAK 38]

\[ \text{case B} \quad \text{case A} \]

Intersection with $8b = 0$ determines the temperature of 'Pseudo TE'.

We have seen in section 4.6 that the temperature dependence in eq. (8.3) is the result of the $T$ dependence of capture only. The cascade rate from a PLTE upper system is temperature independent. But capture is the leading production term in the CRC domain and it is always behind in populating an upper level; this will have consequences for the cascade from that upper level to lower levels. So the cascade temperature dependence is a second order effect. It is in principle possible to get a better approximation of the distribution function by employing eq. (8.6) in an iterative way. We will not follow this line but study the results of the CRC model of Seaton and Baker and Memmel.
The model, presented in [SEA 59b], deals with the calculation of the cascade contribution via all possible routes leading from a certain upper level \( u \) to a lower level \( p \).

The total cascade contribution to a level \( p \) is then given by

\[
\eta_{u} n_{u} \sum_{\nu} n_{u} A(u, p) = \eta_{u} n_{u} \sum_{\nu} n_{v} C_{vp},
\]

where \( C_{vp} \) is the probability that population of \( u \) is followed by a radiative transition to \( p \) via all possible routes. By convention \( C_{pp} = 1 \). The cascade matrix \( C_{vp} \) is calculated for hydrogenic systems employing analytical formulae for the oscillator strength (cf. eq. (3.22-23)) and the relation expressed by eq. (4.2). In this way the cascade contribution from an infinite number of levels can be obtained in an analytical way.

A similar model calculation in which the cascade contribution from an infinite number of levels was taken into account was already carried out in 1938 by Baker and Menzel [BAK 38].

In fig (8.5) some results of [BAK 38] and [SEA 59b] are compared with our formulae (8.2) and (8.3). It can be seen that the temperature dependence is more severe than that predicted by the quasi LTE treatment which can be understood as a result of the indirect \( T_e \) dependency of the cascade contribution.

The results of [SEA 59b] and [BAK 38] can be approximated by an analytical formula of the form:

\[
b = \frac{3}{2} \ln \frac{p}{T} - \frac{1}{3}
\]

in case A

\[
\xi_a = 0.25 \quad \xi_b = 1.63 \ln(Ry/kT) + 0.75 - 0.62(Ry/kT_e)^{0.75} + 0.63/p
\]

in case B

\[
\xi_a = 1.84 \quad \xi_b = 1.53 \ln(Ry/kT_e) + 0.53 - 0.22(Ry/kT_e)/p
\]

These analytical expressions reproduce the model calculations within 15% for \( p > 2 \) and \( \xi < 0.5 \). See fig (8.5).
The departure factor $b(p)$ as a function of the photon number density $n$ for opacity cases A and B for several temperatures:
1) $T_e = 5 \times 10^5 \text{ K}$; 2) $T_e = 2 \times 10^6 \text{ K}$; 3) $T_e = 6 \times 10^6 \text{ K}$ and 4) $T_e = 3.2 \times 10^6 \text{ K}$

Triangles [BAK 36]; crosses [DEN 57b]. Dashed lines: quasi-PLTE values; eqs. (8.4); full lines: eqs. (8.8)

### 8.4 The cold CRD

For low values of $f_n(p)$, i.e. large values of $\epsilon$, we arrive in quadrant III where the cold CRD balance dominates. In this domain capture is much too slow to supply the equilibrium amount of decay processes, large departures from the PLTE density can be expected which consequently results in a breakdown of the cascade. The quasi-PLTE approach is not valid in this domain.

In search of the main features of the distribution function we first neglect cascade contribution and retain capture as the only population process.

By employing the eqs. (4.17) and (4.19b) we find that the approximation

$$n_n(p) = n_n(p) + \frac{\omega(-\epsilon)}{\epsilon_p}$$

holds. Together with the rate of radiative destruction as presented in
eq. (8.2) we find that in this approximation the balance (8.1) reads
\[
n(p) (3 \ln p - \xi) = n_p^0 \frac{\exp(-e_p)}{e_p} \exp(-e_p K),
\]
with the solution
\[
b(p) \exp e_p = \left[ e_p (3 \ln p - \xi) \right]^{-1}.
\]
By inserting \( e_p = \frac{2^3}{2} \frac{2^3}{2} \frac{2^3}{2} \frac{2^3}{2} \frac{2^3}{2} \) in this equation and employing approximation \( 3 \ln p - \xi \approx 2 \sqrt{p} \) we find
\[
b(p) \exp e_p = \left[ 1.5 \frac{\sqrt{p}}{Z^2 s_y} \right].
\]
This equation shows the \( p^{1.5} \) - dependency as predicted by Fujimoto in [Fuj 80b].

In fig. 8.6 we compare this analytical expression with model calculations obtained from [SEA 59b] and [DRA 77] by which it appears that there are large differences between the model calculations and the expression (8.12) for low \( p \) values. Apparently, the cascade contribution is not negligible.

Fig. 8.6
\( b(p) \exp e_p \) as a function of the \( p \) in crosset. [SEA 59b] pure CCR: \( T = 2.5 \times 10^5 \) K
Squares [DRA 77] \( n = 10^{20} \) m\(^{-3}\)
\( T = 2 \times 10^3 \) K

Full lines eq. (8.11)
\( n = p^{1.5} \) refers to [Fuj 80b]

The arrows refer to the levels for which \( e_p = e_p \) = 1 (cf. section 4.7).

The influence of the cascade contribution from the level \( p+1 \) on the population density of the level \( p \) can be estimated. Under the assumption that the population density of the level \( p+1 \) can be described by eq. (8.11) the balance of the level \( p \) reads.
\[ n(p) = n_{\infty}(p) \exp\left(-\frac{\varepsilon}{3 \ln(p - 3)}\right) \]
\[ = n_{\infty}(p) \exp\left(-\frac{\varepsilon}{3 \ln(p - 3)}\right) \]
\[ \times \exp\left(-\frac{\varepsilon}{3 \ln(p - 3)}\right) \]
\[ \times \exp\left(-\frac{\varepsilon}{3 \ln(p - 3)}\right) \]
\[ \times \frac{A(p+1, p)}{A(p+1, p)} \]
\[ \times \frac{A(p+1, p)}{A(p+1, p)} \]
\[ \times \frac{A(p+1, p)}{A(p+1, p)} \]

For low \( p \) values the second term between brackets is comparable to one and cannot be neglected. For large \( p \) values the second term can be approximated by \( 3 \ln(p+1) - \frac{\varepsilon}{3 \ln(p - 3)} \) and approaches zero for large \( p \) values. This is found back in fig. 8.6, which shows large deviations for low \( p \) values and smaller deviations for upper levels. The fact that cascade is not negligible in the cold CRC domain is supported by fig. 8.7 obtained from [Fuj 80b]. This figure gives insight in the various processes for the cold CRC hydrogen system (low \( p \)-values) and shows that about 50% of the production is due to cascade.

From fig. 8.6 we can deduce that the population density per statistical weight is an increasing function of \( p \), which means that there is a pronounced density inversion in the system. A view of Seitz's tables [Sea 59b] and figures 8.5(a) and 8.5(b) tells us that the inversion carries on till far into the hot CRC. We come back to this in section 8.7.

---

The contributions of the various processes to the \( a \) production and the \( b \) destruction of level \( p = 5 \) as a function of \( n_0 \). The hatched areas correspond to radiative transitions; \( \alpha \) denotes capture. A result of model calculations for a \( a \) plasma with \( T = 10^5 \) K as presented in [Fuj 80b]. Compare this with fig. 8.1, where \( T = 1.26 \times 10^5 \) K.
8.5 The domain of the cold excitation saturation balance

In quadrant II we meet with the cold excitation saturation balance. Since $\mathcal{E}_e > 1$, collision processes occur more than once in a radiative lifetime. But these are cold collisions because $\tau_{ee} < 1$, and deexcitation processes will prevail over excitation processes.

This results in a net recombination flow, i.e. a flow in the system pointed in downward direction, a phenomena sometimes denoted by collisional cascade (cf. adjacent vignette). The features of this domain were studied in [MAN 69], [BIB 73], [Fuj 80b] and [SIJ 84].

Hansbach and Keck [MAN 69] used a Pokker Planck treatment to describe the kinetics of the cold collisions. The rate coefficients were obtained in the same study by the analysis of three body trajectory calculations (cf. section 5.10). The distribution function obtained in [MAN 69] is expressed in incomplete factorials for which we apply the approximation

$$b(p) \approx \left( \frac{e_p}{2p} \right)^{3/2} \exp(-e_p) . \quad (8.15)$$

In [BIB 73] the distribution function is also obtained by a Pokker Planck treatment. The incomplete factorial in this case can be approximated by

$$b(p) \approx 0.75 e_p^{-2/3} \exp(-e_p) . \quad (8.16)$$

The differences in the results of [MAN 69] and [BIB 73] can be traced back to the different rate coefficients of electron induced transitions (cf. section 7.5).

Fujimoto used in [Fuj 80b] a numerical CR model based on rate coefficients of [MAN 69] and found that the results of his numerical calculation reflect a distribution function with a

$$n(p) \propto e_p^{-6} \quad \text{dependence} . \quad (8.17)$$

This is indeed a dependency which can be found in eq.(8.15) valid for large $e$ values.

Figure 8.8 shows the results of measurements as obtained by Binnew and Hirschberg [BIN 62] in a low temperature He afterglow. For high levels the slope in the log $\eta$ versus $E$ plot approaches a constant value which was interpreted as reflecting the Saha equilibrium. The temperatures obtained from the Saha equation (cf. eq.(2.33)) are shown in the same figure. In fig. 8.9 the same measurements are shown in a
Fig. 8.8
Measured population density as a function of \( n_{\text{nn}} p \) and the ionization potential \( |e_p| \) of the \( p^\bullet \) states in a neal glow as presented in [MIN 62].

A log \( b \) versus \( E \) plot. It can be seen that deviation from equilibrium occurs at the same value of \( e \) and after the transformation as shown in that fig. 8.9 all \( b \) values of different temperatures lie on the same curve. This is a support for the theory which predicts that the kinetics and the distribution function can be expressed in terms of \( e \).

Fig. 8.9
The results of [MIN 62] presented in a log \( b \) vs \( n \) plot and after a transformation in a log \( b \) vs \( e \) plot:

\[ e_{p} = |p|^{2} / 2 \]

The transformation is depicted by the arrows. The temperatures are obtained from the slopes in fig. 8.8.
In fig. 8.10 theoretical curves of [MAN 69] and [BIB 73] are compared with these experimental results. The figure does not provide an obvious support of one of the theories at the expense of the other.

**Fig. 8.10**
A comparison of the experimental results of [MAN 69] (crosses, circles and triangles) with the theoretical formulae of [MAN 69], eq. 8.15 (dashed) and [BIB 73], eq. 8.16 (dash/dot).

The predicted values as presented in [MAN 69] are too high and those of [BIB 73] are too low. In [MAN 69] it is stated that for lower levels radiative decay has to be taken into account which results in a lowering of the theoretical value. According to [BIB 73] opacity is also of importance and this moves their theoretical curve in an upward direction towards the experimental values. In fig. 8.11 we sketched a corresponding domain curve which reflects two axis intersections, i.e. two knee points. So radiative decay processes are indeed of importance in the determination of the distribution function. The role of the opacity, which we will not consider, is determined by the ground state density and the plasma dimension.

We may conclude that the domain of the cold ESB in recombining systems is characterized by a distribution function which rapidly decreases for \( p = 1 \).

**Fig. 8.11**
A sketch of the domain curve which belongs to \( T_e = 0.13 \) ev and \( n_e = 6.2 \times 10^{18} \text{m}^{-3} \), i.e. the 'lowest condition' of [MAN 69].
The critical levels are shown.
8.6 The collisional hot quadrant

In quadrant I we find the levels which are dominated by hot collisions. The bound electrons in these levels are subjected to collisions with free electrons which occur more frequently than once in a radiative lifetime, i.e. \( N_e > 1 \). The free electrons are the leading particles in the collisions; their kinetic energy is much larger than that of the bound electrons, i.e. \( T_e > 1 \). This means that stepwise transitions will dominate over jumpwise transitions.

Quadrant I is the most occupied quadrant. The upper part of any system lies in this quadrant in which two different balances have their domain: the improper excitation saturation balance (ESB) and the proper balance of ionization and three particles recombination. The latter has to retain the partial local thermal equilibrium (PLTE). The task of the improper ESB is to prepare the advent of PLTE. It is active at the boundaries of quadrant I with quadrant II and IV where it has to smooth out the equilibrium departures caused in the adjacent quadrants. The ionization/recombination balance is less effective in eliminating equilibrium departures since jump processes are much less effective than step processes.

