

**LIMITING CASES: SYMMETRY, ISOTROPY, EQUILIBRIUM,
PLANE WAVES**

In a one-dimensional planar or spherically-symmetric atmosphere the radiation field is azimuthally invariant, hence the pressure tensor becomes *diagonal*

$$\mathbf{P}(\mathbf{r}, v, t) = \begin{pmatrix} p_R & 0 & 0 \\ 0 & p_R & 0 \\ 0 & 0 & p_R \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 3p_R - E_R & 0 & 0 \\ 0 & 3p_R - E_R & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (1-40)$$

where $p_R(z, v, t) \equiv (4\pi/c)K(z, v, t)$ (1-41)

and, in turn,

$$K(z, v, t) \equiv \frac{1}{2} \int_{-1}^1 I(z, \mu, v, t) \mu^2 d\mu \quad (1-42)$$

is the second moment of the radiation field in Eddington's notation.

Exercise 1-9: (a) Derive equation (1-40) for the conditions stated. (b) Show that the same expression for \mathbf{P} is obtained in spherical symmetry relative to the orthogonal triad $(\hat{\phi}, \hat{\theta}, \hat{\mathbf{f}})$. (c) Verify that the tensor shown in equation (1-40) is consistent with equation (1-32).

It is clear from equation (1-40) that, for a *one-dimensional* atmosphere, only two scalars (p_R and E_R) are sufficient to specify the full radiation pressure tensor. Further, for such atmospheres, derivatives with respect to (x, y) or (θ, ϕ) , in the planar and spherical cases respectively, are identically zero, and the only nonvanishing components of the divergence of the radiation pressure tensor are

$$(\nabla \cdot \mathbf{P})_z = \partial p_R(z, v, t) / \partial z \quad (1-43a)$$

in planar geometry—or, in spherical geometry,

$$(\nabla \cdot \mathbf{P})_r = [\partial p_R(r, v, t) / \partial r] + [3p_R(r, v, t) - E_R(r, v, t)] / r \quad (1-43b)$$

In this book we shall confine attention strictly to one-dimensional problems, and with the exception of further formal development of the equations of radiation hydrodynamics in §15-3, the full tensor description of the radiation field will not be required; for ease of expression, we shall therefore refer to the single scalar p_R as "the" radiation pressure.

Exercise 1-10: Show that, for any diagonal tensor A , in spherical coordinates $(\nabla \cdot A)_r = (\partial A_{rr} / \partial r) + (2A_{rr} - A_{\theta\theta} - A_{\phi\phi}) / r$; use this result to derive equation (1-43b).

In general, p_R as defined by equation (1-41) will *not* equal \bar{P} defined by equation (1-32), but the two become equal if the radiation field is isotropic. For an isotropic field, I is independent of μ , and equations (1-7) and (1-41) immediately yield $p_R = \frac{1}{3}E_R$, so that equation (1-40) reduces to

$$\mathbf{P}(\mathbf{r}, v, t) = \begin{pmatrix} p_R & 0 & 0 \\ 0 & p_R & 0 \\ 0 & 0 & p_R \end{pmatrix} \quad (1-44)$$

That is, *when the radiation field is isotropic, the radiation pressure tensor is diagonal and isotropic*, and may be replaced, for all purposes of computation, by a scalar *hydrostatic pressure*, or even eliminated entirely in terms of E_R . If in addition to being isotropic the radiation field has its *thermal equilibrium* value, then the monochromatic radiation pressure is

$$p_R^*(z, v, t) = \frac{1}{3} E_R^*(z, v, t) = (4\pi/3c)B_v(T) \quad (1-45)$$

and the total radiation pressure is

$$p_R^*(z, t) = \frac{1}{3} a T^4 \quad (1-46)$$

a result first obtained by thermodynamic arguments (160, 55; 565, 123).

From equations (1-7) and (1-41) we see that p_R is an average of $I(\mu)$ weighted by μ^2 whereas E_R is a straight average. If the radiation field becomes peaked in the direction of radiation flow out of the atmosphere, the larger values of μ become more heavily weighted in p_R (recall $\mu = 1$ for $\theta = 0$) and p_R will *exceed* its isotropic limit of $\frac{1}{3}E_R$. The most extreme departure from isotropy occurs when the radiation flows in a plane wave. For a wave in the outward direction we can write $I(z, v, \mu) = I(z, v) \delta(\mu - 1)$; then $K(z, v) = J(z, v) = H(z, v)$, and $p_R(z, v) = E_R(z, v)$. This extreme limit is approached in the outermost layers of very extended stellar envelopes (or in nebulae) in which the radiation field originates from a stellar surface that occupies only a very small solid angle as seen from the point in question.

Exercise 1-11: (a) Show that for a plane wave moving along one of the coordinate axes, the radiation pressure tensor has only one non-zero component. (b) Show that the pressure tensor is isotropic if the angular dependence of the radiation field is given by $I(\mu) = I_0 + I_1\mu$. This result is important because the radiation field is accurately described by an expression of the stated form in the *diffusion limit* which obtains at great depth in the atmosphere (cf. §2-5).

Exercise 1-12: Suppose an observer is at distance r from the center of a star of radius r_* which has a uniformly bright surface (i.e., I is independent of μ). Derive analytical expressions for J , H , and K in terms of $\theta_* \equiv \sin^{-1}(r_*/r)$, and show that in the limit $(r/r_*) \rightarrow \infty$, $J = H = K$.

VARIABLE EDDINGTON FACTORS

From the results derived above it follows that the ratio $p_R(r, v, t)/E_R(r, v, t)$ or $K(r, v, t)/J(r, v, t)$ is a dimensionless number whose value is fixed by the degree of isotropy of the radiation field, and typically ranges between $\frac{1}{2}$ and 1. It will be shown later (§6-3) that this ratio can be used in certain numerical methods to reduce the number of independent variables in the transfer problem; further, it may be used to effect a closure of the system of moment equations derived from the transfer equation. It is useful, therefore, to define the *variable Eddington factor*

$$f(r, v, t) \equiv K(r, v, t)/J(r, v, t) \quad (1-47)$$

or, in abbreviated notation $f_v = K_v/J_v$.

Exercise 1-13: (a) Consider an expansion of the form $I(\mu) = I_0 + \sum_n I_n \mu^n$; show that $f = \frac{1}{2}$ if the sum includes only odd powers n . (b) Suppose that $I(\mu) \equiv I_1$ for $(0 \leq \mu \leq 1)$ and $I(\mu) \equiv I_2$ for $(-1 \leq \mu \leq 0)$; show again that $f = \frac{1}{2}$. This representation of I provides a rough description (the *two-stream approximation*) of a stellar radiation field, for we may let $I_2/I_1 \rightarrow 0$ at the surface and $I_2/I_1 \rightarrow 1$ at depth. (c) Show that, for a slab of infinite extent in (x, y) and finite extent in z , f may drop below $\frac{1}{2}$.

2

The Equation of Transfer

As radiation passes through the gas composing a stellar atmosphere, it interacts with the material and is absorbed, emitted, and scattered repeatedly. These phenomena determine how *radiative transfer* occurs in the atmosphere. In this chapter, macroscopic quantities that define radiation-matter interactions are introduced (§2-1), and the *equation of transfer* (which describes the transport of radiation through the medium) is developed (§2-2). Using this equation, we can compute the emergent spectrum from a star, and calculate how the angle-frequency variation of the radiation field changes with depth in the atmosphere. The *time-dependent* equation of transfer will be derived in order to obtain moment equations (§2-3) that describe the *dynamical* behavior of the radiation field, but the discussion will then be restricted to *static* atmospheres in all subsequent work through Chapter 13. In Chapters 14 and 15 radiative transfer and its dynamical effects in *steady* (i.e., time-independent) flows will be considered.

2-1 The Interaction of Radiation with Matter

DISTINCTION BETWEEN SCATTERING AND ABSORPTION-EMISSION PROCESSES

In the interaction of radiation with matter, energy may be removed from, or delivered into, the radiation field by a wide variety of physical processes. For the present, it is adequate to characterize these processes by macroscopic coefficients; as will be seen in Chapters 4 and 7, these coefficients are specified by atomic cross-sections and occupation numbers of energy levels of the constituents of the stellar material. It is worthwhile, from the outset, to make a distinction between "true" *absorption* and *emission* on one hand and the process of *scattering* on the other for, as we shall see repeatedly in the development of the theory, the physical nature of the interaction between the atmospheric material and radiation is quite different in these two cases. However, it is also important to realize that in spectral lines the dichotomy between these processes can be established uniquely only when we consider a transition between two specified atomic states, with no coupling to any other states allowed. As soon as *sequences* of transitions among several interacting states are considered, fundamental ambiguities arise, and it is no longer possible to describe a given line as an "absorption" or a "scattering" line in a rigorous way; nor would it be important or useful to do so. Nevertheless, it is fruitful to have at least an intuitive notion of the contrast between these two basic processes, obtained by consideration of some definite examples.

We may identify as *scattering processes* those in which a photon interacts with a scattering center (perhaps producing a change in the scatterer's internal excitation state) and emerges from the interaction in a new direction with (in general) a *slightly* altered energy. The essential point is that in this process, the energy of the photon is not converted into kinetic energy of particles in the gas. In contrast, we shall identify *absorption processes* as those in which the photon is destroyed by conversion of its energy (wholly or partly) into the thermal energy of the gas. In this process we say that the photon has been *thermalized*. The crucial physical point to note is that the local rate of energy emission in *scattering processes* depends mainly upon the *radiation field* (which may have originated at some other remotely situated point in the atmosphere) and has only a weak connection with the local values of the thermodynamic properties (e.g., temperature) of the gas. *Absorption processes*, on the other hand, feed photon energy directly into the thermal kinetic energy of the gas, and hence are more intimately coupled to local thermodynamic properties of the material. Conversely, the inverse of absorption, *thermal emission*, transfers energy from the thermal pool of the gas directly into the radiation field. Thermal absorption and emission processes thus tend to produce *local equilibrium* between the radiation and material; but scattering

processes allow photons to move from one part of the atmosphere to some other part without coupling to local conditions, and thus tend to delocalize the control of the gas-radiation equilibration process, and to introduce global properties of the atmosphere (e.g., the presence of boundaries) into the problem.

To illustrate the ideas developed above, let us consider the following as typical examples of *scattering processes*.

(a) The interaction of a photon with an atom in bound state *a* leading to the excitation of a higher bound state *b* (the photon's energy being converted to internal excitation energy of the atom), followed by a direct return to state *a* with the emission of a photon. In general the emitted photon will propagate in a different direction from that of the incident photon. Further, both the lower and upper states *a* and *b* of an atom in a radiating gas will not be perfectly sharp, but will have finite energy widths arising, for example, from the finite lifetime of each state produced by radiative decay, or from interactions of the atom with other particles of the plasma in which it is imbedded. Each of the bound states can, therefore, be considered to consist of a distribution of substates, with radiative transitions possible from any substate of one level to any substate of the other. Thus if the decay of the upper level occurs to a different substate of the lower level than that from which the excitation occurred, or if there is a redistribution of the excited electron from the original excited substate to some other substate (because, say, the atom suffers an elastic collision with another particle) then the emitted photon's energy may be slightly different from the incident photon's. Similarly, motions of the scattering centers with respect to the fixed laboratory frame can change the emitted photon's energy from the incident energy if the projection of the scatterer's velocity along the direction of propagation is different for the two photons, for then a differential Doppler shift can occur. (Example: imagine the incident photon to be moving in the *same* direction as *v* of the scatterer and the emitted photon to move in the *opposite* direction. The emitted photon will be *redshifted* by an amount $\Delta v = -2v_0v/c$ relative to the incident photon). Changes in photon direction and frequency during scattering are described by *redistribution functions* (see below). Note that in this process no significant part of the photon energy is imparted to the material.

(b) Scattering of a photon by a free electron (Thomson or Compton scattering) or by an atom or molecule (Rayleigh scattering). Thomson scattering may be viewed as the result of the free charge oscillating in the electromagnetic field of the radiation, Compton scattering as a collision of a photon with a free charged particle, and Rayleigh scattering as a resonance of a permitted "oscillation" of the bound system with the field. The remarks made in (a) above concerning redistribution and lack of coupling of radiant energy to the thermal pool apply here as well.

Similarly, we may consider the following to be examples of *thermal absorption processes* (and their inverses as thermal emission).

(a) A photon is absorbed by an atom in a bound state, and ionizes the bound electron, allowing it to escape with finite kinetic energy into the continuum. In this process of *photoionization* or *bound-free absorption*, the photon is destroyed and the excess of its energy over the electron's binding energy goes initially into the electron's kinetic energy, and ultimately into the general thermal pool after the electron suffers elastic collisions that establish a thermal velocity distribution for the particles. The inverse process, of a free electron dropping to a bound state with the creation of a photon whose energy equals the sum of the electron's kinetic and binding energies, is called direct *radiative recombination*. These processes clearly transfer energy back and forth between the radiation field and the thermal pool of the material.

(b) A photon is absorbed by a free electron moving in the field of an ion, resulting in an alteration of the electron's kinetic energy relative to the ion. The electron then, classically speaking, moves off on a different (hyperbolic) orbit around the ion. This process is known as *free-free absorption* because the electron is unbound both before and after absorbing the photon. The inverse process, leading to the emission of a photon, is referred to as *bremssstrahlung*.

(c) A photon is absorbed by an atom, leading to a transition of an electron from one bound state to another; this process is called *photoexcitation* or *bound-bound absorption*. The atom is then de-excited by an inelastic collision with another particle. Energy is put into the motion of the atom and the collision partner and thereby ends up as part of the thermal pool. The photon is said to have been *destroyed* by a *collisional de-excitation*. The inverse process leads to the collisional creation of a photon at the expense of the thermal energy of the gas.

(d) Photoexcitation of an atom with subsequent *collisional ionization* of the excited atom into the continuum. Photon energy again contributes to the thermal energy of particles. The inverse processes is called (three-body) *collisional recombination*.

To illustrate the conceptual limitations of the kinds of arguments given above, let us now consider some ambiguous cases. Suppose an atom has three bound levels *a*, *b*, and *c*, in order of increasing energy, and a photoexcitation from *a* to *c* occurs. Then suppose that *c* decays radiatively to *b*, and *b* then decays radiatively to *a*; this process is called *fluorescence*. Here a single photon of energy $h\nu_{ac} = E_c - E_a$ is degraded into two photons of energies $h\nu_{ab} = E_b - E_a$ and $h\nu_{bc} = E_c - E_b$. Was the original photon scattered or absorbed? By our original definition it has not been "scattered" and, moreover, the new photons may have vastly different properties (e.g., probability of escape through the boundary surface) from the original, so

that the nonlocal behavior of the radiation field has been altered. On the other hand, no contribution has been made to the thermal energy of the gas. Alternatively, consider the same process, but now with a collisional de-excitation *c* → *b* followed by an emission *b* → *a*. The original photon can be said to have been destroyed (absorbed); but is the emitted photon "thermally" emitted when most of the original energy was derived from the radiation field? Many other more complex and subtle cases may be constructed, which, taken together show the limits of usefulness of the absorption-vs-scattering description.

In fact, a truly consistent picture emerges only when we write down the full *equations of statistical equilibrium* (cf. Chapter 5), which describe all possible processes (both radiative and collisional) that couple an arbitrary state *i* to some other state *j*, and solve these together with the equations (*transfer equations*) that describe how the radiation is absorbed, emitted, and transported through the atmosphere. To do this is, in general, quite difficult, and formulation of successful methods of solution of the problem will occupy the bulk of this book. (The full import of these comments will emerge only when the student has studied the material through Chapter 12; nevertheless they should be borne in mind at all stages of subsequent development).

THE EXTINCTION COEFFICIENT

To describe the removal of energy from the radiation field by matter let us introduce a macroscopic coefficient $\chi(r, v, t)$ called the *extinction coefficient*, or *opacity*, or sometimes (loosely) the *total absorption coefficient*. This coefficient is defined such that an element of material, of cross-section dS and length ds , removes from a beam with specific intensity $I(r, n, v, t)$, incident normal to dS and propagating into a solid angle $d\omega$, an amount of energy

$$\delta E = \chi(r, n, v, t) I(r, n, v, t) dS ds d\omega dv dt \quad (2-1)$$

within a frequency band dv in a time dt . The extinction coefficient is the product of an atomic absorption cross-section (cm^2) and the number density of absorbers (cm^{-3}) summed over all states that can interact with photons of frequency v . The dimensions of χ are cm^{-1} , and $(1/\chi)$ gives a measure of the distance over which a photon can propagate before it is removed from the beam—i.e., a *photon mean-free-path* (cf. §2-2).

The frequency variation of χ may be extremely complicated, and may include thousands or millions of transitions (bound-bound, bound-free, and free-free). For *static media* in which there are no preferred directions imposed on an atomic scale (e.g., by a magnetic field), the *opacity is isotropic*. For *moving media*, the *opacity has an angular dependence* introduced by the

Doppler shift that radiation experiences in the fluid frame relative to its original frequency in the stationary laboratory frame; this Doppler shift obviously depends on the projection of the velocity vector onto the direction of the incident beam. In what follows we consider only static atmospheres.

As outlined earlier in this section, it is sometimes useful to distinguish between "absorption" and "scattering"; hence we introduce volume coefficients $\kappa(r, v, t)$ and $\sigma(r, v, t)$ that describe [via equation (2-1)] the rate at which energy is removed from the beam by "true absorption" and "scattering," respectively. The total extinction is given by

$$\chi(r, v, t) = \kappa(r, v, t) + \sigma(r, v, t) \quad (2-2)$$

That is, both processes are assumed to occur independently and to add linearly. In actual practice χ is sufficient to describe energy removed from the beam; the distinction between κ and σ is useful mainly in defining the emission coefficient.

In the calculation of χ it is necessary to include a correction for *stimulated emission* (see §§4-1 and 4-3). This is a quantum process in which radiation induces a downward transition from the upper state at a rate proportional to the product of a cross-section, the upper-state population, and the specific intensity. Because the process is proportional to $I(r, n, v, t)$ and effectively cancels out some of the opacity, it is convenient to include it in the definition of χ . Stimulated emission occurs only when the emitting system exists in a definite upper state (whether bound or free). There is thus no stimulated emission in Thomson scattering (free electrons) or Rayleigh scattering (involves virtual states) but there is stimulated emission in spectrum lines, even if they are described with a "scattering" coefficient.

If we know the value of $\chi(r, v, t)$ [or of $\kappa(r, v, t)$ and $\sigma(r, v, t)$], we have a complete *macroscopic* description of the rate at which material removes energy from a beam of radiation. But it is crucial to emphasize that the "completeness" of the description is *illusory*. The reason this unpleasant comment must be made is that the simple picture we obtain from equation (2-1) glosses over the fact that the level populations, which "determine" the rate of energy removal from the radiation field by their contribution to χ , are, in turn, *determined by* the radiation field via photoexcitations, photoionizations, radiative emission, radiative recombination, and related processes. Thus, in reality, the interaction of the radiation field with the absorbing material is *nonlinear*. The problem just described still remains (though more subtly) even if it is assumed that we can calculate level populations by local application of thermodynamic equilibrium relations that depend only on the density and temperature. (This is the so-called *local thermodynamic equilibrium* or *LTE* approximation.) The reason is that the temperature is determined by overall balance between energy emitted and energy absorbed

by the material, and thus by the nature of the radiation field and its response to the global properties of the atmosphere (e.g., boundaries, scattering, gradients, etc.). The remarks made in this paragraph carry over with equal force in the macroscopic description of emission. Again, the full significance of these comments will emerge only with considerable further development (see particularly §§5-1 and 5-3).

THE EMISSION COEFFICIENT

To describe the emission of radiation from the stellar material, we introduce a macroscopic *emission coefficient* or *emissivity* $\eta(r, n, v, t)$ defined such that the amount of energy released from an element of material of cross-section dS and length ds , into a solid angle $d\omega$, within a frequency band dv , in direction n in a time interval dt , is

$$\delta E = \eta(r, n, v, t) dS ds d\omega dv dt \quad (2-3)$$

The dimensions of η are ergs $\text{cm}^{-3} \text{sr}^{-1} \text{hz}^{-1} \text{sec}^{-1}$. As was true for the opacity, *thermal emissivity* is *isotropic* for *static media* (without imposed preferred directions) but is *angle-dependent* for *moving material* owing to Doppler-shift effects. For radiation emitted in scattering processes, there is normally an explicit angle-dependence, even for static media. The emissivity is calculated by summing products of upper-state populations and transition probabilities over all relevant processes that can release a photon at frequency v . In writing the transfer equation we shall usually use the unembellished symbol η to denote the total emissivity; if electron scattering terms appear explicitly in the same equation, η will then denote all other emission. Subscripts "c" and "l" may on occasion be used to denote continua and lines, respectively. Again, we must realize that the simplicity of this description is deceptive, for the reasons given above in the discussion of the extinction coefficient.

An important relation exists between the emission and absorption coefficients in the case of strict *thermodynamic equilibrium* (T.E.). If we consider an adiabatic enclosure in steady-state equilibrium containing a homogeneous medium, we know that the material will have the same temperature T throughout (otherwise it would be possible to devise processes to extract work from the temperature gradient, in violation of the second law of thermodynamics). Further, we may expect the radiation field to be isotropic and homogeneous throughout the enclosure (including at the surface of the walls), for if it were not, beams traveling in opposite directions would not be exactly similar and a directional transport of energy would result, from which work could be extracted, again in violation of the second law of thermodynamics. Consideration of the energy absorbed and emitted in

angle-frequency ranges $d\omega dv$ by an element of material, in time dt , now shows that if a steady-state thermal equilibrium is to be achieved (no net gain or loss of energy by the matter), the thermal emission must be given by

$$\eta'(v) = \kappa(v)I(n, v) \quad (2-4)$$

which is known as *Kirchhoff's law*. For an enclosure in strict T.E. at temperature T the intensity of the radiation field is given by the Planck function $B_v(T)$, so that

$$\eta^*(v) = \kappa^*(v)B_v(T) \quad (2-5)$$

which is the *Kirchhoff–Planck relation*. This result has been obtained without reference to the composition of the material and is valid (in T.E.) for all materials. [See the excellent discussion of the interaction of matter and radiation in T.E. in (160, 199–206) and in an article by Milne in (416, 93–96).]

Strictly speaking, the Kirchhoff–Planck law applies only in the case of a system in T.E. But if the material is subject only to small gradients over the mean free path a photon can travel before it is destroyed and thermalized by a collisional process (as is true, e.g., in the interior of a star), then we could expect equation (2-5) to be valid to a high degree of approximation at local values of the thermodynamic variables specifying the state of the material. In such a case we write

$$\eta'(r, v, t) = \kappa^*(r, v, t)B_v[T(r, t)] \quad (2-6)$$

The hypothesis of *local thermodynamic equilibrium* (or LTE) just mentioned makes the *assumption* that the occupation numbers of bound and free states of the material, the opacity, the emissivity—indeed all of the thermodynamic properties of the material—are the same as their T.E. values at the local values of T and density, throughout the entire atmosphere, out to the outermost regions. Only the radiation field is allowed to depart from its T.E. value of $B_v[T(r)]$, and is obtained from a solution of the transfer equation. Such an approach is manifestly *internally inconsistent*, although LTE expressions remain valid for certain quantities even in the general case. For example, equation (2-6) is a valid expression for the continuum emission coefficient even in the presence of departures from LTE so long as the velocity distribution of recombining (or, for free-free emission, colliding) particles is Maxwellian; the equation is not valid for line emission, and further, the LTE formula for the opacity is not correct. The use of LTE is a computational expedient that simplifies the calculation of models of stellar atmospheres, and has been widely applied. (We shall employ it in places to provide a prototype with which we can introduce basic mathematical techniques of solving transfer problems, and will discuss models built assuming LTE in §§7-2 through 7-4.) But it must be stressed that stellar atmospheres are regions

in which there are large gradients of material properties, and an open boundary through which radiation freely escapes; the radiation field is therefore highly anisotropic and has a markedly non-Planckian character. One might argue for using LTE, even though the radiation field is obtained from solving a *nonlocal* transfer equation, if one could show that some mechanism, specifically collisions among the particles, *enforced* LTE populations. As already mentioned above, and as we shall see in detail in §5-3 and in Chapters 7 and 11–14, this will not, in general, be the case. Rather, the radiation field determines the state of the material, and hence equation (2-6) becomes invalid; in the end we must carry through a general analysis in which we specify the thermodynamic state of the gas and the distribution function of the radiation field simultaneously by solving the coupled equations of transfer and statistical equilibrium.

Let us now consider radiation scattered by the material. For simplicity of notation, we suppress explicit reference to t , though all of the quantities may be time-dependent. As described earlier, in scattering processes both the direction and frequency of a photon may change. These changes are described by a *redistribution function*

$$R(v', n'; v, n) dv' dv (d\omega'/4\pi)(d\omega/4\pi)$$

which gives the joint probability that a photon will be scattered from direction n' in solid angle $d\omega'$ and frequency range $(v', v' + dv')$ into solid angle $d\omega$ in direction n and frequency range $(v, v + dv)$. We shall derive redistribution functions and discuss them in detail in Chapter 13, but it is helpful to mention some of the general properties of these functions at the present time. We shall normalize R such that

$$(4\pi)^{-2} \oint d\omega' \oint d\omega \int_0^\infty dv' \int_0^\infty dv R(v', n'; v, n) = 1 \quad (2-7)$$

The redistribution function contains within it both a normalized *absorption profile* $\phi(v)$, and a normalized *emission profile* $\psi(v)$ for the scattering process. From the physical definition given above, it is evident that if we integrate over all emitted frequencies and angles we must obtain the probability for absorption from solid angle $d\omega'$ and frequency range v' —i.e., $\phi(v')dv'd\omega'/4\pi$. Thus

$$\phi(v') = (4\pi)^{-1} \oint d\omega \int_0^\infty dv R(v', n'; v, n) \quad (2-8)$$

which by virtue of equation (2-7) is normalized such that $\int \phi(v')dv' = 1$. If $\sigma_0(r)$ denotes the total scattering coefficient, we may write $\sigma(r, v') = \sigma_0(r)\phi(v')$. The joint probability that an amount of energy $\sigma_0(r)I(r, n', v')$ will be removed from the beam in solid angle $d\omega'$ at frequency v' , and scattered into $d\omega$ at frequency v , is $\sigma_0(r)R(v', n'; v, n)I(r, n', v')dv'dv(d\omega'/4\pi)(d\omega/4\pi)$. Hence if we

integrate over all incoming frequencies and angles, we find the total amount of energy emitted at frequency v into solid angle $d\omega$, namely

$$\eta^S(r, n, v) dv(d\omega/4\pi) = \sigma_0(r) dv(d\omega/4\pi) \oint(d\omega'/4\pi) \int_0^\infty dv' R(v', n'; v, n) I(r, n', v') \quad (2-9)$$

Exercise 2-1: Show that the total emission rate $\int dv \oint d\omega \eta(r, n, v)$ equals the total energy removed from the beam $4\pi\sigma_0(r) \int \phi(v') J(r, v') dv'$ —i.e., that the scattering process is *conservative*.