The stepwise character of the excitation processes is essential for quadrant I. It makes it possible to define an excitation flow \( J \) and to construct a continuity equation for the excitation space which describes how this flow changes in its course through the excitation space. These changes are affected by the presence of sources and sinks. The ionization \( I \) and radiative decay \( D \) are the sinks, the sources are the capture cascade \( CC \) and three particles recombination \( R \).

By means of the continuity equation

\[
\text{div } J = R + CC - T - D,
\]

the divergence of the flow is related to sources and sinks.

Since flow, sinks and sources are related to the population density, this continuity equation provides a differential equation for the distribution function. Together with the boundary conditions the distribution function can be determined. But first we have to determine \( J, R \) and \( I \) as functions of the level density. The capture, cascade and decay which were already discussed in section 8.3 will be retained to study how the transition from quadrant IV to I takes place.

As there are two location parameters, \( p \) and \( z \), in the excitation...
space (cf. sect. 7.2) we can construct the continuity equation in both
the \( p \) and \( K \)-representations. In this section we treat the \( p \)
representation while section 9.6 is devoted to the solution as
function of \( E \).

We start the construction of the continuity equation with the
determination of the \( \text{lhs of eq.}(6.18) \). The excitation flow is in a
first order approximation equal to the stepflow which is defined as
follows (cf. fig. 8.12): Consider a fictitious intersection between \( p \)
and \( p+1 \) in the excitation space. There are stepwise excitation
processes crossing this intersection in upward direction, \( p \rightarrow p+1 \), and
stepwise deexcitation processes in the opposite direction. We define
the stepflow \( J(p,p+1) \) at location \( p \) of the excitation space as the net
number of stepwise excitation processes per unit time and plasma
volume i.e.

\[
J(p,p+1) = n_e \left[ n(p)K(p,p+1) - n(p+1)K(p+1,p) \right].
\]  

(8.19)

In the case of thermal equilibrium \( p \) and \( p+1 \) are populated according
to the Saha equation and by the principle of DL the stepflow \( J(p,p+1) \)
must be zero. This implies

\[
J^g(p,p+1) = 0 = n^g(p)K(p,p+1) - n^g(p+1)K(p+1,p).
\]  

(8.20)

With this, eq. (8.19) can be written as

\[
J(p,p+1) = n_0 n^g(p)K(p,p+1) (\delta b(p) - \delta b(p+1))
\]  

(8.21)

where we applied the relation (cf. eqs. (2.71-72))

\[
\delta b(p) = n(p)/n^g(p) - 1
\]

In a continuous description \( \delta b(p) - \delta b(p+1) \) can be expanded,
which gives

\[
\delta b(p) - \delta b(p+1) = -(\delta b(p)' + \delta b''(p) + \ldots)
\]  

(8.22)

The primes denote the derivative with respect to \( p \). Since the
relative overpopulation \( \delta b \) approaches zero for increasing \( p \) values,
we can neglect higher order derivatives for sufficiently high \( p \)
values. With

\[
K(p,p+1) = k_{p,p+1} p^{-2.4}
\]  

(8.23)
according to eq. (3.47) and the relation $g(p) = 2g_e p^2$ (cf. table 3.1; $g_e$ is the statistical weight of the core) the stepflow gets the form

$$J(p, p'^{+}) = -2n_e g_e Z^{-2} \eta^2(p) k_{p, p'^{+}p}^0 b'(p)$$  \hspace{1cm} (8.24a)$$

With this stepflow the bulk of the excitation flow $J(p)$ is determined and we suppose $J(p)$ to have a structure similar to (8.24a) and equals

$$J(p) = -2n_e g_e Z^{-2} \eta^2(p) k_p^0 b'(p)$$  \hspace{1cm} (8.24b)$$
in which $k_p$ contains also contributions from $\Delta p^{\pm}$ processes but as a consequence of the $\Delta p^k$ dependency of the excitation rate coefficients as reflected in eq. (5.47), we expect that $k_p$ is close to $k_p^0$. In comparison with $p^0 b'$ the weak dependence of the product $\eta^2(p) k_p^0$ can be neglected, the subscripts can be omitted and the l.h.s of eq. (8.18) can be written as

$$\text{div } J(p) = J'(p) = -2n_e g_e Z^{-2} \eta^2(p) b'(p)$$  \hspace{1cm} (8.25)$$

The ionization sink $I(p)$ can be found employing eq. (5.51) which gives

$$I(p) = n_e n(p) = 2n_e g_e Z^{-2} \eta^2(p) p^0 b(p)$$  \hspace{1cm} (8.26)$$
The recombination source $R(p)$ can be found by realizing that $R(p) = I(p)$ in equilibrium. By employing (8.26) for $b = 1$ we get

$$R(p) = 2n_e g_e Z^{-2} \eta^2(p) p^0$$  \hspace{1cm} (8.27)$$

Note that $R(p)$ is independent of the equilibrium departure factor $b(p)$, that $I(p)$ is proportional to $b(p)$ and that $J(p)$ is proportional to the derivative of $b(p)$.

The radiative part of the continuity equation (8.18) is given by

$$\text{CC} - D = n \sum_{u} n_u A(p, u) + \sum_{u, p} n_u A(u, p) - n(p) \sum_{u, p} \delta_{p, u} A(p, u)$$  \hspace{1cm} (8.28)$$

Applying eqs. (8.2) and (8.3) this can be written as

$$\text{CC} - D = n(p) \sum_{u} n_u^{-1} \left( \frac{1}{\text{E} n_p} - \frac{1}{\text{C}} \right) - b(p) = n(p) \sum_{u} n_u^{-1} \left( \frac{1}{\text{E} n_p} - \frac{1}{\text{C}} \right) - b(p)$$  \hspace{1cm} (8.29)$$
in which
\[ \tau_p = \left( \sum_{\nu = 1}^{\infty} \int_0^p A(p, \nu) \right)^{-1} \]
is the effective radiative lifetime. Together with the eqs. (8.23-27)
the continuity equation becomes
\[ n_e \frac{d^2}{dp^2} (p \delta b) + n_e \frac{d}{dp} (p \delta b) \left[ \frac{1}{3} \ln p - \frac{q}{z} \right] = \frac{d}{dp} \left[ \frac{\frac{d}{dp} (p \delta b)}{3 \ln p - \frac{q}{z}} \right]. \tag{8.30} \]

Putting the collisional terms left and the radiative terms right we obtain
\[ \frac{d}{dp} \left( \delta b \right) = \left( \frac{\frac{d}{dp} (p \delta b)}{3 \ln p - \frac{q}{z}} \right) \]
by which we arrived using the fact that \( \tilde{N}_e = 2 n_e \frac{d}{dp} \frac{d}{dp} \frac{\delta b}{\delta \nu} \tau_p \), where \( \tilde{N}_e \) is the number of collisions in a radiative lifetime. (cf. eq. (3.72)).

This equation has more or less the same structure as that given in (3.64) where it was solved by numerical integration for one single plasma condition typical for planetary nebulae.

We will not give a solution of eq. (8.22) but classify parts and shapes of the distribution function as predicted by this differential equation. First we realize that eq. (8.31) shows a competition between radiative and collisional processes. For value of \( \tilde{N}_e \ll 1 \) the lhs is not important and we have the solution
\[ \delta b = \frac{\frac{d}{dp} (p \delta b)}{3 \ln p - \frac{q}{z}} \tag{8.32} \]

which is the same as the CRC solution found in eq. (8.5). This is not surprising since \( \tilde{N}_e \ll 1 \) means that we are in the CRC domain. For values of \( \tilde{N}_e \gg 1 \) the rhs of (8.31) can be neglected and we get the differential equation
\[ p^2 \delta b'' + 6 p \delta b' - \frac{\frac{d}{dp} (p \delta b)}{3 \ln p - \frac{q}{z}} = 0 \tag{8.33} \]

Apart from the \( \delta b = 0 \) solution which reflects LTE we can write the solution of eq. (8.31) as
\[ \delta b(p) = b_0 (p)^{-\frac{q}{z}} \tag{8.34} \]

The value of \( b_0 \) is determined by the boundary condition at the low \( p \).
side, i.e. the boundary with CRC. For very hot systems this results in \( b_0 < 0 \) while for cold and intermediate hot systems the inequality \( h_0 > 0 \) holds.

Substitution of eq. (8.34) in (8.33) predicts that \( \lambda \) should satisfy the equation

\[
x^2 - 5x - \frac{8}{6} = 0
\]

(8.35)

with the solution

\[
x = 2.5(1 + \sqrt{1 + 0.16 \frac{8}{6}})
\]

(8.36)

The second mathematical solution \( x = 2.5(1 - \sqrt{1 + 0.16 \frac{8}{6}}) \) has no physical meaning. It predicts an explosion of \( \delta b \) as \( p \) increases and this violates the high \( p \) side boundary condition which demands that the equilibrium departure \( \delta b \) should approach zero for increasing \( p \) tending to infinity.

We stress the fact that the exponent depends only on the ratio (cf. eq. (5.33))

\[
\frac{\delta}{\kappa} = 17.7 \frac{\psi_0}{\psi_k}
\]

(8.37)

This parameter which we call the competition parameter expresses the competition between ionization and excitation. As expressed by eqs. (5.48), (5.52) and (8.37) the exponent has the following properties:

- It is not directly dependent on the charge number \( z \) and statistical weight of the core. Only a very weak dependency on \( z \) will be present due to the shape function \( \psi_0 \) and \( \psi_k \) but this is diminished by the factor 0.16. So provided that \( p \) is large enough, the distribution function is not dependent on atomic properties.

- If the excitation space is sink free, i.e. \( \epsilon/k = 0 \), we find \( \lambda = 5 \). The presence of a sink will result in a value \( \lambda > 5 \).

It should be realized that we did not make any assumption about the direction of the flow or the sign of the relative overpopulation \( \delta b \) so eq. (8.34) gives a result for both ionizing and recombining plasmas. This is related to the so-called complementary properties of the \( r^* \) and \( r^1 \) coefficients (cf. section 7.4) which states that in the limit of high \( \epsilon_k \) values the relation \( r^*(p) + r^1(p) = 1 \) holds, so if

\[
r^*(p) = 1 - b_0 \rho^{-\lambda}
\]

(8.38)

applies for recombining systems, we get

\[
r^1(p) = b_0 \rho^{-\lambda}
\]
for a comparable situation in ionizing systems.
In section 9.4 where we deal with ionizing systems we continue the
discussion of the value of the exponent.
As stated in the beginning of this section the ESB has to eliminate
the equilibrium departures caused in the adjacent quadrants II and IV.
As an example we discuss the connection between the CRC balance and
the ESB, i.e. the boundary between quadrant IV and I. To be more
specific we consider the intermediate hot CRC, that is a balance in
which the capture and cascade processes are not sufficient to retain
the equilibrium number of decay processes so that an underpopulation
will be present at the I/IV boundary. This underpopulation has to be
eliminated by the ESB with as a result a flow in downward direction.
The continuity equation
\[ \text{div } J = R - I + C - D \]
describes the behaviour of the flow. In the CRC domain, where
collisions are less effective than radiative processes this equation
predicts that \( C = D = 0 \) which gives a distribution function \( b = b_{0}^{CRC} \) as
described by eq. (8.5). If we enter quadrant I stepwise collisional
processes become important and tend to reduce \( b \) with as a final
goal that \( b = 0 \), i.e. \( R = I > 0 \). In the transition region between
the CRC balance on one side and the LTE on the other side, we get a
population density such that
\[ 0 < |b| < |b_{0}^{CRC}| \]  
(8.39)
holds. This means that \( C = D < 0 \) whereas \( R = I > 0 \). So, sources and sinks
tend to compensate each other resulting in
\[ \text{div } J = 0 \]  
(8.40)
which delivers
\[ b = 1 - b_{0}^{5} \]  
(8.41)
The competition between radiative and collisional sinks and sources
will be large at a boundary \( p_{\text{ir}}^{5} \) which we define such that the decay
rate equals the ionization rate, i.e.
\[ n_{e}G(p) = a_{e}^{5}p_{\text{ir}}^{2} \gamma z^{-2} = a_{e}^{5}p_{\text{ir}}^{2}(3 \ln p_{\text{ir}} - \zeta) \]  
(8.42)
Employing eq. (5.52) and (4.7) we get the boundary value

\[ P_{tr} = 2.86 \times 10^3 \; \frac{v_e}{a_e} \; e^{-0.15 \; \frac{v_e}{a_e} - 0.077}. \]  

(8.43)

Comparing this with the collisional radiative boundary \( P_{cr} \) we see that \( P_{tr} \) always lies in the ESR domain and that its position is higher if \( a_e \) is lower.

Results of extensive model calculation as presented in [E1970] are shown in the figs. (8.13a) and (8.13b). These calculations were effectuated for a case B hydrogen plasma as found in planetary nebulae and \( H^\prime \) regions. We selected two temperatures. In the same figs. we presented CRC solutions as given by the analytical formula eq. (8.8).