Equation (2-9) gives the full angle-frequency dependence of the emission profile. It is usually difficult to treat radiative transfer problems in the degree of generality implied here, and useful simplifications of the problem can be made. For example, if we are primarily interested in redistribution in frequency and not in angle, we could assume that $I(r, n, v)$ is nearly isotropic, and replace it in equation (2-9) with $J(r, v)$. Then the emission into $dv dw$ is

$$\eta^S(r, v) = \sigma_0(r) \int_0^\infty R(v', v) J(r, v') dv' \quad (2-10)$$

where the *angle-averaged redistribution function*

$$R(v', v) \equiv (4\pi)^{-1} \oint R(v', n'; v, n) d\omega' = (4\pi)^{-1} \oint R(v', n'; v, n) dw \quad (2-11)$$

gives the redistribution probability from $(v, v + dv')$ to $(v, v + dv)$ and is normalized such that

$$\int_0^\infty dv' \int_0^\infty dv R(v', v) = \int_0^\infty \phi(v') dv' = 1 \quad (2-12)$$

The function $R(v', v)$ is rendered independent of angle as a result of integrating over either $d\omega'$ or $d\omega$; this follows from the fact that (cf §13-2) $R(v', n'; v, n)$ depends only on the angle between n' and n . Equation (2-10) provides an extremely useful approximation in line transfer problems because the crucial phenomenon there is the frequency diffusion of photons from the opaque line core (where they are trapped) to the more transparent line wings (whence they may escape from the atmosphere at depths where I is, in fact, very nearly isotropic). In the angle-averaged approximation the emission profile

$$\psi(v) \equiv \eta(r, v) / \int_0^\infty \eta(r, v) dv$$

is given by

$$\psi(v) = \int_0^\infty R(v', v) J(r, v') dv' / \int_0^\infty \phi(v') J(r, v') dv' \quad (2-13)$$

which shows that the distribution of emitted photons depends upon the frequency profile of the incoming radiation.

In the limiting case that the intensity is independent of frequency, we obtain *natural excitation*, with

$$\psi^*(v) = \int_0^\infty R(v', v) dv' \quad (2-14)$$

If we have $R(v', v) = R(v, v')$, as occurs in most cases of interest (cf. §13-3), then $\psi^*(v) = \phi(v)$; that is, for *natural excitation*, the *emission and absorption profiles are identical* (a result that is *not true in general!*). Natural excitation prevails, of course, in T.E., and it is usually thought of in that context. There are, however, other physical circumstances in which the result $\psi(v) = \phi(v)$ is recovered. In particular, suppose that there is a complete reshuffling of atoms in their excited state in such a way that there is *no correlation between the frequencies of incoming and scattered photons*; then both have frequencies *independently distributed* over the absorption profile $\phi(v)$. This situation is referred to as *complete redistribution*, or *complete noncoherence*. A good approximation to this case occurs, for instance, when atoms are so strongly perturbed by collisions during the scattering process that the excited electrons are randomly redistributed over substates of the upper level. In this case, both the absorption and emission probabilities *independently* are proportional to the number of substates available at each frequency within the line [i.e., to $\phi(v)$ itself], and the joint absorption–emission probability $R(v', v)$ is the product of these two independent distributions—i.e., $R(v', v) = \phi(v')\phi(v)$. For *complete redistribution*, the emissivity is

$$\eta^S(r, v) = \sigma_0(r)\phi(v) \int_0^\infty \phi(v') J(r, v') dv' \quad (2-15)$$

from which we see clearly that the emission and absorption profiles are identical. Complete redistribution is also a good approximation within the Doppler core of a spectrum line, and actually provides an excellent first approximation in line transfer problems. We shall, in fact, assume complete redistribution in our discussion of line formation until Chapter 13.

Another class of problems arises when we focus attention on the angular redistribution of the emitted radiation, but assume that the scattering is essentially *coherent* (i.e., $v' = v$). This is the situation of interest, e.g., in scattering of light by large particles in a planetary (including earth's) atmosphere. We can then write

$$R(v', n'; v, n) = g(n', n)\phi(v') \delta(v - v') \quad (2-16)$$

where δ is the Dirac function and g is an *angular phase function* normalized such that

$$(4\pi)^{-1} \oint g(n', n) d\omega' = 1 \quad (2-17)$$

30 The Equation of Transfer

Two important phase functions are those for isotropic scattering

$$g(\mathbf{n}', \mathbf{n}) \equiv 1 \quad (2-18)$$

and the *dipole* phase function (which applies for Thomson and Rayleigh scattering)

$$g(\mathbf{n}', \mathbf{n}) = \frac{3}{4}(1 + \cos^2 \Phi) \quad (2-19)$$

where $\cos \Phi = \mathbf{n}' \cdot \mathbf{n}$. The phase functions for scattering by large particles (i.e., whose size is comparable to a wavelength of light) are often extremely complicated and show large, rapid variations as a function of angle (312; 359, Chap. 4).

For *coherent scattering*, equation (2-9) reduces to

$$\eta^S(\mathbf{r}, \mathbf{n}, v) = \sigma(\mathbf{r}, v) \oint I(\mathbf{r}, \mathbf{n}', v) g(\mathbf{n}', \mathbf{n}) \frac{d\omega'}{4\pi} \quad (2-20)$$

In a spectrum line, coherent scattering would occur only if the lower state of the line were sharp, the upper state were not perturbed during emission, and the scattering atoms were at rest in the observer's frame. This is not the case, however, and line scattering is much more accurately described by complete redistribution (except in the far line wings where ϕ varies slowly over the range corresponding to a Doppler shift). On the other hand, for continuum scattering (e.g., by electrons) the frequency distribution of radiation is smooth and essentially constant over the typical frequency shifts occurring in the scattering process. For this reason continuum scattering processes are customarily treated as if they were coherent (though this may be inadequate near a spectrum line). Moreover, as the angular redistribution effects from a dipole phase function are usually very small in a stellar atmosphere, it is customary to assume that continuum scattering is also isotropic, and to write

$$\eta^S(\mathbf{r}, v) = \sigma(\mathbf{r}, v) J(\mathbf{r}, v) \quad (2-21)$$

2-2 The Transfer Equation

DERIVATION

Let us now consider the problem of radiative transport. Choose an inertial coordinate system and examine the flow of energy through a fixed volume element in a definite time interval. Let us assume that the radiation field is, in general, time-dependent. If we suppose the material to be at rest, then both χ and η will be isotropic (unless we consider anisotropic scattering). In moving material one must account for changes in photon frequency and

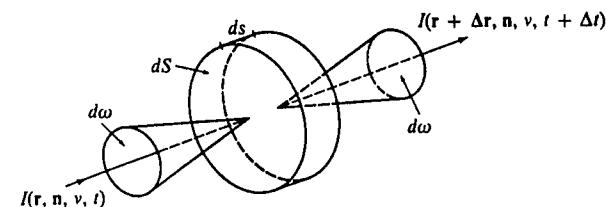


FIGURE 2-1
Element of absorbing and emitting material considered in derivation of transfer equation.

direction (Doppler shift and aberration) resulting from the transformation between the laboratory frame and the fluid frame. These effects depend upon $\mathbf{n} \cdot \mathbf{v}$; hence both χ and η will have an explicit angle-dependence in this case. Now calculate the energy in a frequency interval dv , passing in a time dt through a volume element of length ds and cross-section dS oriented normal to a ray traveling in direction \mathbf{n} into solid angle $d\omega$ (see Figure 2-1). The difference between the amount of energy that emerges (at position $\mathbf{r} + \Delta \mathbf{r}$ at time $t + \Delta t$) and that incident (at \mathbf{r} and t) must equal the amount created by emission from the material in the volume minus the amount absorbed. That is,

$$[I(\mathbf{r} + \Delta \mathbf{r}, \mathbf{n}, v, t + \Delta t) - I(\mathbf{r}, \mathbf{n}, v, t)] dS d\omega dv dt \\ = [\eta(\mathbf{r}, \mathbf{n}, v, t) - \chi(\mathbf{r}, \mathbf{n}, v, t) I(\mathbf{r}, \mathbf{n}, v, t)] ds dS d\omega dv dt \quad (2-22)$$

Let s denote the path-length along the ray; then $\Delta t = \Delta s/c$, and

$$I(\mathbf{r} + \Delta \mathbf{r}, \mathbf{n}, v, t + \Delta t) = I(\mathbf{r}, \mathbf{n}, v, t) + [c^{-1}(\partial I/\partial t) + (\partial I/\partial s)] ds \quad (2-23)$$

Substituting equation (2-23) into equation (2-22) we have the *transfer equation*

$$[c^{-1}(\partial I/\partial t) + (\partial I/\partial s)] I(\mathbf{r}, \mathbf{n}, v, t) = \eta(\mathbf{r}, \mathbf{n}, v, t) - \chi(\mathbf{r}, \mathbf{n}, v, t) I(\mathbf{r}, \mathbf{n}, v, t) \quad (2-24)$$

The derivative along the ray may be re-expressed in terms of an orthogonal coordinate system:

$$\frac{\partial I}{\partial s} = \left(\frac{\partial x}{\partial s} \right) \left(\frac{\partial I}{\partial x} \right) + \left(\frac{\partial y}{\partial s} \right) \left(\frac{\partial I}{\partial y} \right) + \left(\frac{\partial z}{\partial s} \right) \left(\frac{\partial I}{\partial z} \right) = n_x \frac{\partial I}{\partial x} + n_y \frac{\partial I}{\partial y} + n_z \frac{\partial I}{\partial z} \quad (2-25)$$

where (n_x, n_y, n_z) are the components of the unit vector \mathbf{n} . We may thus rewrite equation (2-24) as

$$[c^{-1}(\partial I/\partial t) + (\mathbf{n} \cdot \nabla)] I(\mathbf{r}, \mathbf{n}, v, t) = \eta(\mathbf{r}, \mathbf{n}, v, t) - \chi(\mathbf{r}, \mathbf{n}, v, t) I(\mathbf{r}, \mathbf{n}, v, t) \quad (2-26)$$

For a one-dimensional planar atmosphere $n_z = (dz/ds) = \cos \theta = \mu$; further, the derivatives $(\partial/\partial x)$ and $(\partial/\partial y)$ are identically zero, and we obtain

$$[c^{-1}(\partial/\partial t) + \mu(\partial/\partial z)]I(z, n, v, t) = \eta(z, n, v, t) - \chi(z, n, v, t)I(z, n, v, t) \quad (2-27)$$

or, for the time-independent case,

$$\mu[\partial I(z, n, v)/\partial z] = \eta(z, n, v) - \chi(z, n, v)I(z, n, v) \quad (2-28)$$

Equation (2-28) is the “standard” transfer equation for plane-parallel model-atmospheres calculations; the coordinate z increases *upward* in the atmosphere (i.e., toward an external observer). For static media, the specification (z, n, v) in η and χ may be reduced to (z, v) only. Note that if η and χ are given, equation (2-28) is an *ordinary differential equation*, which may be solved for all relevant choices of μ and v . When η includes scattering terms, the transfer equation becomes an *integro-differential equation* containing angle and frequency integrals of I .

THE TRANSFER EQUATION AS A BOLTZMANN EQUATION

The basic equation describing particle transport in kinetic theory is the *Boltzmann equation*; we shall now show that the transfer equation is just the Boltzmann equation for photons. Suppose we have a particle distribution function $f(r, p, t)$ that gives the number density of particles in the phase volume element $(r, r + dr), (p, p + dp)$. We follow the evolution of f within a particular phase-space element for a time interval dt , in which $r \rightarrow r + v dt$ and $p \rightarrow p + F dt$, where F denotes externally imposed forces acting on the particles. The phase-space element evolves from

$$(d^3r)_0(d^3p)_0 \rightarrow (d^3r)(d^3p) = J[(d^3r)_0(d^3p)_0]$$

where J is the *Jacobian* of the transformation.

Exercise 2-2: Show that to first order in dt the Jacobian of the transformation of a phase volume element is $J = 1$.

In view of the result of Exercise 2-2 we see that the phase-space element is deformed, but its phase volume is *unchanged*. If all external forces F are continuous, then the deformation of the phase-space element is continuous, and all particles originally within the volume remain there; as the volume itself is unchanged, the particle density is unchanged. But if, in addition, collisions occur, individual particles may be reshuffled from one element of phase space to another “discontinuously”; i.e., their neighbors may be totally unaffected during the same time interval. Therefore, the change in the particle

number density within a phase-space element must equal the *net* number introduced into the element by collisions; i.e.,

$$\begin{aligned} \frac{\partial f}{\partial t} + \left(\frac{\partial x}{\partial t} \right) \left(\frac{\partial f}{\partial x} \right) + \left(\frac{\partial y}{\partial t} \right) \left(\frac{\partial f}{\partial y} \right) + \left(\frac{\partial z}{\partial t} \right) \left(\frac{\partial f}{\partial z} \right) \\ + F_x \left(\frac{\partial f}{\partial p_x} \right) + F_y \left(\frac{\partial f}{\partial p_y} \right) + F_z \left(\frac{\partial f}{\partial p_z} \right) = \left(\frac{Df}{Dt} \right)_{\text{coll}} \end{aligned} \quad (2-29)$$

or, in more compact notation

$$(\partial f/\partial t) + (\mathbf{v} \cdot \nabla_p)f + (\mathbf{F} \cdot \nabla_p)f = (Df/Dt)_{\text{coll}} \quad (2-30)$$

For a “gas” consisting of photons (with rest-mass zero), in the absence of general relativistic effects, $\mathbf{F} \equiv 0$, and photon propagation in an inertial frame occurs in straight lines with $\mathbf{v} = cn$, while the frequency remains constant. The distribution function f_R can be written in terms of the specific intensity by means of equation (1-2). The analogues of “collisions” are photon interactions with the material, and the net number of photons introduced into the volume will be the energy emitted minus the energy absorbed, divided by the energy per photon. Thus for photons equation (2-30) becomes

$$(chv)^{-1}[(\partial I/\partial t) + c(\mathbf{n} \cdot \nabla)I] = (\eta - \chi I)/(hv) \quad (2-31)$$

which is identical to the transfer equation (2-26). In effect the transfer equation is a Boltzmann equation for a fluid that is subject to no external forces but which suffers strong collisional effects. As will be seen in §2-3, the *moments* of the transfer equation yield *dynamical equations* for the radiation field, just as moments of the Boltzmann equation for a gas lead to equations of hydrodynamics.