**Fig. 8.13**
The line factor for a \( H \)-plasma case B as a function of the proton \( P \) for two values of \( T_e \) and two values of \( n_e \) (in \( m^{-3} \)) obtained from [E1970].

The CRC pure \( b \)-values (dashed curves) are calculated with eq. (8.8).

**Fig. 8.14** The functions of Fig. 8.13 in the \( b \)-representation.
Figures 8.16a and 8.16b show the 6b representation of the same results in comparison with the slopes of \( p^{-5} \) and \( p^{-6} \) and the boundary values of \( P_{Cp} \) and \( P_{Pl} \) as predicted by our equations (7.18) and (8.43). From the figure we can deduce that:

- the position of the boundary \( P_{Cp} \) is correct.
- the pure CRC solution gives a good description for \( p < P_{Cp} \) so the presence of LTE in upper levels is not of influence.
- for \( P_{Cp} < p < P_{Pl} \) the slope of a sink free space, i.e. \( p^{-5} \) is present.
- for \( p > P_{Pl} \) the tendency to the steeper slope of \( p^{-6} \) can be observed.

Concluding we may state that these extensive model calculations, presented in a large variety of tables and graphs can also be described analytically by the following recipe which provides a three line approximation (cf. fig. 8.15):

- first determine for specific \( n \) and \( T \) values the position of \( P_{Cp} \).
- below this value the distribution function is given by the analytical expression eqs. (8.6).
- for \( p > P_{Cp} \) we can use \( b(p) = 1 - b_0 p^{-5} \) in which \( b_0 \) is determined by \( b(P_{Cp}) = 0 \).

8.7 Inversion and stimulated emission.

As we have seen in the preceding (cf. the figures 8.6 and 8.13) it appears that the distribution function in intermediate hot and cold systems shows inversion, i.e. the density of higher levels exceeds that of lower levels. We may expect that in particular a pronounced inversion will arise at the boundary level \( P_{Cp} \). At that boundary level the distribution function possesses a kinkpoint with a kink in upward direction.

The existence of inversion can effectuate stimulated emission which has to occur in nature if the CK models give the appropriate description. That was the conclusion of Coldberg in [COL 66] following the results of model calculation of Seaton which were initially presented to describe planetary nebulae. Since these nebulae are tenuous gases with very small densities, they are in spite of 'astronomical sizes' too small to give rise to substantial values of the optical depth. This implies that stimulated emission can not be
detected in these nebulae. But nowadays there is a lot of experimental evidence (cf. [Gor 80], [Sha 77]) that stimulated emission indeed exists in the radiofrequency spectrum of $H^0$ regions. These are astrophysical objects of extensive clouds (typical $10^{16} m$) in which young stars are embedded. Due to the low electron density and temperature the clouds will be in the CRC phase. And the incident radiation originated by the young stars can be amplified under appropriate conditions.

As we saw in section 2.6.2 the change of intensity of radiation as given in the slab approximation reads

$$\Delta I = \left( j \kappa - \frac{I_0}{b_0} \right) (1 - \exp(-\kappa l)). \quad (8.44)$$

In this equation the intensity of the external source is $I_0$ and the emissivity and the absorption coefficient of the cloud are given by $j$ and $\kappa$. This absorption coefficient plays an important role. It is related to the LTE value (cf. eq. (2.28a)) by

$$\kappa = \kappa_b (1) \beta_{ul}$$

where

$$\beta_{ul} = \left( \exp(hv/kT) - b(u)/b(l) \right) (\exp(hv/kT) - 1)^{-1}. \quad (8.45)$$

The $b(u)$ and $b(l)$ refer to the equilibrium departure of the upper and lower level respectively. If $b(u)/b(l) > 1$ (inversion) this results in negative values of $\beta$ and $\kappa$. Following eq. (8.44) this implies positive $\Delta I$-values, i.e. amplification of the background radiation.

In the figs. 8.16 calculations of $b(p)$ and $g$ as presented in [Sha 79] are reproduced. They show that the maximum of $g$ can be found at that $p$-value for which the relation $|b| = \frac{1}{2} |\beta_{CRC}|$ approximately holds. However there is still another criterion for the existence of stimulated emission. The optical depth depends also on the emission profile. In the discussion of the escape factor and optical depth of a transition as presented in section 2.6.2 we have seen that a Lorentzian profile with its large wings makes the optical depth extra small. Since the Lorentzian profile shape is effectuated by collision broadening, it can be expected that this limitation of the stimulated emission will occur at the boundary of $p_s$ for which $\beta = 1$. So the maximum of the probability for stimulated emission is lower than the optimum in the $g$ plot, and it is more in the neighbourhood of the
boundary $P_{cr}$ which can be calculated analytically. So if stimulated emission is present this selects the $P_{cr}$ level, which determines the electron density of the $\sigma$ region.

We see that the analytical approach of features related with CR models is rather successful. To stress this fact we regard the results of extensive calculations as presented in [FUR 79] in which conditions for inversion in laboratory plasmas are studied. Figure 8.17 shows under which condition inversion exists between lower levels. We added the values of $P_{cr}$ and give the following interpretation.
Fig. 8.17
Upper bounds of the electron temperature vs the electron density for various level pairs when an inversion is expected as presented in [PUR 79]. We added the critical densities $n_{c}(p)$ for the levels $p = 2, 3, 4$ and 5.

- Low $T_e$ values are favourable for inversion; this is already reflected in our simple representation of eq. (8.5) in which $\xi$ is presented as a function of $T_e$.
- The curves are rather flat in the left part of the fig. 8.17 which is related to the fact that the electron density has no influence on the shape of the distribution function in the CRC domain.
- The highest values, i.e. the peaks in fig. 8.17 occur at $p_{cr}$ for the upper level. For instance we can expect inversion between the levels 4 and 5 if level 5 enters ESB. That is not surprising as we have seen in the preceding that $p_{cr}$ represents the knee point in the distribution function. And coming from cold or medium hot CRC to ESB (i.e. from low to high $n_{e}$-values in fig. 8.17) this knee point induces a kink in upward direction.
- The fact that the range of $T_e$ for which inversion can occur is limited can be seen as a consequence of the fact that very hot CRC does not imply inversion (cf. fig. 8.3). This maximum $T_e$-value in fig. 8.17 is of the same order of magnitude as that of the pseudo $T_e$ value of Baker and Mansell (16 eV in fig. 8.17 and 19 eV in fig. 8.4).

All these conclusions are possible in the frame work of our analytical CRC analysis. To draw these conclusions with the help of numerical calculation is far more difficult. The tremendous amount of formulas, tables and graphs are not suitable to get insight in elementary structures.

We conclude that the analytical approach supported by numerical calculations provides a good understanding of the distribution function.
Chapter IX  Ionizing plasmas

9.1 Introduction
This chapter is devoted to the distribution function of purely ionizing plasmas and deals with the properties of the $r'(p)$ coefficient.
Features of the distribution function will be studied in relation with underlying balances.

The domains of the balances are shown in adjacent figure. The study will proceed along the clockwise curve as indicated in the adjacent domain plane where section numbers and keywords are shown.

9.2 The domain of the corona balance
9.2.1 General
In ionizing systems the lower part of the domain plane is governed by the corona balance. If we compare this balance

$$ n(p) \int \varphi_A(p,l) = \sum_{\nu} n_{\nu} K(1,p) + \sum_{\nu} n(\nu) A(u,p) $$

(9.1)

with the other improper balances, we see that the production and destruction are of a completely different character. The production is (mainly) collisional and the destruction is radiative. In this respect the corona balance is the most improper balance.
As we will see this remarkable character results in two main features - there is no obvious boundary between cold and hot corona - the shape of the distribution function is strongly dependent on the atomic structure, i.e. on the quantum defect.

In the study of the features of the corona domain it is useful to distinguish between (cf. section 2.6.3)
Case A: transparency for all radiation and
Case B: transparency except for resonant radiation.
We first consider case A
9.2.2 Transparent corona

By relating the population density to that according to Saha we divide eq. (9.1) by \( n^2(p) \) which results in

\[
b(p) = \frac{1}{a(n)} \frac{b(0)}{A(0)} + \frac{1}{n^2} \int b(u)n^2(u)A(u,p) \, du \frac{n^2(0)}{A(0)} \tag{9.2}
\]

in which we used the principle of DB in \( n^2(p) = n^2(p)K(p,1) \) and the notation \( b(0)A(0) = A(p) \). Equation (9.2) is the \( n=0 \) limit of the general structure of \( r'(p) \). The general structure of \( r'(p) \) is given in eq. (6.34b).

The first term in eq. (9.2) is the leading term. It describes the production direct from the ground state. The second term reflects the cascade coming from higher levels. But it is also a contribution from the groundstate (via higher levels). This cascade contribution can be estimated by assuming that the \( b(u) \)-values are comparable with \( b(p) \).

In section 4.6 we studied the cascade contribution and found that (cf. eqs. (4.22) and (4.24))

\[
\int_{0}^{u} n^2(u)A(u,p) \, du \approx \frac{1}{3} n^2(p)A(p) \tag{9.3a}
\]

Fig. 9.1

The contributions of the various processes to the a) production and b) destruction of the level \( p = 5 \) are functions of \( n_0 \). The hatched areas correspond to radiative transitions. Results of model calculations are presented in [TJU 79a].
\[ E \cdot b(u)n_e^6(u)A(\nu, p) \propto \frac{1}{3} b(p) \cdot n_e^2(p) A(p) \quad (9.3b) \]

Since \( b(u) \) is a decreasing function of \( u \) this 30\% contribution ascribed to cascade is an overestimation. By analysis of an extensive CR model calculation it was found in [Fuj 79a] (cf. fig. 9.1) that 20\% of the level production is due to cascade, a percentage which is nearly independent of \( T_e \).

The leading processes of the coronal balance are depicted in the adjacent vignette

\[ \text{Eq. (9.2) shows the following properties:} \]

- The \( b(p) \) factor is proportional to \( n_e \).
- and proportional to the groundstate overpopulation \( b(1) \).
- Since \( K(p, l) \) is a deexcitation rate, \( b(p) \) is only a weak function of the electron temperature.

We will study the leading term in more detail for hydrogenic systems.

By employing the principle of detailed balancing (DB) we find that the deexcitation rate equals (cf. eq. (3.44))

\[ K(p, l) = \text{Rate}(T_e) A_{lp} \Phi(1, p; T_e) g(1)/g(p) \quad (9.4) \]

in which \( \text{Rate}(T_e) \) is defined by eq. (5.40), \( \Phi \) represents a shape factor which depends on the shape of the cross section and \( A_{lp} = 2\pi r_p E_{lp}^{-1} \) (cf. eq. (5.24)). By employing the analytical formula of the oscillator strength as given in eq. (3.20) we find that

\[ A_{lp} = 3.8 \cdot 10^{-3} \cdot n_e^6 \quad (9.5) \]

in which \( \gamma = E_{lp}/|E_1| \) and \( E_1 = 2\pi \gamma \). For the total decay rate we use an analytical representation based on the eq. (4.7) which is given by

\[ A(p) = 1.6 \cdot 10^{10} \cdot n_e^{-4.5} \quad (9.6) \]

So we find the \( r^l(p) = b(p)/b_1 \) coefficient to be

\[ r^l(p) \propto \frac{n_e^6 K(p, l)}{A(p)} = 3.8 \cdot 10^{-23} \cdot n_e^{-6} \cdot \Phi(1, p; T_e) \quad (9.7) \]

In the case of the hydrogen atom (Z=1) we can use the shape function according to [DRa 77] which was discussed in section 5.12 and given in fig. 9.2. For the temperature range \( 0.4 \leq T_e \leq 400 \text{eV} \) we can employ the
\( \psi = 0.6 \times 0.5 = 0.6 \times 0.5 \times 0.5 \times 0.5 \)

By inserting this formula in equation (9.6) and multiplying the result with 1.2 (cascade contribution) we find that

\[ r^1(p) = 7 \times 10^{-24} n_e^{-0.5} \times 0.5 \quad (9.8) \]

In fig. 9.3 we compared this analytical formula with results of numerical CR calculation of [DRA 77] from which we may conclude that

- there is not much difference between the distribution function obtained in [DRA 77] and our analytical approximation based on the same cross sections,
- the temperature dependency is rather limited,
- for \( p > 5 \) the dependency as predicted in [FJ 79a] can be found back.

\[ 10^4 \times 10^5 \]

\( r^1(p) \) coefficient as obtained by the analytical eq. (9.8) (solid curve) and numerical results of [DRA 77] for several values of \( T_e \).
The fact that \( r^1(p) \) is more or less constant over a large \( T \) range implies that the determination of the electron temperature must be possible since

\[
\alpha(p) = r^1(p) \beta(p) \eta_0(p)
\]

and \( \eta_0(p) \) contains the Boltzmann factor. However there are limitations of this technique:
- Absorption of radiation may not exist.
- The electron density should be not too high. Otherwise corona is replaced by the excitation saturation balance.
- The electron (ion) density should not be too low. In the range \( n_e < n_e^{*}(p) \) the atomic states of a level are not equally populated and the structure of the \( K \) and \( A \) rates are more complex (cf. section 2.4.4).
- Since the corona balance dominates in the lower part of the energy scheme it will be sensitive to atomic properties. Due to the quantum deficiency states with the same pm but different orbit quantum number do generally not have the same energy.