SPHERICAL GEOMETRY

In a *spherically symmetric* medium, the specific intensity will be independent of the coordinates Θ and Φ of the triplet (r, Θ, Φ) which specifies a position in the atmosphere, and of the azimuthal angle ϕ of the pair (θ, ϕ) which specifies the direction of the beam relative to the local outward normal $\hat{\mathbf{r}}$. Thus $I(r, n, v, t)$ reduces to $I(r, \theta, v, t)$. In writing the transfer equation, starting from the general form of equation (2-24), we must now account for the variation of θ along a displacement, and employ the general form $ds = dr \hat{\mathbf{r}} + r d\theta \hat{\theta}$. As is clear from the geometry of the situation (see Figure 2-2), $dr = \cos \theta ds$, while $r d\theta = -\sin \theta ds$ (note that $d\theta \leq 0$ for any ds), so that

$$(\partial/\partial s) \rightarrow \cos \theta(\partial/\partial r) - r^{-1} \sin \theta(\partial/\partial \theta) = \mu(\partial/\partial r) + r^{-1}(1 - \mu^2)(\partial/\partial \mu) \quad (2-32)$$

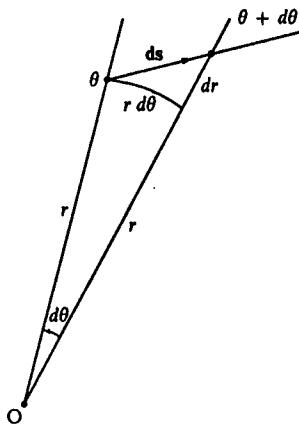


FIGURE 2-2
Geometric relations among variables used in derivation of transfer equation in a spherically symmetric medium.

where, as usual, $\mu = \cos \theta$. Hence the transfer equation for a *spherically symmetric atmosphere* is

$$[c^{-1}(\partial/\partial t) + \mu(\partial/\partial r) + r^{-1}(1 - \mu^2)(\partial/\partial \mu)]I(r, \mu, v, t) = \eta(r, v, t) - \chi(r, v, t)I(r, \mu, v, t) \quad (2-33)$$

which simplifies in an obvious way in the time-independent case. Note that now, even with η and χ specified, equation (2-33) is a *partial differential equation* in r and μ . However, this added complexity can be avoided by using the (straight-line) characteristic paths that reduce the spatial operator to a single derivative with respect to pathlength (see §7-6). In fact, equation (2-33) is not structurally different from equation (2-28) and can be solved almost as easily.

Exercise 2-3: (a) Consider an atmosphere which is *axially symmetric* but not *spherically symmetric* (e.g., a rotationally flattened star). Show that now $I(r, n) = I(r, \Theta, \theta, \phi)$. (b) For the general case where $I(r, n) = I(r, \Theta, \Phi, \theta, \phi)$ (e.g., a rotationally flattened star illuminated by a companion), show that the transfer equation in spherical coordinates, accounting for all the spatial derivatives, is

$$c^{-1}(\partial I/\partial t) + \mu(\partial I/\partial r) + (\gamma/r)(\partial I/\partial \Theta) + (\sigma/r \sin \Theta)(\partial I/\partial \Phi) + r^{-1}(1 - \mu^2)(\partial I/\partial \mu) - (\sigma \cot \Theta/r)(\partial I/\partial \phi) = \eta - \chi I$$

where $\gamma \equiv \cos \phi \sin \theta$ and $\sigma \equiv \sin \phi \sin \theta$.

OPTICAL DEPTH AND THE SOURCE FUNCTION

For the remainder of §2-2 let us confine attention to the time-independent planar transfer equation (2-28). Writing $d\tau(z, v) \equiv -\chi(z, v) dz$, we define an

optical depth scale $\tau(z, v)$ which gives the integrated absorptivity of the material along the line of sight as

$$\tau(z, v) = \int_z^{z_{\max}} \chi(z', v) dz' \quad (2-34)$$

The negative sign is introduced so that the optical depth increases *inward* into the atmosphere from zero at the surface (where $z = z_{\max}$), and thus provides a measure of how deeply an outside observer can see into the material [cf. equations (2-47) and (2-52)]. Recalling that χ^{-1} is the photon mean-free-path, we recognize that $\tau(z, v)$ is just the *number of photon mean-free-paths* at frequency v along the line of sight from z_{\max} to z . In addition, we define the *source function* to be the ratio of the total emissivity to total opacity,

$$S(z, v) = \eta(z, v)/\chi(z, v) \quad (2-35)$$

To simplify the notation we shall for the present suppress explicit reference to z and μ , and denote frequency dependence with a subscript v . The equation of transfer may then be written in its standard form

$$\mu(\partial I_v/\partial \tau_v) = I_v - S_v \quad (2-36)$$

From the discussion of §2-1 we can write prototype expressions for the source function which we use to study methods of solving equation (2-36). Suppose first we have strict LTE. Then from equation (2-6) we have

$$S_v = B_v \quad (2-37)$$

If we have a contribution from thermal absorption and emission plus a contribution from a coherent, isotropic, continuum scattering term (say from Thomson scattering by free electrons or from Rayleigh scattering) then we could write

$$\chi_v = \kappa_v + \sigma_v \quad (2-38)$$

$$\text{and } S_v = (\kappa_v B_v + \sigma_v J_v)/(\kappa_v + \sigma_v) \quad (2-39)$$

For a spectrum line with an overlapping background continuum we have

$$\chi_v = \chi_c + \chi_l(v) = \chi_c + \chi_l \phi_v \quad (2-40)$$

where χ_c and χ_l denote the continuum and line opacities, respectively. If we assume that a fraction ϵ of the line emission occurs from thermal processes and the remainder is given by angle-averaged complete redistribution [equation (2-15)], we can write

$$\eta_v = \chi_c B_v + \chi_l \phi_v \left[\epsilon B_v + (1 - \epsilon) \int \phi_v J_v dv \right] \quad (2-41)$$

and

$$S_v = \left(\frac{r + \epsilon \phi_v}{r + \phi_v} \right) B_v + \left[\frac{(1 - \epsilon) \phi_v}{r + \phi_v} \right] \int \phi_v J_v dv = \xi_v B_v + (1 - \xi_v) \int \phi_v J_v dv \quad (2-42)$$

where $r \equiv \chi_c / \chi_i$. (We may ignore the frequency variation of the continuum over a line-width.) In equations (2-39) and (2-42) we have examples of the explicit appearance of integrals of the radiation field over angle and frequency, which shows the integro-differential nature of the transfer equation. It must be stressed that the source functions in equations (2-37), (2-39), and (2-42) are *only illustrative*; they are based on essentially heuristic arguments, and a physically rigorous formulation can be provided only after the equations of statistical equilibrium (Chapter 5) are developed.

BOUNDARY CONDITIONS

Solution of the transfer equation requires the specification of *boundary conditions*. Two problems of fundamental astrophysical importance are (a) the *finite slab* (in planar geometry) or *shell* (spherical geometry), and (b) a medium (e.g., a stellar atmosphere) that has an open boundary on one side but is so optically thick that it can be imagined to extend to infinity on the other side—the *semi-infinite atmosphere*.

For the finite slab of total geometrical thickness Z and total optical depth T_v (defined to be zero on the side nearest the observer), a unique solution is obtained if the intensity incident on both faces of the slab is specified. Writing θ for the angle between a ray and the normal directed toward the observer, and $\mu \equiv \cos \theta$, we must specify the two functions I^+ and I^- such that

$$I(\tau_v = 0, \mu, v) = I^-(\mu, v), \quad (-1 \leq \mu \leq 0) \quad (2-43)$$

at the upper boundary, and

$$I(\tau_v = T_v, \mu, v) = I^+(\mu, v), \quad (0 \leq \mu \leq 1) \quad (2-44)$$

at the lower boundary. For a shell of outer radius R and inner radius r_c , equation (2-43) still applies at $r = R$.

Exercise 2-4: (a) At the inner boundary of a spherical shell, $r = r_c$, show that the lower boundary condition is given by $I(r_c, +\mu, v) \equiv I(r_c, -\mu, v)$ if the central volume $r \leq r_c$ is *void*; this is Milne's "planetary nebula" boundary condition. (b) If the volume contains a *point source* (a star) of intensity I_0 , show that the result in (a) must be augmented by $I(r_c, +\mu, v) = I_0(v) \delta(\mu - 1)$. (c) Extended results (a) and (b) to the case of the volume being partially filled by an *opaque source* on the

range $0 \leq r \leq r_*$, ($r_* \leq r_c$) with intensity $I_0(\mu', v)$ where μ' is the angle cosine at the opaque surface; this case simulates an envelope around a star. (d) Show in case (a) above that the flux is *identically zero* at all points $r \leq r_c$.

In the semi-infinite case (planar or spherical), the radiation field incident upon the upper boundary must be specified by an equation of the form of (2-43); for stellar atmospheres work, it is customary to assume $I^- \equiv 0$ (clearly this would *not* be done, e.g., in a binary system). For a lower boundary condition one may replace equation (2-44) by a *boundedness condition* in analytical work where the limit $\tau_v \rightarrow \infty$ is taken. Specifically we impose the requirement that

$$\lim_{\tau_v \rightarrow \infty} I(\tau_v, \mu, v) e^{-\tau_v/\mu} = 0 \quad (2-45)$$

The reasons for this particular choice will become clear in the discussion below. Alternatively, at great depth in the atmosphere we may write $I(\tau_v, \mu, v)$ in terms of the *local* value of S_v and its gradient, or may specify the *flux*; these conditions follow naturally from physical considerations in the *diffusion limit* where the photon mean free path is much smaller than its optical depth from the surface (see §2-5).

SIMPLE EXAMPLES

Before writing the formal solution of the equation of transfer, it is instructive to consider a few simple examples in planar geometry.

(a) Suppose no material is present. Then $\chi_v = \eta_v = 0$, and equation (2-28) reduces to $(\partial I_v / \partial z) = 0$ or $I_v = \text{constant}$. This result is consistent with the proof in §1-1 of the invariance of the specific intensity when no sources or sinks are present.

(b) Suppose that the material emits at frequency v , but cannot absorb. Then equation (2-28) is $\mu (\partial I_v / \partial z) = \eta_v$, and for a finite slab the emergent intensity is given by

$$I(Z, \mu, v) = \mu^{-1} \int_0^Z \eta(z, v) dz + I^+(0, \mu, v) \quad (2-46)$$

The physical situation described above occurs in the formation of optically forbidden lines in nebulae. Atoms may be excited to *metastable levels* by collisions; because nebular densities are so low, the chances of a second collision leading to de-excitation are very small, so the atoms can remain unperturbed in these levels for long periods of time, and large numbers of atoms may accumulate in these states. Eventually some of the atoms decay via "forbidden" transitions, which have very small but nonzero transition probabilities, and emit photons. Because the line is forbidden, the probability of reabsorption is negligible, and the photon escapes. Thus photons are created

at the expense of the energy in the thermal pool, and none are destroyed by absorption.

(c) Suppose that radiation is absorbed but not emitted by the material. Then $\mu(\partial I_v/\partial z) = -\chi_v I_v$, and defining $d\tau_v = -\chi_v dz$, the emergent intensity from a finite slab of total optical thickness T_v is

$$I(\tau_v = 0, \mu, v) = I^+(T_v, \mu, v) \exp(-T_v/\mu) \quad (2-47)$$

Equation (2-47) applies, for example, to radiation passing through a filter in which photons are absorbed and degraded into photons of some very different frequency (e.g., extreme far-infrared heat radiation) before being re-emitted, or are destroyed and converted into kinetic energy of the particles in the absorbing medium.

FORMAL SOLUTION

Let us now obtain a formal solution of the equation of transfer; we confine attention exclusively to planar geometry. Regarding S as given, equation (2-36) is a linear first-order differential equation with constant coefficients, and must therefore have an integrating factor. The integrating factor is easily shown to be $\exp(-\tau_v/\mu)$, so that

$$\partial[I, \exp(-\tau_v/\mu)]/\partial\tau_v = -\mu^{-1}S_v \exp(-\tau_v/\mu) \quad (2-48)$$

Integration of equation (2-48) yields

$$I(\tau_1, \mu, v) = I(\tau_2, \mu, v)e^{-(\tau_2-\tau_1)/\mu} + \mu^{-1} \int_{\tau_1}^{\tau_2} S_v(t)e^{-(t-\tau_1)/\mu} dt \quad (2-49)$$

If S_v is given, equation (2-49) provides a complete solution of the planar transfer problem.

We may apply equation (2-49) at an arbitrary interior point in a semi-infinite atmosphere. For $\mu \geq 0$ (outgoing radiation), set $\tau_1 = \tau_v$ and $\tau_2 = \infty$, and impose the boundedness condition of equation (2-45); the result is

$$I(\tau_v, \mu, v) = \int_{\tau_v}^{\infty} S_v(t)e^{-(t-\tau_v)/\mu} dt/\mu, \quad (0 \leq \mu \leq 1) \quad (2-50)$$

For incoming radiation, ($-1 \leq \mu \leq 0$), set $\tau_2 = 0$ and apply the upper boundary condition $I^- \equiv 0$; we then obtain

$$I(\tau_v, \mu, v) = \int_0^{\tau_v} S_v(t)e^{-(\tau_v-t)/(-\mu)} dt/(-\mu), \quad (-1 \leq \mu \leq 0) \quad (2-51)$$

One of the most important applications of equation (2-50) is the expression for the emergent intensity seen by an external observer ($\tau = 0$),

$$I(0, \mu, v) = \int_0^{\infty} S_v(t)e^{-t/\mu} dt/\mu \quad (2-52)$$

The physical significance of equation (2-52) is that the emergent intensity is a weighted average of the source function along the line of sight; the weighting function is the fraction of the energy emitted at each depth that penetrates to the surface along a ray whose optical slant-length is (τ/μ) . Mathematically speaking, equation (2-52) shows that the specific intensity is the *Laplace transform* of the source function, a property that may be used to solve for S in certain classes of problems.

Considerable insight can be gained by supposing the source function is a linear function of depth: $S_v(\tau_v) = S_{0v} + S_{1v}\tau_v$; then equation (2-52) yields

$$I(0, \mu, v) = S_{0v} + S_{1v}\mu = S_v(\tau_v = \mu) \quad (2-53)$$

which is known as the *Eddington-Barbier relation*. This result states that the emergent intensity is characteristic of the value of the source function at about optical depth unity along the line of sight (recall that τ_v represents the *normal* optical depth, so that *slant* optical depth unity for a ray penetrating at angle $\cos^{-1}\mu$ occurs at $\tau_v = \mu$). The Eddington-Barbier relation has been widely applied in empirical analyses of the solar and stellar spectra, and provides a basic conceptual framework for many interpretive methods. In the case of the sun, when we observe, at a fixed frequency, the variation in intensity from disk center ($\mu = 1$) to the limb ($\mu \rightarrow 0$) we can (in principle) infer information about $S_v(\tau_v)$ for $0 \lesssim \tau_v \lesssim 1$. For stars, we cannot observe the center-to-limb variation, but it is clear that if we observe at different frequencies (e.g., within a spectral line), we encounter unit optical depth in higher layers for frequencies with high opacity (e.g., line-center) and in deeper layers for frequencies with low opacity (e.g., line-wings). If we then know something about the frequency-variation of S_v , we can infer information about its depth-variation; for example, in LTE, $S_v = B_v$ and the frequency-variation over a narrow line can be ignored, so that one can, in principle, infer the run of the temperature with depth. Although it is extremely useful conceptually, the Eddington-Barbier relation should not be applied indiscriminately and used literally to argue that $I(0, \mu, v)$ is identical to $S_v(\tau_v = \mu)$, because (a) there are always significant contributions to $I(0, \mu, v)$ from other depths (i.e., there is an intrinsic "fuzziness" in the problem), and (b) the assumptions from which it follows may not be valid. A detailed critique of the limitations of the Eddington-Barbier relation can be found in (18, 121–130) and (20, 20–30).

Exercise 2-5: Suppose the source function is to be represented by a power-series expansion about the point τ_* ; i.e., $S(\tau) \approx S(\tau_*) + S'(\tau_*)(\tau - \tau_*) + \frac{1}{2}S''(\tau_*)(\tau - \tau_*)^2$. Calculate the emergent intensity and show that the choice $\tau_* = \mu$ is "optimum" in the sense that it eliminates the contribution of S' and minimizes the contribution of S'' to $I(0, \mu)$.

Another instructive example to consider is a finite slab of optical thickness T , within which S is constant, and upon which there is no incident radiation.

The normally emergent intensity is $I(0, 1) = S(1 - e^{-T})$. For $T \gg 1$, $I = S$. This result is sensible physically, for the radiation that emerges consists of those photons emitted over a mean-free-path from the surface; the emission rate is η and the mean-free-path is χ^{-1} , hence $I = \eta/\chi = S$. For $T \ll 1$, $e^{-T} \approx 1 - T$, so $I \approx ST$. Again this result is physically reasonable, for in the optically thin case we can see through the entire volume; hence the energy emitted (per unit area) must be the emissivity per unit volume η times the total path-length Z , or $I = \eta Z = (\eta/\chi)(\chi Z) = ST$. Note that this result is consistent with equation (2-46).

THE SCHWARZSCHILD–MILNE EQUATIONS

By integration of the formal solution for the specific intensity over angle, concise expressions for the moments of the radiation field may be derived. Thus by substitution of equations (2-50) and (2-51) into equation (1-4) we have for the mean intensity

$$J_v(\tau_v) = \frac{1}{2} \int_{-1}^1 I_v(\tau_v, \mu) d\mu = \frac{1}{2} \left[\int_0^1 d\mu \int_{\tau_v}^{\infty} S_v(t) e^{-(t-\tau_v)/\mu} \frac{dt}{\mu} + \int_{-1}^0 d\mu \int_0^{\tau_v} S_v(t) e^{-(\tau_v-t)/(-\mu)} \frac{dt}{(-\mu)} \right] \quad (2-54)$$

Equation (2-54) is reduced to a more useful form by interchanging the order of integration, and making the substitution $w = \pm 1/\mu$ in the first and second integrals respectively. Then

$$J_v(\tau_v) = \frac{1}{2} \left[\int_{\tau_v}^{\infty} dt S_v(t) \int_1^{\infty} dw \frac{e^{-w(t-\tau_v)}}{w} + \int_0^{\tau_v} dt S_v(t) \int_1^{\infty} dw \frac{e^{-w(\tau_v-t)}}{w} \right] \quad (2-55)$$

The integrals over w are of a standard form and are called the first *exponential integral*. In general, for integer-values of n , the n th exponential integral is defined as

$$E_n(x) \equiv \int_1^{\infty} t^{-n} e^{-xt} dt = x^{n-1} \int_x^{\infty} t^{-n} e^{-t} dt \quad (2-56)$$

In terms of $E_1(x)$, equation (2-55) can be rewritten as

$$J_v(\tau_v) = \frac{1}{2} \int_0^{\infty} S_v(t) E_1|t_v - \tau_v| dt \quad (2-57)$$

Equation (2-57) was first derived by K. Schwarzschild and is named in his honor; Schwarzschild's paper (416, 35) is one of the foundation stones of radiative transfer theory, and merits careful reading. Because the integral appearing in equation (2-57) occurs so often in radiative transfer theory it has

been abbreviated to an operator notation:

$$\Lambda_v[f(t)] \equiv \frac{1}{2} \int_0^{\infty} f(t) E_1|t - \tau| dt \quad (2-58)$$

Exercise 2-6: (a) Show that equations (2-50) and (2-51) are equivalent to

$$I(r, n) = \int_0^{s_{\max}} \eta(r') \exp[-\tau(r, r')] dr' - r|$$

where $r'(s) \equiv r - sn$, $\tau(r', r) \equiv \int_0^{r'-r} \chi[r'(s)] ds$, and s_{\max} is the distance along the ray to any boundary surface in the direction $(-n)$; $s_{\max} = \infty$ for outward-directed rays in a semi-infinite medium. (b) Substitute the above result into the definition of $J(r)$ [equation (1-3)] to derive Peierls's equation:

$$J(r) = (4\pi)^{-1} \int_V \{\eta(r') \exp[-\tau(r', r)]/|r' - r|^2\} d^3 r'$$

where V denotes the entire volume containing material.

By an analysis similar to that used to obtain equation (2-57) we can derive expressions for F_v and K_v first obtained by Milne (416, 77):

$$F_v(\tau_v) = 2 \int_{\tau_v}^{\infty} S_v(t) E_2(t_v - \tau_v) dt_v - 2 \int_0^{\tau_v} S_v(t) E_2(\tau_v - t_v) dt_v \quad (2-59)$$

$$\text{and} \quad K_v(\tau_v) = \frac{1}{2} \int_0^{\infty} S_v(t) E_3|t_v - \tau_v| dt_v \quad (2-60)$$

We also define the corresponding operators

$$\Phi_v[f(t)] \equiv 2 \int_t^{\infty} f(t) E_2(t - \tau) dt - 2 \int_0^t f(t) E_2(\tau - t) dt \quad (2-61)$$

$$\text{and} \quad X_v[f(t)] \equiv 2 \int_0^{\infty} f(t) E_3|t - \tau| dt \quad (2-62)$$

Exercise 2-7: Derive equations (2-59) and (2-60).

The mathematical properties of the exponential integrals are discussed in detail in (4, 228–231) and (161, Appendix I), and the properties of the Λ , Φ , and X operators are discussed in (361, Chap. 2). A few of the most important results are mentioned in the following exercise.

Exercise 2-8: (a) Differentiate equation (2-56) to prove $E'_n(x) = -E_{n-1}(x)$. (b) Integrate equation (2-56) by parts to show that $E_n(x) = [e^{-x} - xE_{n-1}(x)]/(n-1)$ for $n > 1$. (c) Show that the asymptotic behavior ($x \gg 1$) of $E_n(x)$ is $E_n(x) \sim e^{-x}/x$.

Some interesting physical insight can be gained by considering a linear source function $S(\tau) = a + bt$; with the results of Exercise 2-8, it is easy to show that

$$\Lambda_v(a + bt) = (a + b\tau) + \frac{1}{2}[bE_3(\tau) - aE_2(\tau)] \quad (2-63)$$

$$\Phi_v(a + bt) = \frac{4}{3}b + 2[aE_3(\tau) - bE_4(\tau)] \quad (2-64)$$

and $X_v(a + bt) = \frac{4}{3}(a + b\tau) + 2[bE_5(\tau) - aE_4(\tau)] \quad (2-65)$

Exercise 2-9: Verify equations (2-63) through (2-65).

From the expressions written above (which will be applied in Chapter 3 and later work), we can note some important results. First, because the exponential integrals decay asymptotically as e^{-x}/x , it is evident from equation (2-63) that $J(\tau) = \Lambda_v(S)$ strongly approaches the local value of $S(\tau)$ for $\tau \gg 1$; that is, the Λ -operator tends to reproduce the source function at depth. In contrast, at the surface, $E_2(0) = 1$ and $E_3(0) = \frac{1}{2}$, and we obtain $\Lambda_0(S) = \frac{1}{2}a + \frac{1}{3}b$; in particular, if $b = 0$, then $J(0) = \frac{1}{2}a = \frac{1}{2}S$. Physically this reflects the fact that J at the surface is the average over a hemisphere containing no radiation (none incident from empty space) and a hemisphere in which $I = S$ (no gradient in S). When a gradient is present, $J(0)$ may lie above or below $S(0)$ depending on the sign and magnitude of the gradient. In a general way, J will depart most strongly from S at the surface. Second, we see from equation (2-64) that for $\tau \gg 1$, $H \rightarrow \frac{1}{3}b$. That is, the flux at depth depends only on the gradient of the source function (see also §2-5). The flux at the surface is $H(0) = \frac{1}{2}a + \frac{1}{3}b$; clearly the surface flux will be larger, the faster the source function rises inward. Note also that the effect of a gradient, relative to the case $b = 0$, is larger for $H(0)$ than for $J(0)$. (Why?)

Finally, it must be stressed that the solution of the transfer equation as given by equations (2-50) and (2-51) or (2-57) and (2-59) is only formal, and its apparent simplicity is illusory. For example, suppose the source function contains a scattering term as in equation (2-39) or (2-42). Then it is clear that the source function, which is required to compute the radiation field, depends upon the radiation field, and hence upon the solution of the transfer equation. In such cases we cannot calculate I or J by simple quadrature, but must find the solution of an integral equation or of the corresponding differential equation.

Exercise 2-10: Assume a source-function of the form of equation (2-39). Show that $J_v(\tau_v)$ satisfies the integral equation

$$J_v(\tau_v) = \Lambda_{v,v}[\rho_v(\tau_v)J_v(\tau_v)] + \Lambda_{v,v}\{[1 - \rho_v(\tau_v)]B_v(\tau_v)\}$$

where $\rho_v \equiv \sigma_v/(\kappa_v + \sigma_v)$

Complications of this kind are also introduced by other physical constraints on the solution. For example, we shall see in §2-4 that the requirement of energy balance couples together the radiation field and the temperature structure of the atmosphere. Thus even if strict LTE is assumed, and S_v is set equal to B_v and presumed to be independent of J_v , we are not in general able to specify the run of $T(\tau_v)$ and hence of $B_v[T(\tau_v)]$ until the radiation field is already known. Here again the source function required to compute the radiation field depends upon the field itself. When the more general non-LTE situation is considered, these problems become more subtle and complex, for now material properties (opacity, emissivity, etc.) depend directly upon the radiation field, for it determines occupation-numbers in atomic states. The transfer problem, in short, is fundamentally nonlinear in real stellar atmospheres. The development of methods to treat complicated interactions of the types just described will occupy a major part of this book.

2-3 Moments of the Transfer Equation

The angular moments of the transfer equation yield results of deep physical significance and great mathematical utility. The basic time-dependent transfer equation (2-26) may be rewritten as

$$c^{-1}[\partial I(\mathbf{r}, \mathbf{n}, v, t)/\partial t] + \sum_j n_j [\partial I(\mathbf{r}, \mathbf{n}, v, t)/\partial x_j] \\ = \eta(\mathbf{r}, \mathbf{n}, v, t) - \chi(\mathbf{r}, \mathbf{n}, v, t)I(\mathbf{r}, \mathbf{n}, v, t) \quad (2-66)$$

where x_j denotes the j th cartesian coordinate. To obtain the zero-order moment equation, we integrate equation (2-66) over all solid angles $d\omega$, and use the definitions in equations (1-4) and (1-19) to write

$$(4\pi/c)[\partial J(\mathbf{r}, v, t)/\partial t] + \nabla \cdot \mathcal{F}(\mathbf{r}, v, t) \\ = \oint [\eta(\mathbf{r}, \mathbf{n}, v, t) - \chi(\mathbf{r}, \mathbf{n}, v, t)I(\mathbf{r}, \mathbf{n}, v, t)] d\omega \quad (2-67)$$

where we have allowed for the possibility that χ and η may depend upon angle (as they will for moving media). If we integrate equation (2-67) over

all frequencies, and recall equation (1-8), we find

$$\begin{aligned} [\partial E_R(\mathbf{r}, t)/\partial t] + \nabla \cdot \mathcal{F}(\mathbf{r}, t) \\ = \int_0^\infty dv \oint d\omega [\eta(\mathbf{r}, n, v, t) - \chi(\mathbf{r}, n, v, t)I(\mathbf{r}, n, v, t)] \end{aligned} \quad (2-68)$$

This is an *energy equation* for the radiation field, and it closely resembles the standard energy equation for a moving fluid (cf. §15-1). The terms in the equation have a straightforward physical interpretation: the time rate of change of the radiation energy density equals (a) the total energy emitted into the field by the material, (b) minus the total absorbed from the field by the material, (c) minus the net flow of energy through the surface containing a volume element (the divergence of the flux). If the medium is *static*, χ and η are *isotropic* and the integrals on the righthand side simplify to yield

$$[\partial E_R(\mathbf{r}, t)/\partial t] + \nabla \cdot \mathcal{F}(\mathbf{r}, t) = 4\pi \int_0^\infty [\eta(\mathbf{r}, v, t) - \chi(\mathbf{r}, v, t)J(\mathbf{r}, v, t)] dv \quad (2-69)$$

For a *time-independent* radiation field in a *one-dimensional planar static medium*, equation (2-67) reduces to the "standard" result

$$[\partial H(z, v)/\partial z] = \eta(z, v) - \chi(z, v)J(z, v) \quad (2-70)$$

or, abbreviating the notation and using equations (2-34) and (2-35),

$$(\partial H_v/\partial \tau_v) = J_v - S_v \quad (2-71)$$

For *spherical geometry* (in a time-independent static atmosphere), by use of the appropriate expression for the divergence, we find

$$r^{-2}[\partial(r^2 H_v)/\partial r] = \eta_v - \chi_v J_v \quad (2-72)$$

Equations (2-70) through (2-72) will be employed repeatedly to obtain solutions of the transfer equation, and equation (2-69) will be used to develop the equations of radiation hydrodynamics (cf. §15-3).