### 9.2.3 Corona case B

In case B all resonant radiation will be absorbed while the plasma is transparent for all other bound-bound transitions. So we are faced with a special situation in which the transition \( 1 \rightarrow 2 \) is completely collisional while transitions between (lower) excited states are both collisional and radiative of character. This particular domain presented as a radiative domain perturbed by (stepwise) collisions can also be regarded as a collisional domain with radiative obstruction (cf. 9.4).

Since the excitation to the first excited state \( p=2 \) is not compensated by (effective) radiative decay, the level density will increase, i.e. it moves towards the Boltzmann value which belongs to the balance

\[
A_1 + e \rightarrow (2_{1,2}) \rightarrow A_2 + e
\]

If the temperature is so high that \( T_{\text{e}}(2) > T \), excitation to \( 1 \) higher levels is more likely than the deexcitation back to the groundstate and stepwise processes will dominate. This leads to a so-called ladder climbing process in the excitation space.
In order to understand the main features of the distribution function we first recall the situation in which radiative decay can be neglected. Following the technique given in section 8.6 we define the step flow as

$$J(p,p+1) = n_e n_e(p) K(p,p+1) - n_e n_e(p+1) K(p+1,p), \quad (9.11)$$

which applying the principle of GB can be written as

$$J(p,p+1) = n_e n_e(p) K(p,p+1) (b(p) - b(p+1)). \quad (9.12)$$

By equating $b(p+1) - b(p) = b'(p)$, the derivative of $b$, we get

$$J(p,p+1) = -n_e n_e(p) K(p,p+1) b'(p). \quad (9.13)$$

So, in order to generate a flow in upward direction a decrease of $b$ with increasing $p$, i.e., $b' < 0$, is needed. The larger the flow the steeper $b$ should be.

In the case of corona we have a downward radiative decay which obstructs the ladder climbing flow. So if the excitation flow is suppressed to the system due to opacity (there is no radiative way back to the ground state) the decrease as function of $p$ will be extra large.

The global features of the distribution function can be studied by the one step approximation presented in [BIE 79]. This model is based on the assumptions that

- the flow is constant in the excitation space
- ionization can be neglected
- radiative decay processes can be treated in a stepwise manner.

So the stepwise flow across the fictitious intersection between $p$ and $p+1$ will be

$$J(p,p+1) = n_e n_e(p) K(p,p+1) [b(p) - b(p+1)(1 + \lambda(p,p+1))]. \quad (9.14)$$

In the same way we can relate $b(2)$ to $b(3)$, $b(3)$ to $b(4)$ etc., i.e., calculate the distribution function. For more details of this approach we refer to [BIE 79].

To understand the main features of the distribution function we consider two limiting cases.

First the situation for which $A(p+1,p) \gg n_e K(p+1,p)$, i.e., radiative processes are by far dominant. In that case we may write eq. (9.14) as
\[
0 \approx \frac{J(p,p+1)}{b(p) n^R(p) K(p,p+1)} = 1 - \frac{b(p+1)}{b(p)} (1 + \frac{A(p+1,p)}{n_e K(p+1,p)}) ,
\]

which expresses that the flow can be seen as a small difference between two large terms. This gives

\[
b(p+1) = \frac{b(p)}{1 + \frac{A(p+1,p)}{n_e K(p+1,p)}} ,
\]
a very steep function. In the case of \(A(p+1,p) \ll n_e K(p+1,p)\) we get

\[
J(p,p+1) = -n_e n^R(p,p+1) \delta b'(p)
\]

Since \(J(p,p+1)\) is supposed to be independent of \(p\) and \(n^R(p,p+1)\) scales with \(p^6\) this results in

\[
\delta b = p^{-5}
\]

And this is the same result as that of the solution of the continuity equation for a sink free excitation space as discussed in section 8.6. If ionization is taken into account we find \(\delta b = p^{-3}\) (cf. section 9.3.2). The actual distribution function has to describe a continuous transition from the limiting case as reflected by eq. (9.16) to a \(p^{-6}\) -dependency. It has a knee point at the same \(p_{cr}\) -value as the case A would have. This is outlined in fig. 9.4.

**Fig. 9.4.** A comparison between the distribution function and underlying balances for case A and case B
due to opacity (case B) the excitation 1+2 will not be balanced by radiative decay 2+1 and a flow in the excitation space is needed to remove the population of level 2. Since collisional transitions are obstructed by backward radiative processes, the slope of the distribution function must be extra large to make the steeper collisional flow possible.
9.3 The excitation saturation balance in ionizing systems.

In the upper half plane we meet with domains where electron collisions occur more than once in a radiative lifetime.

The distribution function of ionizing systems can be described by the $r^1$ value. Since both production and destruction are both collisional and proportional to $n_e$, the $r^1$ coefficient will be $n_e$ independent.

In the study of the main features of these population coefficients we have seen that in the $n_e^+$ limit the $r$ coefficients are complementary, that is

$$r^+(p) + r^1(p) = 1.$$  \hspace{1cm} (9.19)

So all information obtained in the study of the $r^+$ coefficient (section 8.5 and 8.6) can now be used to understand the $r^1$ coefficient.

9.3.1 The cold excitation saturation balance

In the study of the cold recombining ESR we have seen that $r^+$ is a rapid decreasing function of $p$. So descending the system and crossing the bottleneck $r^+$ approaches zero rapidly (cf. section 8.5).

So the ionizing complement

$$r^1(p) = 1 - r^+(p),$$  \hspace{1cm} (9.20)

will approach unity for decreasing $p$ values. This means that

$$b(p) = b(1)$$  \hspace{1cm} (9.21)

i.e. the lower part of the system will be populated according to Boltzmann. In a more direct approach this can be understood by realizing that the balance

$$A_1 + e + (E_{12}) \rightarrow A_2 + e$$  \hspace{1cm} (9.22)

is not much disturbed by other processes.

Demotion back to the groundstate is more likely than excitation $2 \rightarrow 3$, so the balance will be in equilibrium which implies that the level 2 is in Boltzmann equilibrium with the groundstate. Here we are faced with a particular situation in which two levels are in Boltzmann relation with each other but not in equilibrium with the continuum, i.e. not populated according to Saha.
9.3.2 The hot ionizing excitation saturation balance

In the hot ESB of recombining systems we found that the power law

\[ n^*(p) = 1 - b_0 p^{-k} \quad (9.23) \]

gives a good description of the distribution function.

The underlying improper balance is depicted in the adjacent vignette. Production is realized by deexcitation of the adjacent upper level and destruction consists of deexcitation to the adjacent lower level. Since the \( \tau^i(p) \) is complementary we find that

\[ \tau^i(p) = b_0 p^{-k} \quad \text{or} \quad \dot{\delta} b(p) = b_0 \delta b p^{-k} \quad (9.24a) \]

The vignette shows the production/destruction balance. It is the complement of the \( \tau^a \) vignette. Applying eq. (9.24a) and recalling that\( b(p) = \tau^a(p) + \tau^i(p) b(i) = \gamma(p)/n^a(p) \)
(cf. section 6.7) we can write the distribution function as

\[ n(p) = n^a(p) + n^i(p) b_0 \delta b p^{-k} \quad (9.24b) \]

which shows that the population density can be regarded as a superposition of an equilibrium value and an overpopulation. This overpopulation of the level \( p \) is a result of the overpopulation of the ground state \( \delta b \) which is distributed over the levels as a result of the stepwise excitation flow.

The value of \( k \) can be found (cf. eq. (8.36)) from

\[ k = 2.5(1 + \sqrt{1 + 0.16 s/k}) \quad (9.25) \]

in which the competition parameter \( s/k \) expresses the importance of the ionization sink with respect to the excitation flow. We recall that atomic properties such as the charge number and the statistical weight of the core are eliminated in the ratio \( s/k \) which suggests that \( k \) is independent of the atomic structure.

A particular value was found to be that of \( k=3 \), it corresponds to a sink free excitation space.

By inserting \( s \) and \( k \) values as found by semi empirical approximations, \( s=6 \) appears to be a good value in the description of the distribution function of ionizing systems. Figure 9.3 shows that this is indeed
observed in a lot of experimental situations. In section 9.3 we will pay attention to the fundamental meaning of this value $x=6$.

Fig. 9.3

The population density $\chi(p)$ of excited states as a function of the effective parameter $p$. The quantity $\chi(p) = n(p) \exp(-c_p)$ is proportional to $b(p)$ which is nearly equivalent to $b(p)$ if $b(p) \gg 1$. Note the slope of $p^{-6}$.

Experiments: Na from [XIE 78], He from [XCW 78] and Ar from [MUL 80].

9.4 Flow sink and sources in hot ionizing systems

Much can be learned from an analytical study of the flow, sinks and sources in the excitation space.

In section 9.6 it was shown how the power law was obtained from the solution of the continuity equation in the excitation space

$$\text{div } \mathbf{J} = R - I + CC - D$$

(9.26)

in which $\mathbf{J}$ is the excitation flow based on the stepwise excitation processes. $R$ the recombination source, $I$ the ionization sink, $CC$ the capture cascade source and $D$ the sink caused by the decay processes. The last two terms, which are radiative, can be neglected provided that we are so high in the energy scheme that ionization and recombination dominate over decay. This is the case if $p > p_{ix}$ in which the boundary level $p_{ix}$ is given by eq.(8.43). In ionizing mediums with $n_e = 10^{19}$ m$^{-3}$ we find that $p = 3$ which is rather low in the system. For these collisionally dominated domains the continuity equation can be simplified to
\[ \text{div } J = R - 1 \quad (9.27) \]

The functional dependence of \( J, R \) and \( I \) which were given in eqs. (8.24), (8.26) and (8.27) are reproduced here

\[
J(p) = -2n_e \sigma_n Z^{-2} n^2(p) \mu_e \sigma_n^2 b(p) \quad (9.28a)
\]

\[
I(p) = 2n_e \sigma_n Z^{-2} n^2(p) \mu_e \sigma_n^2 b(p) \quad (9.28b)
\]

\[
R(p) = 2n_e \sigma_n Z^{-2} n^2(p) \mu_e \sigma_n^2 \quad (9.28c)
\]

After inserting \( b(p) = 1 + b_0 b_1 p^{-\delta} \) in eqs. (9.28) we get

\[
J(p) = 12n_e \sigma_n Z^{-2} n^2(p) \mu_e \sigma_n^2 b_0 b_1 p^{-1} \quad (9.29a)
\]

\[
I(p) = 2n_e \sigma_n Z^{-2} n^2(p) \mu_e \sigma_n^2 (1 + b_0 b_1 p^{-\delta}) = R(p) + I^{\text{net}}(p) \quad (9.29b)
\]

\[
R(p) = 2n_e \sigma_n Z^{-2} n^2(p) \mu_e \sigma_n^2 \quad (9.29c)
\]

**Fig. 9.6.**

A comparison between the flow \( J \), sink \( I \) and source \( R \) in a hot, ionizing excitation space according to eq. (9.29), for several values of \( n_e \), in hydrogen.

Also shown is \( I^{\text{net}} \).
in fig. 9.6 the flow, sink and source are compared with each other. We used the approximations \( \frac{d}{dp} \eta_{S}(p) \approx \frac{d}{dp} \eta_{S}(p) \approx 0 \) and \( x=6 \) which corresponds with \( x=6 \). From the eqns. (9.29) and fig. 9.6 the following conclusions can be drawn:

- The ionization sink consists of two parts: the detailed balanced part of \( \eta \) and the net ionization \( \eta_{\text{net}}(p) \) which results from the ionization of the overpopulation.
- The net ionization is positive for every value of \( p \). This is in agreement with the fact that we are dealing with an ionizing plasma.
- For every value of \( p \) the excitation flow \( J \) is larger than the net ionization sink. Moreover \( J \) is a slower decaying function of \( p \) than \( \eta \) (\( p^{-1} \) instead of \( p^{-2} \)). But the net ionization is inexorable: once being ionized the history of the electron in the excitation space is finished. The decrease of the excitation flow as a function of \( p \) is due to the disappearance of the electrons out of the excitation space. The change in the flow is

\[
\Delta J = - \int \eta_{\text{net}} \, dp
\]  

which in fact is an integral representation of the continuity equation.

- The intersection of \( \eta_{\text{net}} \) and \( \eta \) can be used to define the boundary between the domain of the ESB and PTE. In this boundary level denoted by \( p_{0} \) where the overpopulation equals the Saha density, i.e., \( \mathfrak{b}(p_{0})=2 \). It can be seen in fig. 9.6 that while the ionization sink changes dramatically at the advent of PTE, the excitation flow is not influenced by the degree at which PTE is established. Even far in the PTE for instance at the level with \( 10 \) overpopulation, i.e., \( b=1.01 \), the excitation flow is only reduced by a factor 2. The small surplus over Saha is mainly removed stepwise. This fact is used in our cut-off procedure as presented in section 6.5. By an analytical treatment the excitation flow was kept to its unattenuated value.

- The total ionization coefficient (cf. sections 6.7, 6.8 and 7.3) can be calculated in an analytical way. We have to distinguish between two cases.

If the lower part of the system is not completely dominated by the ESB and the plasma is transparent we get for the total (or effective) ionization

\[
\eta_{e}^{S} - \eta_{e}^{S} \approx \eta_{\text{net}} + J(p_{\text{cr}})
\]  

(9.31)
in which \( p_{\text{cr}} \) is the collisional/radiative boundary level, i.e. the boundary between corona and ESB. This equation is based on the fact that transparent corona is 'closed' for the excitation flow. If saturation is complete, i.e. the whole system is collisional, we get the relation

\[ n_{\text{e}}^0 n_{\text{cr}}^0 - n_{\text{e}}^0 n_{\text{cr}}^+ = I_{\text{net}} - J_{\text{e}} \tag{9.32} \]

which also applies for corona case B (cf. section 9.2.3).

9.5 On the fundamental meaning of the power law

The function \( \delta_0 = b_0 \delta b_0 \delta p \) is found as a result of experiments (cf. fig. 9.5) of numerical CR models (cf. [FUJ 79b]), and of the solution of the continuity equation in excitation space.

But there is more; it can be shown that this power law has a fundamental meaning (cf. [MUL 83] and [SIL 84]). For that purpose we write the distribution in the \( E \) representation, such that

\[ f(E) dE = n(p) g(p) dp \tag{9.33} \]

represents the number of bound electrons with energy between \( E \) and \( E + dE \). Using \( g(p) = 2 g_p^2 \) and \( E = -\text{Ry} \delta_p^2 \) the distribution function \( 1 + b_0 \delta b_0 \delta p \) can be transformed into

\[ f(E) = g_n \delta^g |E|^{-5/2} (\text{Ry} \delta^2)^{3/2} + g_n b_0 \delta b_0 n^g |E|^{1/2} (\text{Ry} \delta^2)^{-3/2} \tag{9.34} \]

\[ f^6 \]

\[ \delta^g \]

in which \( f^6 \) represent the equilibrium value according to Saha, and \( \delta^g \) the overpopulation.

It is remarkable that this overpopulation has the same energy dependence as that of the Maxwell distribution of free electrons (cf. eq. (2.24) where \( f(E) \) scales with \( |E|^{1/2} \)). This surprising result can be understood by noting that in the ESB the interaction between bound and free electrons occurs more frequently than typical atomic events like radiative decay. And in the study of hot electron-atom collisions as presented in chapter V it appeared that there is no substantial difference between the energy transfer from a free to a bound electron on one hand and the energy transfer between two free electrons on the other hand. Apparently, the frequent e-e interactions result in the fact that the energy distribution of free electrons is imposed on the overpopulated bound electrons.
The Fokker-Planck equation

In the last section we have seen that the power law $\Delta b \propto p^{-6}$, obtained by an analytical approximation, gives a good description of both numerical and experimental results. Moreover, in the $E$-representation a fundamental meaning becomes visible. We recall that this power law was obtained by solving of a continuity equation for the excitation space (section 8.6) which, in a differential way, describes a discrete space. Especially in the $p$-representation this approach is questionable since the discreteness remains unchanged, the smallest step remains $\Delta p = 1$ for increasing $p$. Now we are faced with the question if it is possible to get the bound Maxwell distribution directly from the continuity equation in the $E$-representation. In this representation the excitation space becomes more and more continuum-like approaching the continuum since $\Delta E \propto p^{-3}$ decreases with increasing $p$. So the $E$-representation of the problem seems to be more appropriate for a continuity equation. For this purpose we use the Fokker-Planck formalism which describes the course of a particle in a sink-free space.

The probability that the particle is between $E$ and $E+\Delta E$ at time $t$ is given by $P(E,t) \ \Delta E$. At the time $t+\Delta t$ this probability function will be

$$P(E,t+\Delta t) = \int_{-\infty}^{E} P(E-\Delta E, t) \ P(E-\Delta E, \Delta E) \ \Delta E \quad (9.35)$$

in which $P(E-\Delta E, \Delta E)$ is the probability that the particle initially with energy $E-\Delta E$ reaches $E$ in the duration $\Delta t$. This function should obey the relations

$$\int_{-\infty}^{E} P(E-\Delta E, \Delta E) \ \Delta E = 0 \ \text{and} \ \frac{\partial P}{\partial t} = 0 . \quad (9.36)$$

The latter reflects that we deal with a Markoff process. This means that the event which happens at time $t$ is independent of the particle's history. By expanding $P(E-\Delta E, \Delta E)$ and $P(E-\Delta E, t)$ in powers of $\Delta E$ and $P(E,t+\Delta t)$ in powers of $\Delta t$ it can be found that

$$\frac{\partial P}{\partial t} = \frac{1}{2} \frac{\partial^2}{\partial E^2} \left( P \ <\Delta E^2> \right) + \frac{1}{2} \frac{\partial^2}{\partial E \partial \Delta E} \left( P \ <\Delta E > \right) \quad (9.37)$$

in which terms of $O(\Delta E^3)$ and $O(\Delta E^4)$ are neglected.

We will use eq. (9.37) in the quasi steady state (QSS) description of the excitation space in the following way
- Instead of the probability 'history' of one particle we apply eq. (9.37) to the energy distribution of the bound electrons \( f(E) \).
- The lhs can be neglected (QHS).
- In the limit of \( \Delta t \to 0 \) the rhs of eq. (9.37) can be regarded as
  \[
  J(E) = f(E) - \frac{1}{2} \frac{\partial}{\partial E} f(\Delta E^2). 
  \]  
  (9.38)

The mean energy supply to the bound electron per unit time is denoted by \( \langle \Delta E \rangle \) and the change of the mean square of the energy per unit time is denoted by \( \langle \Delta^2 E \rangle \).
- The excitation space contains sinks and sources which have to be added to the Fokker-Planck equation. For the ionization sink we can write
  \[
  I(E) = I(p) \frac{d \rho}{dE} = n_e f(E) Ry \frac{\partial}{\partial E} |E|^{-1} \]  
  (9.39)

in which \( I(p) \) is defined by eqs. (5.51) and \( p^2 = \frac{Z^2 Ry}{|E|} \). Using the principle of DB this provides the recombination source \( R(E) \) if \( f \) is substituted by \( f^R(p) \), the energy distribution function according to Saha (cf. eq. 9.34).

The energy gain of a bound electron due to stepwise transitions is discussed in chapter V (cf. eq. 5.43). We have seen that
  \[
  \langle \Delta E \rangle = n_e \sum K(p,q) E_{pq} = n_e \frac{\partial}{\partial E} |E| \]  
  (9.40)

which was possible using the sum rule (3.17) and eq. (5.43). The square of the energy gain per unit time is given by
  \[
  \langle \Delta^2 E \rangle = n_e \sum K(p,q) \frac{\partial^2}{\partial p \partial q} |E| = \frac{1}{3} n_e \frac{\partial}{\partial E} |E| \]  
  (9.41)

in which sum rule (3.19) was used. The continuity equation
  \[
  \frac{dJ}{dE} = I(E) - R(E) \]  
  (9.42)

can now be written as
  \[
  n_e \frac{\partial}{\partial E} \left( \frac{7/3 f'}{2/3 f'' |E|} \right) = n_e \frac{\partial}{\partial E} f(E) |E|^{-1} (f - \frac{\partial}{\partial E} |E|) \]  
  (9.43)

in which we neglected the terms which result from the \( E \)-dependence of \( \frac{\partial}{\partial E} |E| \). The primes denote differentiation with respect to \( E \).
substituting $f = f^0 + \delta f$ we find that

$$\left(\frac{7}{3} f^0 - \frac{2}{3} v^0 |E| + \left(\frac{7}{3} f^1 - \frac{2}{3} v^1 |E|\right) = \frac{n \eta}{\beta} \delta f |E|^{-1} \right) \tag{9.44}$$

The Saha distribution $f^0(E)$ which scales with $|E|^{-1/2}$ (cf eq. 9.33) is indeed a solution of this equation ($\delta f = 0$ and $\exp(|E|/\beta)$ is put equal to unity). The overpopulation with the Maxwellian form scaling with $|E|^{1/2}$ is a solution provided that $\eta \beta = 1$.

The limitations of this technique are determined by the cut-off in the expansion of eq.(9.37), the problem of the proper transition from step to jump processes (cf. fig. 9.7) and the exact behaviour of the rate of the collisional transition. These problems are related to each other. In the treatment of the cross section we have seen that rates of all jump processes can be put together in what we call the rate for the 'leap from $p\rightarrow p+1$. With the sum rules we can take step processes together in what we call the local activity.

The question of the boundary between leap and local deserves further study.

---

**Fig. 9.7**

A flow which comes in at a level $p$ can partially skip $p+1$, going directly to $p+2$. So the level $p+1$ is missing some population 'input', but this is (partially) compensated by the skip process $p+1 \rightarrow p$. In the same way the process $p+2 \rightarrow p+3$ is (partially) compensated by the process $p+2 \rightarrow p$ etc.

With the factorization treatment all the stepwise processes $(\Delta p \lesssim p)$ can be lumped together in the 'local flow' $J(E)$. All jump processes to destinations far enough can be lumped in the 'leap sink' $J^*(E) \rightarrow E = 0$. The boundary where the local flow ends and the leap sink begins is subject to further study.
X. Experimental results from an Argon plasma

10.1 Introduction
In the preceding we presented a systematic treatment of collisional radiative balances and classified the main features of the distribution functions in relation with the underlying balances. This chapter can be seen as an illustration in which experimental results of an ionizing argon plasma will be compared with the proposed systematics.

It is based on the results on Ar I and Ar II, as obtained in the Eindhoven hollow cathode arc for which detailed information is available on densities, temperatures and transport phenomena of the plasma. Besides the evaluation of Ar I and Ar II systems using the traditional numerical CR approach is one of the best developed ones. Moreover it is interesting to make a comparison between two systems, Ar I and Ar II, of the same element in the same plasma. It can be seen that there are large differences. The Ar I system is ionizing and the excitation saturation balance dominates the main part of the system whereas a large part of the Ar II bottom is still globally in the corona domain. We will see that the Ar I system can be treated in a hydrogenic way, while this approach fails completely for the Ar II system, a system which is very complicated. Metastable and resonant levels with very short lifetimes are next to each other. But the energy spacing is not so small that levels are statistically distributed. This capriciousness of the Ar II system can be regarded as essential for the possibility of the construction of an Ar II laser.

10.2 Experiment and diagnostics
In Fig. 10.1 the experiment is shown schematically. A magnetized arc is formed between a hollow, self heated cathode and a flat anode. The axial magnetic field can be varied between 0.05 and 0.5 T. The filling pressure is typically 10⁻² - 1 Pa argon, the flow 1-10 cc NTP/s, and the plasma current 10-250 A. The cathode can be moved axially and laterally, so that the plasma can be moved through the optical systems. This is of particular interest in scattering and fluorescence experiments.

Typical values for plasma parameters are summarized in table 1. For further details we refer to published data [POT 79] and [YOG 84].
Diagnostics which are relevant to the present experiment are:

- Thomson scattering: \( n_e, T_e \) electron density and temperature.
- Fabry-Perot line analysis: \( T_i, T_n \) ion- and neutral temperature
- Spectroscopy: \( n_e(p), n_i(p) \) (absolute densities)
- Fluorescence: \( n_e(p), n_i(p) \) for non-radiative states

- Ar II laser lines
- Dye laser: 3d' - 4p'

**FIG. 10.1**

Sketch of the hollow cathode discharge. TS = Thomson scattering diagnostic, OS = optical spectroscopy, FI = Fabry-Perot interferometry, OP = optical probes, CS = collective scattering diagnostic, Fl. = fluorescence experiments.