Exercise 2-11: Derive equation (2-72) directly from equation (2-33).

The *first-order-moment equation* with respect to the i th coordinate axis is obtained by multiplying equation (2-66) by n_i and integrating over $(d\omega/c)$, which yields

$$\begin{aligned} c^{-2}[\partial \mathcal{F}_i(\mathbf{r}, v, t)/\partial t] + \sum_j [\partial P_{ij}(\mathbf{r}, v, t)/\partial x_j] \\ = c^{-1} \oint [\eta(\mathbf{r}, n, v, t) - \chi(\mathbf{r}, n, v, t)I(\mathbf{r}, n, v, t)] n_i d\omega \end{aligned} \quad (2-73)$$

or, in vector notation,

$$\begin{aligned} c^{-2}[\partial \mathcal{F}(\mathbf{r}, v, t)/\partial t] + \nabla \cdot \mathbf{P}(\mathbf{r}, v, t) \\ = c^{-1} \oint [\eta(\mathbf{r}, n, v, t) - \chi(\mathbf{r}, n, v, t)I(\mathbf{r}, n, v, t)] \mathbf{n} d\omega \end{aligned} \quad (2-74)$$

Recalling that the momentum density in the radiation field is $\mathbf{G}_R = c^{-2}\mathcal{F}$ (see §1-3), we see that equation (2-74) is analogous to the hydrodynamical equations of motion, and may be viewed as a *dynamical equation* for the momentum in the radiation field at frequency v . When we integrate over all frequencies, we obtain a *total momentum equation* for the radiation, which we shall use in the equations of radiation hydrodynamics (cf. Chapter 15):

$$\begin{aligned} c^{-2}[\partial \mathcal{F}(\mathbf{r}, t)/\partial t] + \nabla \cdot \mathbf{P}(\mathbf{r}, t) \\ = c^{-1} \int_0^\infty dv \oint d\omega [\eta(\mathbf{r}, n, v, t) - \chi(\mathbf{r}, n, v, t)I(\mathbf{r}, n, v, t)] \mathbf{n} \end{aligned} \quad (2-75)$$

Equation (2-75) states that the time rate of change of the total momentum density in the radiation field is equal to the negative of the volume force exerted by radiation stresses (cf. §1-4) plus a term that must represent the net momentum gain (or loss) from interacting with the material [see further discussion following equation (2-76)]. As in equation (2-68), equation (2-75) allows for the possibility of material motions. If the medium is at rest, then the integral over η vanishes (which merely states that the net momentum loss from the material by *isotropic* emission is zero, as is physically obvious), while the second term reduces to an integral over the flux:

$$c^{-2}[\partial \mathcal{F}(\mathbf{r}, t)/\partial t] + \nabla \cdot \mathbf{P}(\mathbf{r}, t) = -c^{-1} \int_0^\infty \chi(\mathbf{r}, v, t) \mathcal{F}(\mathbf{r}, v, t) dv \quad (2-76)$$

The physical significance of the integral on the righthand side of equation (2-76) can readily be seen by the following argument. Consider a beam of specific intensity I , entering an element of absorbing material of surface area dS , at an angle θ relative to the normal. The energy absorbed by material of opacity χ from a solid angle $d\omega$ and frequency band dv in time dt is

$$dE = \chi I dS \cos \theta ds dw dv dt$$

where $ds = (dz/\cos \theta)$ is the slant-length of the ray through the element of thickness dz along the normal. The component of momentum deposited in the material along the direction of the normal is $c^{-1} dE \cos \theta$; hence the momentum deposition per unit volume per unit time is

$$(c^{-1} \cos \theta dE)/(dz dS dt) = c^{-1} \chi I \cos \theta dw dv$$

If we sum over all angles and frequencies, we obtain precisely the integral in equation (2-76). We have thus shown that the integral is the *radiation force, per unit volume, on the material*; this interpretation is clearly compatible with the overall physical meaning of the equation.

For a *time-independent* radiation field in a *one-dimensional static planar medium*, equation (2-74) reduces to

$$[\partial p_R(z, v)/\partial z] = -(4\pi/c)\chi(z, v)H(z, v) \quad (2-77a)$$

or, integrating over all frequencies

$$[\partial p_R(z)/\partial z] = -(4\pi/c) \int_0^\infty \chi(z, v)H(z, v) dv \quad (2-77b)$$

Alternatively we can write

$$[\partial K(z, v)/\partial z] = -\chi(z, v)H(z, v) \quad (2-78)$$

or

$$(\partial K_v/\partial \tau_v) = H_v \quad (2-79)$$

In *spherical geometry*, under the same assumptions, equation (2-74) reduces, with the aid of the expression derived in Exercise 1-10 for $(\nabla \cdot P)_r$, to

$$(\partial K_v/\partial r) + r^{-1}(3K_v - J_v) = -\chi_v H_v \quad (2-80)$$

Exercise 2-12: Derive equation (2-80) directly from equation (2-33).

Thus far we have examined the moment equations primarily from the standpoint of their dynamical significance; but in the time-independent case they may also be used as tools to solve the transfer equation. By the introduction of moments, the angle-variable is eliminated and the dimensionality of the system to be solved is reduced. As we have seen in §2-2, the mean intensity can be determined from the solution of an integral equation (see Exercise 2-10). This gives the source function, from which the higher moments (e.g., the flux) can be determined by quadrature. The question now arises whether we can solve the moment equations as differential equations. Examination of equations (2-71) and (2-79) immediately reveals an essential difficulty: the moment equation of order n always involves the moment of order $n + 1$, hence there is always one more variable than there are equations to determine them! This difficulty is known as the *closure problem*: one *additional* relation among the moments must somehow be obtained to "close" the system. For solving transfer equations, a variety of methods exist that employ moments of arbitrarily high order, and introduce *ad hoc* closure relations [see, e.g., (361, 90–101; 365)]. However, in this book attention will be confined entirely to the moments J_v , H_v , and K_v (an exception appears in §14-3), and the system will be closed (see §6-3) by eliminating K_v in terms of J_v and

the variable Eddington factor f_v —i.e., $K_v = f_v J_v$. The factor f_v is obtained by iteration and allows us to effect an *approximate closure* of the *exact system* (if the iteration *converges*, the closure is also exact). Alternatively, it will be shown in §6-3 that the transfer equation can be rewritten in terms of *angle-dependent* mean-intensity-like and flux-like variables, and that *exact closure* of an angle-dependent equation that resembles a moment equation can be obtained. This equation is easily discretized and solved. In sum, the solution of the transfer equation in terms of moments or equivalent variables *can* be effected by differential-equation techniques of great generality and power.

2-4 The Condition of Radiative Equilibrium

Deep within the interior of a star, nuclear reactions release a flux of energy that diffuses outward, passes ultimately through the star's atmosphere, and emerges as observable radiation. In normal stars there is no creation of energy within the atmosphere itself; the atmosphere merely *transports* outward the total energy it receives. In a time-independent transport process, the frequency distribution of the radiation, or the partitioning of energy between radiative and nonradiative modes of transfer, may be altered; but *the energy flux as a whole is rigorously conserved*.

There are two basic modes of energy transport in those atmospheric layers in which spectrum-formation takes place: radiative and convective (or some other hydrodynamical mode). In these layers conduction is ineffective and can be ignored (it becomes important in *corona* at temperatures of the order of 10^6 °K). When all of the energy is transported by radiation, we have what is called *radiative equilibrium*; conversely, pure convective transport is called *convective equilibrium*. Whether or not radiative transport prevails over convection is determined by the *stability* of the atmosphere against convective motions.

The criterion for the stability of radiative transport was first enunciated by K. Schwarzschild (416, 25) in another of the fundamental papers of radiative transfer theory. Schwarzschild was able to demonstrate convincingly that the dominant mode of energy transport in the photosphere of the sun is radiative. Since his work, a number of analyses of radiative stability have been carried out for a variety of stellar types; results are summarized in (638, 215; 11, 449; 654, 432). The basic picture that emerges for a star like the sun is that radiative equilibrium obtains to continuum optical depths of order unity, and that below this depth the atmosphere becomes unstable against convection. Convection zones exist below the outer radiative zone in all stars of spectral type later than about F5. For earlier spectral types, radiative equilibrium prevails throughout the entire outer envelope of a star. In this book primary concern will be given to the early-type stars, and accordingly

emphasis will be given to the radiative equilibrium regime. The theory of convective transport is not, at present, in a fully satisfactory form, and only the *mixing-length theory* (a phenomenological approach that has been widely applied in astrophysics) will be described (§7-3).

Let us now consider some of the implications of radiative equilibrium; assume the medium is static and the radiation field is time-independent. From the discussion in §2-1, it is clear that the total energy removed from the beam is

$$\int_0^\infty dv \oint d\omega \chi(r, v) I(r, n, v) = 4\pi \int_0^\infty \chi(r, v) J(r, v) dv \quad (2-81)$$

where χ denotes the total extinction coefficient. The total energy delivered by the material to the radiation field is

$$\int_0^\infty dv \oint d\omega \eta(r, v) = 4\pi \int_0^\infty \chi(r, v) S(r, v) dv \quad (2-82)$$

where equation (2-35) has been used. The condition of radiative equilibrium demands that the total energy absorbed by a given volume of material must equal the total energy emitted; thus at each point in the atmosphere

$$4\pi \int_0^\infty [\eta(r, v) - \chi(r, v) J(r, v)] dv = 0 \quad (2-83a)$$

or $4\pi \int_0^\infty \chi(r, v) [S(r, v) - J(r, v)] dv = 0 \quad (2-83b)$

Exercise 2-13: Suppose that S , is given by equation (2-39). Show that, in the condition of radiative equilibrium, the scattering terms cancel out to yield

$$\int_0^\infty \kappa_v B_v(T) dv = \int_0^\infty \kappa_v J_v dv$$

Using equation (2-83) in equation (2-69) we have, alternatively,

$$\nabla \cdot \mathcal{F} \equiv 0 \quad (2-84)$$

Hence in planar geometry the condition of radiative equilibrium is equivalent to the requirement that the depth derivative of the flux is zero—i.e., the flux is constant. Physically, equations (2-83) and (2-84) have the same meaning, but mathematically the requirement $\mathcal{F} = \text{constant}$ is rather different from the expressions in equations (2-83); either form of the constraint may be used in constructing model atmospheres.

Because the total flux is constant in a planar atmosphere, it may be used as a parameter that describes the atmosphere; an equivalent quantity often employed is the *effective temperature*. From Exercise 1-6 we know that the integrated flux from a black body of absolute temperature T is $\mathcal{F}_{BB} = \sigma_R T^4$.

Although the radiation emerging from a star is by no means Planckian, it is nevertheless customary to define the effective temperature as the temperature a black body would have in order to emit the actual stellar flux—i.e.,

$$\sigma_R T_{eff}^4 \equiv \int_0^\infty \mathcal{F}_v dv = 4\pi \int_0^\infty H_v dv = L/(4\pi R^2) \quad (2-85)$$

Here L is the total luminosity and R is the radius of the star; the atmospheric thickness is assumed to be negligible compared to R . Although T_{eff} has only an indirect physical significance, it is a convenient parameter with which to characterize the atmosphere, for typically the actual kinetic temperature T will equal T_{eff} near the depth from which the continuum radiation emerges (i.e., unit optical depth at frequencies where the opacity is lowest). In spherical geometry equation (2-84) implies

$$r^2 \mathcal{F} = \text{constant} = L/4\pi \quad (2-86)$$

In an extended atmosphere it is no longer really possible to choose a unique radius R for the star and to define a unique value of T_{eff} ; rather, L or the quantity $r^2 \mathcal{F}$ should be regarded as fundamental. However the identification $R = r(\tau_R = \frac{1}{2})$ is sometimes made, and a value of “ T_{eff} ” derived with this radius; here τ_R is the *Rosseland optical depth scale* (cf. §3-2).

Finally, it is important to return to the point raised in the discussion of the formal solution. Suppose that the opacity κ_v is independent of T ; then for physically reasonable distributions of κ_v , the integral $\int \kappa_v B_v(\tau) dv$ (which gives the total thermal emission) will be a monotone increasing function of T . Thus when we fix the total thermal emission at some value, we fix the local value of T . It is then clear from equation (2-83b) (and from the result of Exercise 2-13) that the *local* value of T is determined by the mean intensity, which depends upon the *global* properties of the atmosphere because it follows from a solution of the transfer equation. Thus the temperature at a *given* point in the atmosphere is to some extent determined by the temperature at *all other* points and, at the same time, helps to establish the temperature structure elsewhere. This *nonlocalness* in the problem is a result of radiative transfer, through which photons moving from one point in the medium to another lead to a fundamental coupling (i.e., interdependence) of the properties at those points.