**Table 1. A review of data of the hollow cathode discharge.**

<table>
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<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
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<tr>
<td>( n_e = n_i )</td>
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</tr>
<tr>
<td>( n_p )</td>
<td>neutral particle density</td>
</tr>
<tr>
<td>( T_e )</td>
<td>electron temperature</td>
</tr>
<tr>
<td>( T_i )</td>
<td>ion temperature</td>
</tr>
<tr>
<td>( T_n )</td>
<td>neutral particle temperature</td>
</tr>
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<td>( B_z )</td>
<td>magnetic field</td>
</tr>
<tr>
<td>( I_{pl} )</td>
<td>plasma current</td>
</tr>
<tr>
<td>( V_{sc} )</td>
<td>anode-cathode voltage</td>
</tr>
<tr>
<td>( p_n )</td>
<td>pressure</td>
</tr>
<tr>
<td>( G )</td>
<td>gas flow</td>
</tr>
<tr>
<td>( L_{pl} )</td>
<td>length plasma column</td>
</tr>
<tr>
<td>( R_{pl} )</td>
<td>radius plasma column</td>
</tr>
<tr>
<td>( d_c )</td>
<td>cathode inner diameter</td>
</tr>
</tbody>
</table>
10.3 Results on Ar I population densities

The atomic energy system of Ar I is shown in Fig. 10.2 in which a distinction is made between the $2p_{3/2}$ and $2p_{1/2}$ core. It is interesting to compare this representation of the Ar I system with that presented in Fig. 3.1. Fig. 10.2 shows the excitation energy, i.e., the energy distance from the ground- to excited states whereas Fig. 3.1 shows the ionization potential $|E_p|$ of the levels, i.e., the kinetic energy of the outer electron. The difference between the representations originates from the fact that the $3/2$ and $1/2$ core have different ionization potentials (cf. Fig. 10.2). A study of the radiative decay processes from the $4p$-$4s$ lines shows that in about 10% of these transitions a change in core takes place. So it may be expected that electron collisions will also induce core-change transitions. It is a somewhat open matter whether this electronic coupling between the two core systems is sufficient to ignore the distinction between the different cores. Especially for the lower excited levels it is
expected that the coupling between the cores due to electron collisions is very effective. For higher levels, for which quantum deficiency is relatively unimportant (cf. section 3.1 and fig 3.2) and a hydrogenic description must be possible, we expect that the different cores represent disjunct excitation channels. The change in core of \$\Lambda \Gamma \Gamma \$ is magnetic of character (change in spin) and in section 2.4.2 we have seen that these processes are only important for large threshold transitions i.e. \$E_{1g}/kT \gg 1\$. Moreover it has to be realized, that the geometrical cross section of the outer electron scales with \$p\$ while the size of the core remains constant. So we arrive at the concept that the different cores can be seen as two excitation channels which are probably communicating in the bottom but disjunct in the top.

In Fig. 10.3 the experimental values of the equilibrium departure factor \$b(p)\$ is given as a function of the ionization potential \$|E_p|\$.

The major difference between these conditions is \$n_e\$ as indicated in the caption of the figure.

**Fig. 10.3**

The equilibrium departure \$b(p)\$ of \$\Lambda \Gamma \Gamma \$ levels as a function of the ionization energy for several electron densities.

- \$n_e = 1.6 \times 10^{19} \text{ m}^{-3}\$
- \$n_e = 6.7 \times 10^{19} \text{ m}^{-3}\$
- \$n_e = 1.6 \times 10^{20} \text{ m}^{-3}\$

\$T_e = 3-6 \text{ eV}\$
Fig. 10.4 shows the corresponding values of $\delta b(p)/b(p)-1$ as a function of the effective ppm $p$. Also presented are the values for the position of the boundary levels $p_{\text{ex}}$ as obtained from the hydrogenic formula eq.(7.18). They show that for $n_e = 1.5 \times 10^{20} \text{ m}^{-3}$ the levels of the $4p$-group are still in the domain of the corona balance, which is indeed reflected in the shape of the distribution function. The position of the cold/hot boundary for $T=3000 \text{ K}$ will be $p_{\text{ch}} = 1.2$, which is lower than the first excited level. So in this plasma the $\text{Ar I}$ system is a hot system and levels with $p > p_{\text{ch}}$ are in the domain of the hot ES balance. This is shown in Fig. 10.4 where, apart from the $4p$ level at lower densities, a $p^{-6}$ dependence is observed.

In Fig. 10.4 the $b(p)$ for several levels are plotted against $n_e$ for a wide $n_e$ range. Here a general $n_e^{-2}$ dependence is observed. Since the Saha density scales as $n_e^{2/3}$ this implies constant excited state densities. Though this has not been worked out in detail we expect that this reflects the fact that the source term has to remain (more or less) constant in view of the requirement of existence of the plasma.
It is interesting to pay attention to the boundary between E83 and PLTE. In section 9.4 we introduced the definition of this boundary \( n_{83} \) by \( b(p_{83}) = 2 \). In fig 10.5 we observe that the densities approach \( \delta_{83} \) at lower levels for higher \( n_e \)-densities, again as expected. The advent of the PLTE becomes more visible in the representation of fig 10.6, in which \( n/n_{4p} \) is plotted as a function of \( n_e \).

Since we are able to determine experimentally the groundstate density of the \( \text{Ar} \ I \) system and the electron temperature we can also determine the values of the \( r^1 \)-coefficients. For the 4p levels it can be found [SIJ 84a] that \( r^1(4p) = 6 \times 10^{-5} \).

The population densities and \( r^1 \)-coefficients have also been calculated with traditional numerical CR-models. In these models a cut-off of \( N \) is required at a sufficiently high level. In [SIJ 84a] a study of the influence of the cut-off is reported. The result is shown in fig. 10.7 where the shape of the distribution function is given expressed in a power law \( n = N \) as obtained from the numerical model as a function of
The slope of the distribution function as a function of \( N \), the number of groups included in the model. Slope \( \beta \) corresponds with \( b_p \sim p^{-\beta} \).

The number \( N \) of the considered groups of levels. It turns out that the analytical and experimentally confirmed \( p^{-\beta} \)-dependence is only found numerically for very large \( N \) values. We also applied a cut-off procedure as introduced in section 6.5 which turned out to be successful [Wil 85].

10.4 On the difference between Ar I and H

From the preceding we may conclude that the hydrogenic approach of the Ar I system is successful as far as it concerns the shape of the distribution function. But if we look at the absolute value of the distribution function we see that there are large differences between Ar I and H.

We have seen in section 6.7 that the distribution function can be presented in several ways. In the \( b(p) = n(p)/n^\infty(p) \)-representation the population is related to its equilibrium value and reads

\[
b(p) = r^+(p) + r^-(p) b_0 \quad (10.1)
\]

In the \( b^2 \)-representation, i.e. that of the relative overpopulation we get

\[
\delta b(p) = b(p) - 1 = r^+(p) + r^-(p) - 1 + r^1(p) b_1. \quad (10.2)
\]

For complete saturation (\( 2 > p_T \)) we find with \( r^+(p) + r^-(p) = 1 \) the relation \( r^1(p) = \delta b(p)/\delta b_1 \). If we employ the bound Maxwell relation \( \delta b(p) \sim p^{-\beta} \) and suppose that this holds for the whole H system...
including \( p_0 \) we get for hydrogen:

\[
c^0(p) = b_0 H^{-6} \text{ with } b_0 H = 1
\]  

(10.2)

Applied to the level \( p=2 \) this results in \( r^0(2) = 1/64 \), which agrees within a factor 2 with CR calculation in [DRA 77] (cf. fig. 7.1). Note that the \( T_e \) dependence of \( r^0 \) is very weak if the system is hot (cf. fig. 7.7). In the case of the Ar I system we find that \( r^0(4p) = 6 \times 10^{-5} \) while the effective \( p_{5} \) is only slightly larger than 2 namely \( p(4p) = 2.2 \). So eq. (10.3) does not apply to the Ar I system.

This difference between \( H \) and Ar I can be explained from the different cross-section for the groundstate excitation which in its turn can be traced back to the difference in atomic structure. So we are faced with the question if it is possible to understand the large difference between \( r^0(2) \) in \( H \) and \( r^0(4p) \) in Ar I directly from the atomic structure as reflected in the energy scheme.

To answer this question we first note the following: In the complete UBB there is a flow of bound electrons in excitation space. This flow is connected with the transport of electrons out of the plasma. In the voyage towards the free space the overpopulated bound electrons are distributed over the energy range according to Maxwell. This leads to the relation \( c^0(p) = n_e^0 \) in the non-defected system of \( H \).

In the excitation space of \( H \) the flow is mainly generated by the step transition from \( p=1 \) to \( p=2 \). Since the statistical weight of the groundstate is \( g(1) = 2 \) while \( g(2) = 8 \), this means that the flow is spread out in 4 parts.

In the Ar I system the excitation space is supplied by a transition from the \( 3p^5 \) (ground state) to the \( 3p^4 \) shell. The effective quantum number of the ground state is \( g(3p) = 1 \) and the statistical weight in \( g(3p) = 1 \). In the shell of \( p_{5} \) 4 we have the levels \( 4s, 4p, 4d \) and \( 4f \) which due to quantum deficiency are spread out over the excitation space. Referring to the figs. 3.1 and 3.2 we recall that \( g(p) = 2g_p^2 \) with \( g_p = 6 \), which results in a total amount of \( g(4) = 192 \). So the flow in the excitation space originating from the groundstate is divided in 192 parts which is 48 times larger than in the case of hydrogen.

Now we assume that the population density in such a part is inversely proportional with the number of parts, that Ar I and H may be compared to each other in this way and we expect that the relation
\[ r^1(p) = \frac{1}{48} \left( p^{-6} \right) \text{ or } b_{0}\text{Ar} = \frac{1}{48} \]

holds. This gives a \( r^1(4p) \) value of \( 9 \times 10^{-5} \) which is in good agreement with the measured values.

Conclusions:
1) the results on Ar I densities show the \( p^{-6} \) behaviour
2) the differences between Ar I and H are mainly related to the increase of the statistical weight in the bottom of the system.

10.5 The Ar II system
Extensive measurements and calculations have also been performed on the Ar II system. This system can be classified as abnormal in view of two experimental facts:
1) the system shows inversion
2) the distribution function is by no means hydrogenic.
In the study of the Ar II system we will proceed as follows. First we discuss the Ar II system of energy levels, second we summarize the experimental findings and finally we try to get a picture of the structure of the excitation space.

The energy scheme of the Ar II system is given in fig. 10.8. It shows a large quantum defect and the level \( 5^2 \) is the first level for which the quantum deficiency is limited. There are three core configurations, one \( ^3P \) with a doublet and quartet structure and two others \( (^1D, ^1S) \) with a doublet structure. In some of the older studies only the doublet system of the \( ^3P \) is considered. However the fact that there are strong optical transitions between quartet and doublet systems of this core makes this approach questionable. It is possible that there is also core mixing due to electron collisions. This is important because if all levels can be included irrespective of their core configuration we observe a nearly continuously filled energy space in which the average energy gap between levels is much smaller than in He, the hydrogenic system with \( Z=2 \).

Nevertheless it is instructive to calculate the hydrogenic boundaries. In a hydrogenic approach one would find that for \( T_{\text{e}} = 3\text{eV} \) the position of the cold/root boundary is located at \( p_{\text{c}} = 2.5 \) which corresponds with an excitation energy \( |E_p| = 19 \text{eV} \) in the \( ^3P \) core. This means that \( p_{\text{He}} \) would lie in the \( 4p \) group (cf. fig. 10.8). The position of the
The energy scheme of the AR II system.

Hydrogenic collisional/radiative boundary varies between $\rho_{\text{er}} = 3.4$ and 3.9 if $n_e$ varies between $10^{19}$ and $2 \times 10^{20}$ $\text{m}^{-3}$ which corresponds with the excitation energy of 23.9 and 24.2$\text{eV}$ of the $3p$ system and this is located in that part of the system where quantum deficiency becomes relatively unimportant and a hydrogenic approach better.

The spectroscopy is mainly carried out at the levels of the $4p$ group which in a hydrogenic system would have been dominated by the corona balance. However, as stated in section 9.2, the corona balance is the most improper balance. The production and destruction of a level population are of different nature, i.e. collisional and radiative resp. In the hydrogenic approach we used collisional and radiative properties for degenerated hydrogenic levels for which the states are statistically distributed. It is known from experiments (cf. section 2.4.4. and [KOM 77]) that this statistical distribution is not fully present even in a He$^+$ plasma. So the applicability of a pure hydrogenic approach in this complicated system is out of the question.
10.6 Experimental results in Ar II

A lot of spectroscopic measurements have already been published (cf. [S1J 72], [FOT 78], [OUN 76] and [JOL 78]). Here we take the opportunity to reproduce in Fig. 10.9 results of [WIL 84, 86] for the density of a 4p' level as function of $n_e$. An interesting feature of these results is the knee point in the curve. For low $n_e$-values $n(4p')$ scales with $n_e^2$ while for higher $n_e$-values a scaling with $n_e$ is observed. This knee point reflects that for $n > 10^{19}$ m$^{-3}$ the level is collisionally dominated. In the production/destruction balance $n(4p')D(4p') = P(4p')$, the production scales with $n_e$ while $D$ scales with $n_e^2$. We must conclude that this critical density of 4p' is smaller than that obtained from hydrogenic formula (Eq. 7,16). This behaviour is also observed for other 4p-levels (cf. [S1J 76]).