2-5 The Diffusion Approximation

At great depths in a semi-infinite atmosphere the properties of the radiation field and the nature of the transfer equation become extremely simple. We can obtain in a straightforward way an asymptotic solution that applies

throughout the interior of a star (except, of course, in convective zones), and that provides a lower boundary condition on the transfer problem in the stellar atmosphere. Consider first the properties of the radiation field. At depths in the medium much larger than a photon mean-free-path, the radiation is effectively trapped, becomes essentially isotropic, and (eventually) approaches thermal equilibrium so that $S_v \rightarrow B_v$. Choose a reference point $\tau_v \gg 1$, and expand S_v as a power-series:

$$S_v(\tau_v) = \sum_{n=0}^{\infty} [d^n B_v/d\tau_v^n](\tau_v - \tau_v)^n/n! \quad (2-87)$$

Calculating the specific intensity for $0 \leq \mu \leq 1$ from this source function with equation (2-50) we have

$$I_v(\tau_v, \mu) = \sum_{n=0}^{\infty} \mu^n \frac{d^n B_v}{d\tau_v^n} = B_v(\tau_v) + \mu \frac{dB_v}{d\tau_v} + \mu^2 \frac{d^2 B_v}{d\tau_v^2} + \dots \quad (2-88)$$

A similar result for $-1 \leq \mu \leq 0$ follows from equation (2-51) and differs from equation (2-88) only by terms of order $e^{-|\mu|}$; in the limit of great depth the latter vanish and equation (2-88) applies on the full range $-1 \leq \mu \leq 1$. By substitution of equation (2-88) into the appropriate definitions we find for the moments

$$\begin{aligned} J_v(\tau_v) &= \sum_{n=0}^{\infty} (2n+1)^{-1} (d^{2n} B_v/d\tau_v^{2n}) \\ &= B_v(\tau_v) + \frac{1}{3} (d^2 B_v/d\tau_v^2) + \dots \end{aligned} \quad (2-89a)$$

$$\begin{aligned} H_v(\tau_v) &= \sum_{n=0}^{\infty} (2n+3)^{-1} (d^{2n+1} B_v/d\tau_v^{2n+1}) \\ &= \frac{1}{3} (dB_v/d\tau_v) + \dots \end{aligned} \quad (2-89b)$$

and

$$\begin{aligned} K_v(\tau_v) &= \sum_{n=0}^{\infty} (2n+3)^{-1} (d^{2n} B_v/d\tau_v^{2n}) \\ &= \frac{1}{3} B_v(\tau_v) + \frac{1}{5} (d^2 B_v/d\tau_v^2) + \dots \end{aligned} \quad (2-89c)$$

Note that only even-order terms survive in the even moments J_v and K_v , and only odd-order terms in H_v .

We now inquire how rapidly these series converge. The derivatives can be approximated, at least to order-of-magnitude, by appropriate differences—

i.e., $|d^n B_v/d\tau_v^n| \sim B_v/\tau_v^n$. Then it is clear that the ratio of successive terms in the series is of order $O(1/\tau_v^2)$ or $O(1/\langle \chi_v \rangle^2 \Delta z^2)$ where $\langle \chi_v \rangle$ is the average opacity over the path-length Δz . In terms of the photon mean-free-path $l_v \sim 1/\chi_v$, the convergence factor is $O(l_v^2/\Delta z^2)$. It is clear that the convergence is quite rapid; indeed the estimate just given turns out to be conservative. Also, it is obvious that convergence will be most rapid at frequencies where the material is quite opaque. For a star as a whole one expects Δz to be some significant fraction of a stellar radius, say $\Delta z \sim 10^{10}$ cm, while $\langle \chi \rangle \sim 1$ (which implies a photon mean-free-path of 1 cm), so that the convergence factor of the series is of the order 10^{-20} . It is clear that in the deep interior of the star only the leading terms are required.

In the limit of large depth we may therefore write

$$I_v(\tau_v, \mu) \approx B_v(\tau_v) + \mu (dB_v/d\tau_v) \quad (2-90a)$$

$$J_v(\tau_v) \approx B_v(\tau_v) \quad (2-90b)$$

$$H_v(\tau_v) \approx \frac{1}{3} (dB_v/d\tau_v) \quad (2-90c)$$

$$K_v(\tau_v) \approx \frac{1}{3} B_v(\tau_v) \quad (2-90d)$$

In equation (2-90a) we have retained two terms so as to account for the nonzero flux [cf. equation (2-90c)]. Note that equations (2-90b) and (2-90d) show that $\lim_{\tau_v \rightarrow \infty} [K_v(\tau_v)/J_v(\tau_v)] = \frac{1}{3}$, which is what we would expect for isotropic radiation; we shall show below that the ratio of the anisotropic to isotropic term in $I(\tau, \mu)$ becomes vanishingly small as $\tau \rightarrow \infty$, so that the limit just found is appropriate. Insofar as the specific intensity as given by equation (2-90a) was computed from the formal solution of the transfer equation, in effect using a source function $S_v(\tau_v) = B_v(\tau_v) + (t_v - \tau_v)(dB_v/d\tau_v)$, equations (2-90) should obviate further use of the transfer equation. It is easy to verify that this is so, for by inspection one sees that substitution from equations (2-90) reduces both the transfer equation (2-36) and the zero-order moment equation (2-71) to the single requirement $d^2 B_v/d\tau_v^2 = 0$ (already assumed), while the first-order moment equation (2-79) is identical to (2-90c). Thus, in effect, at great depth the transfer problem reduces to the single equation

$$H_v = \frac{1}{3} \left(\frac{\partial B_v}{\partial \tau_v} \right) = -\frac{1}{3} \left(\frac{1}{\chi_v} \frac{\partial B_v}{\partial T} \right) \left(\frac{dT}{dz} \right) \quad (2-91)$$

It is clear that equations (2-90) and (2-91) can be used, as mentioned in §2-2, to set lower boundary conditions on the transfer equation in a semi-infinite atmosphere.

Equation (2-91) [and also equations (2-90)] is referred to as the *diffusion approximation*, primarily because of its formal similarity to other diffusion equations, which are of the form

$$(\text{flux}) = (\text{diffusion coefficient}) \times (\text{gradient of relevant physical variable})$$

e.g., $\Phi = -\kappa VT$ for heat conduction. The coefficient $\frac{1}{3}\chi_v^{-1}(\partial B_v/\partial T)$ is, in fact, sometimes called the *radiative conductivity*, a designation that is quite appropriate in view of the fact that $\chi_v^{-1} = l_v$ is the photon mean-free-path. Note that equation (2-91) exhibits the essential physical content of our earlier result that the flux computed by application of the Φ -operator to a linear source function depends only on the gradient of S [see discussion following equation (2-65)]. Also it shows that *the mere fact that energy emerges from the star implies that the temperature must increase inward*. Indeed, replacing H with $(L/4\pi R^2)$ and (dB/dz) with $(\sigma_R T_c^4/\pi R)$, and taking $\langle\chi\rangle \approx 1$, it is easy to show that the central temperature T_c of the sun must be of the order of 6×10^6 °K, a result consistent with our earlier statement that the ultimate energy source in a star is thermonuclear energy-release at the center.

In an intuitive picture of diffusion, one usually conceives of a slow leakage from a reservoir of large capacity by means of a seeping action. These ideas apply in the radiative diffusion limit as well. The diffusion approximation becomes valid at great optical depth (i.e., many photon mean-free-paths from the surface) whence many individual photon flights, with successive absorptions and emissions, are required before the photon finally trickles to the surface, and issues forth into interstellar space.

If we integrate equations (2-90a–c) over all frequencies, we obtain $I(\tau, \mu) \approx B(\tau) + 3\mu H$. The ratio of the anisotropic to isotropic terms gives a measure of the “drift” in the radiation flow; this ratio is

$$\frac{\text{Anisotropic term}}{\text{Isotropic term}} \sim \frac{3H}{B} = \frac{3}{4} \left(\frac{\sigma_R T_{\text{eff}}^4}{\pi} \right) / \left(\frac{\sigma_R T^4}{\pi} \right) \sim \left(\frac{T_{\text{eff}}}{T} \right)^4 \quad (2-92)$$

Clearly at great depth, where T becomes $\gg T_{\text{eff}}$, the “leak” becomes ever smaller. The same result is found by a physical argument from a slightly different point of view. If πF is the energy flux carried from an element of material by photons of velocity c , the rate of *energy flow* per unit volume is $(\pi F/c)$; the *energy content* per unit volume is $(4\pi J/c) \approx (4\pi B/c)$, so that $(\text{Rate of energy flow})/(\text{Energy content}) = (F/4B) = \frac{1}{4}(T_{\text{eff}}/T)^4$. Again, we see that diffusion, in the intuitive sense described above, occurs at great depth where $T \gg T_{\text{eff}}$, while *free flow* of radiant energy occurs at the surface where $T \approx T_{\text{eff}}$.

The Grey Atmosphere

The grey atmosphere problem provides an excellent introduction to the study of radiative transfer in stellar atmospheres. The nature of the defining assumptions is such that the problem becomes independent of the physical state of the material, and requires the solution of a relatively simple transfer equation. At the same time, the grey problem demonstrates how the constraint of radiative equilibrium can be satisfied, and the solution can be related to more general and more realistic physical situations. Furthermore, an exact solution of the problem can be obtained, and this provides a comparison standard against which we can evaluate the worth of various approximate numerical methods that can be applied in more complex cases.

3-1 Statement of the Problem

The problem is posed by making the simplifying assumption that the opacity of the material is independent of frequency; i.e., $\chi_v \equiv \chi$. This assumption is of course unrealistic in many cases. Yet as we shall see in later chapters, the opacity in some stars (e.g., the sun) is not too far from being grey and, in

addition, it is possible partially to reduce the nongrey problem to the grey case by suitable choices of *mean opacities*. Thus the solution also provides a valuable starting approximation in the analysis of nongrey atmospheres.

If we assume $\chi_v \equiv \chi$, then the standard planar transfer equation (2-36) becomes

$$\mu(\partial I_v / \partial \tau) = I_v - S_v \quad (3-1)$$

Then by integrating over frequency, and writing

$$I \equiv \int_0^\infty I_v dv \quad (3-2)$$

and similarly for J , S , B , etc., we have

$$\mu(\partial I / \partial \tau) = I - S \quad (3-3)$$

If we impose the constraint of radiative equilibrium [equation 2-83b)], we require

$$\int_0^\infty \chi J_v dv = \int_0^\infty \chi S_v dv \quad (3-4)$$

which, for grey material, reduces to $J \equiv S$. Thus equation (3-3) becomes

$$\mu(\partial I / \partial \tau) = I - J \quad (3-5)$$

which has the formal solution [equation (2-57)]

$$J(\tau) = \Lambda_\tau[S(t)] = \Lambda_\tau[J(t)] = \frac{1}{2} \int_0^\infty J(t) E_1 |t - \tau| dt \quad (3-6)$$

Equation (3-6) is a linear integral equation for J known as *Milne's equation*; the grey problem itself is sometimes called *Milne's problem*. It is important to recognize that, when a solution of equation (3-6) is obtained, it satisfies simultaneously the transfer equation and the constraint of radiative equilibrium. The determination of such solutions in the nongrey case will occupy most of Chapter 7.

If we now introduce the additional hypothesis of LTE, then $S_v \equiv B_v(T)$ —which, from the condition of radiative equilibrium, implies that

$$J(\tau) = S(\tau) = B[T(\tau)] = (\sigma_R T^4)/\pi \quad (3-7)$$

Thus, if we are given $J(\tau)$, the solution of the integral equation (3-6), then the additional premise of LTE allows us to associate a temperature with the radiative equilibrium radiation field via equation (3-7).

Several important results may be obtained from moments of equation (3-5). Taking the zero-order moment and imposing radiative equilibrium we have

$$(dH/d\tau) = J - S = J - J \equiv 0 \quad (3-8)$$

which implies the flux is constant, while the first moment gives

$$(dK/d\tau) = H \quad (3-9)$$

which, because H is constant, yields the exact integral

$$K(\tau) = H\tau + c = \frac{1}{4} F\tau + c \quad (3-10)$$

To make further progress, we must relate $J(\tau)$ to $K(\tau)$. This is easily done on the basis of the discussion in §2-5, where we showed that at great depth the specific intensity is quite accurately represented by $I(\mu) = I_0 + I_1\mu$, which produces a nonzero flux and also implies that, for $\tau \gg 1$, $K(\tau) = \frac{1}{3}J(\tau)$. Thus the fact that $K(\tau) \rightarrow \frac{1}{4}F\tau$ for $\tau \gg 1$ implies that at great depth

$$J(\tau) \rightarrow \frac{3}{4}F\tau \quad (\tau \gg 1) \quad (3-11)$$

That is, asymptotically the mean intensity varies linearly with optical depth. On general grounds we expect the behavior of $J(\tau)$ to depart most from linearity at the surface [note equation (2-63)], which suggests that a reasonable general expression for $J(\tau)$ is

$$J(\tau) = \frac{3}{4}F[\tau + q(\tau)] = \frac{3}{4}(\sigma_R T_{\text{eff}}^4/\pi)[\tau + q(\tau)] \quad (3-12)$$

The function $q(\tau)$, known as the *Hopf function*, remains to be determined; from equation (3-6) it is clear that $q(\tau)$ is a solution of the equation

$$\tau + q(\tau) = \frac{1}{2} \int_0^\infty [t + q(t)] E_1 |t - \tau| dt \quad (3-13)$$

Finally, we notice that because

$$\lim_{\tau \rightarrow \infty} \left[\frac{1}{3} J(\tau) - K(\tau) \right] = \frac{1}{4} F \lim_{\tau \rightarrow \infty} [\tau + q(\tau) - \tau - c] \equiv 0 \quad (3-14)$$

we have $c = q(\infty)$ and hence can write equation (3-10) as

$$K(\tau) = \frac{1}{4} F[\tau + q(\infty)] \quad (3-15)$$

The solution of the grey problem consists of the specification of $q(\tau)$. Given $q(\tau)$, the temperature distribution is obtained by combining equations (3-7) and (3-12) into the relation

$$T^4 = \frac{3}{4} T_{\text{eff}}^4 [\tau + q(\tau)] \quad (3-16)$$

We shall derive approximate expressions for $q(\tau)$ in §3-3 and describe the exact solution in §3-4. First, however, it is useful to delineate the nature, and extent, of the correspondence between the grey and nongrey problems.