Two fluorescence experiments have been added to the spectroscopy. In the first experiment the fluorescence is caused by the irradiation of the plasma with Ar$^+$ lines from an Ar-ion laser. The second concerns fluorescence due to irradiation from a 1 mJ pulsed dye laser tuned at the 3d'$\rightarrow$4p' 611.5 nm line (cf. Fig. 10.11). The prime refers to the D core.

The Ar-ion laser, a 5% all lines Spectrophysics laser, is tuned at one of the four laser transitions 486.0, 476.5, 496.5 and 514.5 nm. The fluorescence signal is detected at 90°. The laser beam waist diameter is 3 mm, the viewing waist is 0.94 mm$^2$ and the fluorescence
volume is 3.5 mm$^3$. The spontaneous emission is observed along the full length of the viewing beam. So a volume correction has been applied to renormalize the spontaneous emission background to the emission of the fluorescence volume only. A second correction is required since the laser line width is much smaller than the Gaussian width of the optical transition.

In most cases a negative fluorescence signal is observed. This shows that the population densities are inverted, which is to be expected for laser transitions in a certain $n_e$ range. In fig. 10.10 the resulting population densities are displayed as a function of $n_e$.

Fig. 10.10
The absolute inversion $N$ of the $4p^2P_{3/2}$ with respect to a $4s4p^2P^0_{1/2}$ line as a function of $n_e$.

The figure shows a quenching of the inversion at $n_e = 5 \times 10^9$ m$^{-3}$. At this electron density the rate of collisional destruction of the 4s' levels is comparable with that of radiative decay.

In the second fluorescence experiment we used a pulsed dye laser with a time duration of approximately 1 ns. A diagram of the levels involved is shown in fig. 10.11. The behaviour of the 4p' level, hereafter denoted by level a, is detected from the 461 nm line. An interesting feature is that the lower level 3d', hereafter denoted by level b, is metastable. So the density of b is substantially higher than that of
a. And we expect the following time behaviour of the upper level (fig. 10.12): If the laser is switched on at time $t=0$, the density of level a increases rapidly until in saturation the levels a and b have the same density per statistical weight, i.e. $n^a(t) = n^b(t)$. In this new situation the common $n$-value will decrease, mainly due to the destruction of the upper level a. The rapid increase followed by the decay is reflected by the peak in the fluorescence signal (cf. fig. 10.12). The decay leads to a 'plateau' which reflects a steady state in which levels a and b coupled by the laser radiation share each other's production and destruction.

![Diagram of levels a and b with laser on and off](image)

Fig. 10.11
The levels involved in the pulsed laser experiment.

Fig. 10.12
The expected time behaviour of the 461 nm line.

Fig. 10.13 shows the time behaviour of the 461 nm line as obtained from the experiment. The 'decay' of the peak is spread out over 300 ns while the decay time of the level a ($4p^a$) is smaller than 10 ns. This difference can be explained by the jitter of the laser pulse and the experiment has learned that it is nearly impossible to measure short decay-times with long laser pulses. In this context we refer to [80K 80] where decay time measurements of a comparable experiment in $H$ are

![Graph of fluorescence over time](image)

Fig. 10.13
The measured time behaviour of the 461 nm line.
The hatched area refers to the integrated peak.
reported. The main result is that the 'decay time' is larger than those predicted by theory.

We confine ourselves to the experimental results of the integrated values at the peak and the plateau and ignore the differential time structure.

In a simple model we assume that the population density of all other levels are unaffected by the laser irradiation and that the intensity of the laser is so high that saturation is reached in a time much smaller than the lifetime of the upper level. Under this assumption we do not need further information of the laser beam. The rate of absorption and stimulated emission level supercedes those of all other processes many times. (cf. section 2.6.3 case C). As a consequence a and b can be regarded as sublevels of one level, denoted by a+b with total statistical weight \( G(a+b) = g(a) + g(b) \) and total density \( N(a+b) = \bar{n}(a) + \bar{n}(b) \). In this level a+b each state has the same density, i.e. \( \bar{n}(a) = \bar{n}(b) \). With the asterisk the quantities during the laser pulse will be marked.

The total density will have a time evolution which can be described by

\[
\frac{d\bar{n}^*(a+b)}{dt} = \bar{P}^*(a) + \bar{P}^*(b) - g(a)\bar{n}^*(a)\bar{D}^*(a) - g(b)\bar{n}^*(b)\bar{D}^*(b),
\]  

(10.5)

in which \( \bar{P}^*(a) \) and \( \bar{D}^*(a) \) reflect the production and destruction of level \( a \) during the laser pulse due to collisional/radiative interactions with all other levels except level \( b \) (cf. fig. 10.14). The transitions between \( a \) and \( b \) are excluded since they do not contribute to \( N(a+b) \).

**Fig. 10.14**

Due to the laser irradiation, the levels \( a \) and \( b \) are coupled and share each other's production and destruction.

For the density per statistical weight we get the following time evolution

\[
\frac{d\bar{n}^*}{dt} = \frac{\bar{P}^*(a) + \bar{P}^*(b)}{g(a) + g(b)} - \frac{g(a)\bar{n}^*(a)\bar{D}^*(a) + g(b)\bar{n}^*(b)\bar{D}^*(b)}{g(a) + g(b)}.
\]  

(10.6)
After a relaxation determined by the common depopulation factor 
\[ D^*(a+b) = (g(a)D^*(a) + g(b)D^*(b))/(g(a) + g(b)) \] the density per statistical weight will tend to 
\[ n^*_{\text{plat}} = \frac{P^*(a) + P^*(b)}{g(a)D^*(a) + g(b)D^*(b)} \] (10.7)

which is the plateau value of \( n^*(a) - n^*(b) \). A quantity of interest is the change in the density of level \( a \) (\( = 4d^* \)) due to the laser interaction. It reads \( \Delta n^*(a) = g(a)\Delta n^*(a) = n^0(a) \) and its plateau value is given by
\[ \Delta n^*_{\text{plat}}(a) = \frac{n^0(b) - n^0(a)g(b)/g(a)}{D^*(a) + g(b)/g(a)D^*(b)} \] (10.8)

in which \( n^0(a) \) is the unperturbed density of level \( a \). This result is obtained using the relation \( P^*(a) = n(b)D^*(b) \) and \( P^*(b) = n(a)D^*(a) \).

Another important quantity is the peak value. In our model in which we assume that the ‘switch time’ of saturation is much smaller than \( D^{-1}(a+b) \) we get
\[ \Delta n^*_{\text{peak}}(a) = (n^0(a) - n^0(a)g(b)/g(a))/(1 + g(b)/g(a))^{-1} \] (10.9)

However due to the laser jitter this peak value is not detectable in our experiment. A related measurable quantity is that of the integrated peak \( \Delta n^*_{\text{peak}}(a) \) (cf. the hatched area under the curve of fig. 10.13). It can be found by integration that
\[ \Delta n^*_{\text{peak}}(a) = \frac{n^0(b) - n^0(a)g(b)/g(a)}{(1 + g(b)/g(a))D^*(a+b)} \] (10.10)

To obtain information of the Ar I II system from the experiment we proceed as follows.

- The ratio of integrated peak and plateau is theoretically given by
  \[ \frac{\Delta n^*_{\text{peak}}(a)}{\Delta n^*_{\text{peak}}(a)} = D^*(b) = \sum_{i \neq a} K(b,i) \] (10.11)

which is found by using eqs. (10.8) and (10.10).

We recall that level \( b \) (\( = 3d^* \)) is metastable which implies that the destruction factor is completely collisional. From the experimental values of integrated peak and plateau we find that
\[ D^*(b) = (3 \pm 1.5) \times 10^{-16} \text{ cm}^{-3} \text{s}^{-1} \] (10.12)
- From the values of the Einstein coefficients $A_{a,i}$ obtained from literature [WIE 69] and the knee point in Fig. 10.9 the depopulation factor of level $a$ can be determined; it is given by

$$D^a(a) = \sum_{i \neq b} A_{a,i} + n_e \sum_{i \neq b} K_{a,i} = 1.2 \times 10^5 + 6.10^{-17} n_e \text{s}^{-1} \quad (10.13)$$

With the equations (10.10-13) and the measured integrated peak values we can determine the density of the lower level. The results are given in Fig. 10.15 where $\alpha^0(b)/\alpha^0(a)$ is plotted as a function of $n_e$. Note that this ratio is large, and for low $n_e$ values the ratio amounts to $2.10^4$.

Fig. 10.16
the ratio of the (unperturbed)
population densities
of the metastable level $b$ and the radiative
level $a$.

10.7 The structure of the excitation space of the Ar II system
In the preceding we presented
- spectroscopic data of 4p levels
- Ar-ion laser fluorescence data of 4s levels
- and data obtained from the pulsed dye laser fluorescence of 3s' and
4p' levels. The accuracy of these experimental facts is sufficient to
permit some conclusions about the excitation kinetics of the Ar II
system.

The main scope crusted by the experiments is that the system is very
complicated and that it contains different classes of levels next to
each other. These different classes are
- the metastable levels mostly with a large statistical weight
- strongly radiating levels for which the lower ones have small
statistical weight
- and an intermediate class, i.e. levels such as the 4p levels, with
a typical lifetime of 10 ns, for which we know that the population
density increases linear with $n_e$ for $n_e > 2.10^{19} \text{s}^{-3}$.

The levels in the latter class leave corona for critical densities
smaller than those in the He II system.
Now we are faced with the challenge to describe the excitation kinetics of the Ar II system. One possible approach is to look at the shape of the distribution function. It is known from experiments [WL 84] that the shape of the distribution function is globally described by $\eta = \rho^{-\beta}$. So it is not at all the shape of the transparent corona for hydrogenics (for which $\eta = \rho^{-0.5}$), and even steeper than that of ESB ($\rho^{-0.5}$).

In section 9.2.2, we have found a very steep function in the description of corona case B (cf. fig.9.4). We recall that the underlying processes are the following: The first excited states are populated by electronic groundstate excitation, and since they can not lose their population by radiation this population has to be removed in upward direction. But due to the radiative decay between excited levels by which this flow is obstructed, the slope has to be extra steep in order to generate this step flow. This case B corona can also be denoted with 'ESB with radiative obstruction'.

This provides a possible explanation for the Ar II system. Many states of the lower excited levels in this system are metastable with consequently large population densities. As in the situation of case B corona this population is stepwise removed in upward direction but this ladder-climbing is obstructed by radiative decay. However it is not expected that this excitation flow reaches the continuum of the Ar$^{2+}$ ion (i.e. the groundstate of the Ar III system). This is because the flow finds strongly radiative holes in its course through the excitation space. And by these leaks the flow will be removed back to the groundstate. So the production of the Ar$^{2+}$ ions is limited. Based on our hydrogenic collisional boundary it is expected that this flow is not even able to reach the undefected part of the system.

So an interpretation which seems to describe the observations is that the Ar II system is partially in ESB but for the lower part globally in corona. That is to say: the excitation to e.g. metastable or weakly radiating levels is lost primarily by deexcitation upwards. This results in an $\eta$-dependence as in ESB rather than an $\eta \propto \rho^{-\beta}$ dependence as in full corona. However the upward climbing excitation finds strongly radiating holes at several levels in the system. So, most of the excitation is finally re-radiated to the ground state even for moderately high electron densities. Only at even higher $\eta$-values the deexcitation upward becomes so fast that the radiative losses can not compete. Moreover, at higher ion densities the effective lifetime increases in view of the increasing opacity. For $R = 1 \text{ cm}$ we estimate this transition to full ESB at $\eta > 5 \times 10^5 \text{ m}^{-3}$. 
Even though this forms only a first attempt to place also the Ar II system in the framework of general CR-classifications the following becomes clear:

1. The relevant critical densities between corona/ESS may shift significantly downward with regard to hydrogenic scaling because of non-hydrogenic positions of the energy levels and small energy differences between the levels.

2. The presence of strongly radiating levels more upward in the system may prevent that the excitation flow reaches the continuum. So the production of Ar$^{2+}$ ions will be limited.
Abbreviations

BB  Boltzmann balance (1.3; 2.2.3)
BEA  binary encounter approximation (5.3)
CB  corona balance (1.3; 9.2)
C-hot  collisional hot (5.2-5.9)
CL  classical
CP  correspondence principle (3.3)
CR  collisional radiative (6.1)
CRC  capture radiative cascade (8.2-8.4)
DA  dipole approximation (5.4)
DB  detailed balancing (1.2; 2.2)
ion. ESB  ionizing excitation saturation balance (1.3; 9.3)
recom. ESB  recombinating excitation saturation balance (1.3; 8.5-8.6)
LTE  local thermal equilibrium (1.3)
PLTE  partial local thermal equilibrium (1.3)
QM  quantum mechanical
QSS($\tilde{S}$)  quasi steady state (solution) (6.4)
R-hot  radiative hot (4.6)
S  Saha balance (1.3; 2.2.4)
SE  semi empirical (5.11)
TE  thermodynamic equilibrium (1.2-1.3)
TDFPT  time dependent perturbation theory (5.5)
qd  quantum defect (3.2)
pqm  principal quantum number (2.2)

The numbers between brackets refer to the sections in which the concepts are introduced or discussed.
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Summary

The science of plasma physics is relatively young and finds itself in the early stage of classification. This classification of plasmas is an enormous task since we deal with the most chaotic state of matter. In this thesis we present a classification based on the atomic state distribution function.

In many plasmas the electrons are dominant in the excitation kinetics; this is the consequence of the small mass and consequently large velocity of the electron. This class of plasmas is denoted by EEK plasmas in which EEK stands for electron excitation kinetics. The study of the distribution function of atomic states in EEK plasmas is essentially the study of the interaction of bound and free electrons, similar particles in different situations. Our study is based on the relation between the distribution function and the underlying processes and starts with the proper understanding of thermodynamic equilibrium (TE). In TE the production and destruction of a level population can be classified in forward and backward processes. A balance which consists of a process and its inverse process is a so-called 'proper balance'. Four types of proper balances are relevant: The 'Maxwell balance' of kinetic energy transfer, the 'Boltzmann balance' of excitation/deexcitation, the 'Saha balance' of ionization/recombination and the 'Planck balance' for interaction of atoms with radiation. If all the proper balances are in equilibrium this detailed balancing results in the distribution function given by the Saha-Boltzmann equation. Deviation from equilibrium can be characterized by the fact that not all proper balances are in equilibrium.

In most cases the new situation is dominated by an improper balance in which forward and backward processes are not each other's inverse. As an example we refer to the corona balance. The population of an excited level in corona is produced by electron excitation of groundstate atoms and destroyed by radiative decay.

In EEK plasmas there are four types of improper balances and each of them manifests itself in a particular way in the shape of the distribution function.

An important feature of improper balances is that they are associated with activity on macroscopic level. For instance, in ionizing plasmas improper balances create a net ionization flow in the system of atomic levels. This results in a production of charged particles which supports the transport of charged particles out of the plasma. In recombining plasmas there is an inward transport of charged particles
which supports the improper recombining balances. Special attention is paid to the distribution function of the ionizing excitation saturation balance. The overpopulated bound electrons are subjected to frequent interactions with free electrons and in the voyages from bound to free space the energy distribution will be taken over from the free electrons. This distribution is denoted by the bound Maxwell distribution.

A practical result of the bound Maxwell distribution is that the boundary between free and bound space can be lowered and that the calculation of the distribution function is limited to the determination of the population density of lower lying levels only. This leads to a modified cut-off procedure, an analytical capping, of the conventional numerical calculation of the distribution function.

The classification theory of the distribution functions in relation with underlying balances is supported by experimental evidence in an ionizing argon plasma. The AR I system provides a pertinent support of the theory. Experimental facts, found in the AR II system can be interpreted in global terms.

This classification theory can be seen as a unification of the work of Siberman, Drawin, Fujimoto and Seaton. Although these different studies resulted from different points of view they appear to be complementary to each other.
Samenvatting
De plasma fysica is een jonge wetenschap en bevindt zich in het ontwikkelings stadium van classificatie. Het classificeren van plasmas is echter geen eenvoudige opgave omdat we met de vaak chaotische verschijningsvorm van materie te maken hebben.
In dit proefschrift wordt een classificatie theorie gepresenteerd die uitgaat van de verdelingsfunctie van atoomaire toestanden. Deze verdelingsfunctie beschrijft de manier waarop atomen verdeeld zijn over de mogelijke interne toestanden.
Het blijkt dat voor een groot aantal plasmas de verdelingsfunctie bepaald wordt door de electronen die door hun kleine massa sneller zijn dan zware deeltjes en zodoende frequenter wisselwerken met atomen. In deze zogenaamde EKK (electron excitatie kinetiek) plasmas wordt de verdelingsfunctie bepaald door de interactie tussen vrije en gebonden electronen; gelijke deeltjes in verschillende omstandigheden.
De verdelingsfunctie van een bepaald EKK plasma geeft dus een beeld van de activiteit van het elektronen-gas in dat plasma.
Om de afwijkingen van evenwicht te begrijpen beschouwen we eerst de situatie van thermodynamisch evenwicht (TE) waarvoor de verdelingsfunctie bekend is. In TE komt de bevolkings-dichtheid van een bepaalde atoomaire toestand tot stand doordat bevolkings- en ontvolkings processen te groepen zijn in heen en teruggaande processen. Een balans gevormd door een proces met het bijbehorende inverse proces wordt een 'eigenlijke balans' genoemd. Er zijn vier soorten eigenlijke balansen. Zo beschrijft de 'Maxwell balans' de heen en teruggaande processen van de kinetische energie overdracht, de 'Holtzmann balans' de excitatie en deexcitatie, de 'Saha balans' de ionisatie/recombinatie terwijl de 'Planck balans' de interactie van atomen met straling aan elkaar relateert.
Als alle eigenlijke balansen in evenwicht zijn dan is de verdelingsfunctie bekend en kan deze worden beschreven door de Saha-Holtzmann vergelijking. Afwijkingen van evenwicht zijn terug te voeren tot het feit dat niet alle eigenlijke balansen in evenwicht zijn. In vaste gevallen kan de situatie geclassificeerd worden door een andere balans, een 'oneigenlijke balans', waarbij de bevolkings- en ontvolkings processen niet elkaar's invers zijn. Vier oneigenlijke balansen zijn van belang. In ioniserende plasmas zijn dat de corona balans en de balans van ioniserende excitatie verzadiging, in recombineerende plasmas zijn dat de balans van electronvangeest-stabilisaties-cascade en die van recombineerende excitatie verzadiging.
Een belangrijke eigenschap van ongeioniseerde belansen is dat zij gepaard gaan met activiteiten op macroscopische schaal. In ioniserende plasmas zal door de aanwezigheid van ongeioniseerde belansen een ionisatietoestroom gegenereerd worden. Dit betekent dat atomen gesplitst worden in geladen deeltjes. Deze productie van geladen deeltjes fungeert als bron voor een naar buiten gericht transport van geladen deeltjes. In recombineerende plasmas is de omgekeerde situatie van toepassing. Het naar binnen gericht transport van geladen deeltjes voedt de recombinitie die door ongeioniseerde belansen gerealiseerd wordt.

In dit proefschrift wordt in het bijzonder aandacht besteed aan de relatie tussen de verdelingsfunctie en de processen die daaraan ten grondslag liggen. Met name is een goed begrip van het gedrag van electronen van groot belang. Enerzijds worden stralingsprocessen duidelijk uit de studie van de aantrekking tussen een electron en een positieve kern, anderzijds is de kennis van het collectief gedrag van electronen van belang in situaties waar botsingen tussen gebonden en vrije electronen vaak voorkomen. Vooral wanneer dit laatste betreft is de studie van de verdelingsfunctie van een ioniserend plasma met hoge electronendichtheid zeer interessant. Het blijkt dat gebonden electronen die onderworpen worden aan een frequentie interacties met vrije electronen ook de energie verdeling van de vrije electronen overnemen. Deze energie verdeling noemen wij de 'gebonden Maxwell' verdeling. Het gedrag van recombineerende plasmas kan men hieruit begrijpen omdat ioniserende en recombineerende plasmas in vele gevallen complementair zijn.

Een praktisch resultaat van de gebonden Maxwell verdeling is dat de grens tussen gebonden en vrije electronen naar beneden kan worden verschoven en dat het bepalen van de verdelings functie, waar het in feite om gaat, gereduceerd kan worden tot het berekenen van de dichtheid van de onderste aangeslagen toestanden.

De classificatie theorie wordt ondersteund door experimentele gegevens van een argon plasma. Het Ar I systeem geeft een goede ondersteuning van de theorie en experimentele gegevens verkregen van het Ar II systeem kunnen globaal geïnterpreteerd worden.

De gepresenteerde classificatie theorie kan gezien worden als een unificatie van het werk dat eerder verricht werd door o.a. Hiberman, Drawin, Fujimoto en Seaton. Deze verschillende studies kwamen vanuit verschillende gezichtspunten tot stand. Ze blijken echter in vele opzichten complementair te zijn aan elkaar.
Dankwoord

Dit proefschrift is tot stand gekomen door de inzet van valen. Een aantal van hen wil ik op deze plaats bedanken.
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Ondervin Neetbaar heeft mij inzicht gegeven in quantum mechanische aspecten van botsingen. Bijzonder leeraan waren de klassieke interpretaties die hij daaraan wist te geven.

Wat betreft het experiment ondersteund werk bedank ik Rien van de Sande. Als ik vanuit Breda na schoollijd nog even snel een experiment wilde doen dan was dat vaak mogelijk na een telefoontje met Rien.
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De figuren in dit boek zijn gemaakt door Rudi Gruijters. Ondanks mijn mierdighheid heeft ze er toch iets moois van weten te maken.

Als laatste (niet least) dank ik Simona. Ondanks eigen drukke verkeersbomen wist zij altijd tijd te vinden om te adviseren en te corrigeren. Daarnaast gaf ze mij de moeite en materiele steun die vooral bij de laatste leodjes zo nodig waren.
CURRICULUM VITAE


In zijn studententijd hield hij zich gedurende een aantal jaren zeer actief bezig met het verenigingsleven, de muziek en het theater. In totaal produceerde hij drie musicals en regisseerde een aantal toneelstukken op de middelbare scholen waar hij werkzaam was.
STELLINGEN

behorende bij het proefschrift van

Joost van der Kullen

Eindhoven, 21 februari 1986
1) Recente modelberekeningen aan de Trichelpuls in de negatieve coronatoren aan dat de electronen verantwoordelijk zijn voor het bevinden van de snelle voorflank. Dit betekent dat dit verschijnsel ook in electropositieve gassen waargenomen moet kunnen worden. Dit is in strijd met de gangbare opvatting* dat in electropositieve gassen geen Trichelpulsen optreden.


2) Gehouden electronen die onderworpen zijn aan frequentie interacties met vrije electronen, nemen de energieverdeling van de vrije electronen over.

Dit proefschrift, hoofdstuk 9.

3) In het natuurkundeonderwijs dient de behandeling van de wet van behoud van energie gepaard te gaan met het bijbrengen van het begrip entropie.


4) De economie van een gecomputeriseerde maatschappij kan alleen functioneren als de opbrengst van de geautomatiseerde industrie verdeeld wordt over de mensen in de vorm van een basisinkomen. Indien men als vrijtijdsbesteding wil participeren in georganiseerde arbeid die schaars is, zal men daarvoor moeten betalen.

5) Als voorbereiding op hun functioneren in een dynamische maatschappij vol specialismen dient het onderwijs aan leerlingen een zo breed mogelijke basis te bieden. In die zin is het systeem van vakkenpakketten zoals geïntroduceerd door de wet op het voortgezet onderwijs, de zogenaamde mammootwet, een stap in de verkeerde richting.

Wet op het Voortgezet Onderwijs (Mamootwet); Staatsblad nr. 40 d.d. 26-2-1963.
6) Door de gevoelsmatige aspecten van de exacte vakken te verwaarlozen, schrikten leerlingen af. Dit geldt met name voor meisjes.

7) De opvatting dat de Nederlandse defensie in 1940 niet op een voldoende niveau was als gevolg van de invloed van de toenmalige pacifistische stromingen, is onjuist.

8) Het vernemen van een regeringsperiode naar de minister-president geeft weinig informatie over het in die periode ontwikkelde regeringsbeleid. Zo krijgt de veel gehoorde kritiek, geleverd door aanhangers van het kabinet-Lubbers op het economische beleid van het kabinet-den Uyl, meer relief indien men de naam van de toenmalige minister van economische zaken vermeldt.

9) Als voorbereiding op een informatica-maatschappij dient men op middelbare scholen naast het vak informatica ook het vak vrijtijdsbesteding te introduceren.
"De experimentele studierichting vrijtijdswetenschappen ex art. 20 WWO" Rapport, uitgegeven door de Katholieke Hogeschool Tilburg, 1984.

10) In de te verwachten chaos van satelliet-TV en computerspelletjes zal het mens-erger-je-niet goed gedijen.