3-2 Relation to the Nongrey Problem: Mean Opacities

The opacity in real stellar atmospheres usually exhibits strong frequency variations, at least when spectral lines are present. Although numerical methods now exist that allow a refined solution of nongrey transfer equations and an accurate determination of the temperature structure in a nongrey atmosphere, the calculations are, at best, laborious, and it is important to ask whether a significant connection exists between the grey and nongrey cases. We shall show in this section that such a connection, though limited in scope, does exist, and that, among other things, it permits the temperature distribution of the deepest atmospheric layers to be determined quite accurately from the grey solution.

Let us first compare side-by-side the grey and nongrey transfer equations. Starting with the transfer equation and calculating the zero and first-order moments we have, in the nongrey and grey cases respectively:

$$\mu(\partial I_v/\partial z) = \chi_v(S_v - I_v) \quad (3-17a)$$

$$\mu(\partial I/\partial z) = \chi(J - I) \quad (3-17b)$$

$$(\partial H_v/\partial z) = \chi_v(S_v - J_v) \quad (3-18a)$$

$$(dH/dz) = 0 \quad (3-18b)$$

$$(\partial K_v/\partial z) = -\chi_v H_v \quad (3-19a)$$

$$(dK/dz) = -\chi H \quad (3-19b)$$

Here variables without frequency subscripts denote *integrated* quantities, as in equation (3-2). We now ask whether it is possible to define a mean opacity $\bar{\chi}$, formed as a weighted average of the monochromatic opacity, in such a way that the monochromatic transfer equation, or one of its moments, when integrated over frequency, has exactly the same form as the grey equation. Several possible definitions have been suggested.

FLUX-WEIGHTED MEAN

Suppose we wish to define a mean opacity in such a way as to guarantee an exact correspondence between the integrated form of equation (3-19a) and the grey equation (3-19b). If such a mean can be constructed, then the relation $K(\bar{\tau}) = H\bar{\tau} + c$ will again be an exact integral, as it was in the grey case. Integrating equation (3-19a) over all frequencies we have

$$-(dK/dz) = \int_0^\infty \chi_v H_v dv = \bar{\chi}_F H \quad (3-20)$$

where the second equality produces the desired identification with equation (3-19b) if we define

$$\bar{\chi}_F \equiv H^{-1} \int_0^\infty \chi_v H_v dv \quad (3-21)$$

The opacity $\bar{\chi}_F$ is called the *flux-weighted* mean. Note that this choice does *not* reduce the nongrey problem completely to the grey problem, for the monochromatic equation (3-18a) does not transform into equation (3-18b) with this choice of $\bar{\chi}$. Further, there is the practical problem that H_v is not known *a priori*, and therefore $\bar{\chi}_F$ cannot actually be calculated until after the transfer equation is solved. This latter difficulty can be overcome by an iteration between construction of models and calculation of $\bar{\chi}_F$. Although the desired goal has not been fully attained, the fact that the flux-weighted mean preserves the *K*-integral is important, for it implies that the correct value is recovered for the *radiation pressure* [cf. equation (1-41)]. It also follows that the correct value of the *radiation force*, which is the gradient of the radiation pressure, is likewise obtained. Thus from equation (2-77) we have

$$(dp_R/d\bar{\tau}) = -\bar{\chi}_F^{-1}(dp_R/dz) = (4\pi/c\bar{\chi}_F) \int_0^\infty \chi_v H_v dv = (4\pi H/c) = (\sigma T_{\text{eff}}^4/c) \quad (3-22)$$

so that use of the flux-mean opacity produces a simple expression for the radiation pressure gradient. This is a result of practical value in the computation of model atmospheres for early-type stars, because in these objects radiation forces strongly affect the pressure (or density) structure of the atmosphere via the condition of hydrostatic equilibrium (or momentum balance in steady flow).

ROSELAND MEAN

Alternatively, suppose we wish to obtain the correct value for the integrated energy flux. From equations (3-19) it follows that this may be done if $\bar{\chi}$ is chosen such that

$$-\int_0^\infty \chi_v^{-1}(\partial K_v/\partial z) dv = \int_0^\infty H_v dv = H \equiv -\bar{\chi}^{-1}(dK/dz) \quad (3-23)$$

or, equivalently,

$$\bar{\chi}^{-1} \equiv \int_0^\infty \chi_v^{-1}(\partial K_v/\partial z) dv / \int_0^\infty (\partial K_v/\partial z) dv \quad (3-24)$$

Again we face the practical difficulty that K_v is not known *a priori*, and hence the indicated calculation cannot be performed until the transfer equation is

solved. But the mean defined in equation (3-24) can be approximated in the following way: at great depth in the atmosphere, $K_v \rightarrow \frac{1}{3}J_v$, while $J_v \rightarrow B_v$. Thus may write $(\partial K_v / \partial z) \approx \frac{1}{3}(\partial B_v / \partial T)(dT/dz)$. We then define the mean opacity $\bar{\chi}_R$ as

$$\frac{1}{\bar{\chi}_R} \equiv \frac{\frac{1}{3} \left(\frac{dT}{dz} \right) \int_0^\infty \left(\frac{1}{\chi_v} \right) \frac{\partial B_v}{\partial T} dv}{\frac{1}{3} \left(\frac{dT}{dz} \right) \int_0^\infty \frac{\partial B_v}{\partial T} dv} = \frac{\int_0^\infty \frac{1}{\chi_v} \frac{\partial B_v}{\partial T} dv}{\int_0^\infty \frac{\partial B_v}{\partial T} dv} \quad (3-25)$$

or $\bar{\chi}_R^{-1} \equiv (\pi/4\sigma_R T^3) \int_0^\infty \chi_v^{-1} (\partial B_v / \partial T) dv \quad (3-26)$

The opacity $\bar{\chi}_R$ is called the *Roseland mean* in honor of its originator. Note that the harmonic nature of the averaging process gives highest weight to those regions where the opacity is lowest, and, where as a result, the greatest amount of radiation is transported—a very desirable feature. Again the use of $\bar{\chi}_R$ or the mean defined by equation (3-24) does not permit a correspondence between equations (3-18a) and (3-18b), and hence does not allow the nongrey problem to be replaced by the grey problem. On the other hand, it is obvious that the approximations made to obtain equation (3-26) are precisely those introduced in the derivation of the diffusion approximation to the transfer equation (2-91); i.e.,

$$H_v = -\frac{1}{3} \left(\frac{1}{\chi_v} \frac{\partial B_v}{\partial T} \right) \left(\frac{dT}{dz} \right)$$

Hence use of $\bar{\chi}_R$ is consistent with the diffusion approximation. Therefore on the Roseland-mean optical-depth scale τ_R we must recover the correct asymptotic solution of the transfer equation and the correct flux transport at great depth. This implies that at great depth ($\tau_R \gg 1$) the temperature structure is quite accurately given by the relation $T^4 = \frac{4}{3}T_{\text{eff}}^4[\tau_R + q(\tau_R)]$; see equation (3-16). It is therefore clear why Roseland mean opacities are employed in studies of stellar interiors. Note also that so long as the diffusion approximation is valid, a simple expression can be written for the radiation force, namely

$$(dp_R/d\tau_R) = (16\pi\sigma_R T^3/3c\bar{\chi}_R)(-dT/dz) \quad (3-27)$$

Exercise 3-1: Derive equation (3-27).

Although the diffusion approximation is nearly exact at great depth, and provides the very useful results just discussed, it *must* of course break down at the surface, and exact flux conservation is *not* guaranteed in the upper layers by use of the Roseland mean, nor will it give the temperature structure

or the radiation force correctly in the outermost regions of the atmosphere. This point must be recognized clearly, for it is precisely these layers in which spectrum-formation occurs, and hence which are of primary interest in the analysis of stellar spectra.

PLANCK AND ABSORPTION MEANS

Several other expressions for mean opacities may be chosen. For example, if we demand that the mean be defined to yield the correct integrated value of the thermal emission, then we require

$$\bar{\kappa}_P \equiv \left[\int_0^\infty \kappa_v B_v(T) dv \right] / B(T) = \pi \int_0^\infty \kappa_v B_v(T) dv / \sigma_R T^4 \quad (3-28)$$

Note that only the true absorption is used, and scattering is omitted. The opacity $\bar{\kappa}_P$ is known as the *Planck mean*; it has the advantage of being calculable without having to solve the transfer equation. On the other hand, $\bar{\kappa}_P$ does not permit a reduction of equation (3-18a) to (3-18b) nor of (3-19a) to (3-19b), and therefore it lacks the desirable features possessed by $\bar{\chi}_F$ or $\bar{\chi}_R$. Nevertheless this mean does have additional significance.

In particular, near the surface of the star, the physical content of the condition of radiative equilibrium is expressed most directly by equation (3-4). In view of this constraint, a correspondence between equations (3-18a) and (3-18b) can be made near the surface if $\bar{\kappa}$ satisfies the relation

$$\int_0^\infty (\kappa_v - \bar{\kappa})(J_v - B_v) dv = 0 \quad (3-29)$$

Once the material becomes optically thin (i.e., $\tau_v < 1$ at all frequencies), J_v becomes essentially fixed, and the integral above will be dominated by those frequencies where $\kappa_v \gg \bar{\kappa}$. If we represent B_v by a linear expansion on a $\bar{\tau}$ -scale, i.e.,

$$B_v(t) = B_v(\bar{\tau}) + (dB_v/d\bar{\tau})(t - \bar{\tau}) \approx B_v(\bar{\tau}) + (dB_v/d\bar{\tau})(\bar{\kappa}/\kappa_v)(t_v - \tau_v),$$

then by application of the Λ -operator we find [cf. equations (2-57), (2-58), and (2-63)],

$$\begin{aligned} J_v(\bar{\tau}) - B_v(\bar{\tau}) &\approx -\frac{1}{2} B_v(\bar{\tau}) E_2(\tau_v) \\ &+ (\bar{\kappa}/\kappa_v)(dB_v/d\bar{\tau}) \left[\frac{1}{2} E_3(\tau_v) + \frac{1}{2} \tau_v E_2(\tau_v) \right] \end{aligned} \quad (3-30)$$

In the limit $\tau \rightarrow 0$, $E_2(\tau) \rightarrow 1$, and $E_3(\tau) \rightarrow \frac{1}{2}$, so the first term yields $-\frac{1}{2}B_v(\bar{\tau})$, while the second becomes least important when $\kappa_v \gg \bar{\kappa}$ [precisely the region of highest weight in equation (3-29)]. Thus to satisfy equation (3-29), $\bar{\kappa}$

should essentially fulfill the requirement

$$\int_0^\infty \kappa_v B_v dv = \bar{\kappa} \int_0^\infty B_v dv \quad (3-31)$$

which shows that the Planck mean is the choice most nearly consistent with the requirement of radiative equilibrium near the surface.

Alternatively, we might demand that the mean opacity yield the correct total for the amount of energy absorbed. We then obtain the *absorption mean*

$$\bar{\kappa}_J \equiv \int_0^\infty \kappa_v J_v dv / J \quad (3-32)$$

Again only the true absorption is included, and scattering is omitted. As was true for $\bar{\chi}_F$, we cannot calculate $\bar{\kappa}_J$ until a solution of the transfer equation has been obtained. Further, $\bar{\kappa}_J$ does not permit a strict correspondence between the grey and nongrey forms of the transfer equation or any of its moments (as was also true for the Planck mean).

SUMMARY

We have seen that no one of the mean opacities described above allows, in itself, a complete correspondence of the nongrey problem to the grey problem. Yet mean opacities provide a useful first estimate of the temperature structure in a stellar atmosphere if we assume, as a starting approximation, $T(\tau_R) = T_{\text{grey}}(\tau_R)$, and then improve this estimate with a *correction procedure* that is designed to enforce radiative equilibrium for the nongrey radiation field. Indeed, the mean opacities $\bar{\chi}_F$, $\bar{\kappa}_P$, and $\bar{\kappa}_J$ appear explicitly in some temperature-correction procedures.

From an historical point of view, it should be recognized that, before the advent of high-speed computers, the nongrey atmosphere problem required far too much calculation to permit a direct attack, and the use of $\bar{\chi}_R$ and $\bar{\kappa}_P$ provided a practical method of approaching an otherwise intractable problem. In fact, the answers obtained in this way often do not compare too unfavorably with more recent results despite the apparent crudeness of the approximation. Only some of the more basic properties of mean opacities have been mentioned here; further information may be found in (419) and (361, §§34–35).

3-3 Approximate Solutions

THE EDDINGTON APPROXIMATION

In §2-5 it was shown that, at great depth in a stellar atmosphere, the relation $J = 3K$ holds; further, in §1-4 (cf. Exercise 1-13), it was demonstrated

that this relation is also valid for a variety of other situations, including the two-stream approximation, which provides a rough representation of the radiation field near the boundary. In view of these results, Eddington made the simplifying assumption that $J \equiv 3K$ everywhere in the atmosphere. Then the exact integral $K = \frac{1}{4}F\tau + c$ implies that in the Eddington approximation $J_E(\tau) = \frac{3}{4}F\tau + c'$. To evaluate the constant c' we calculate the emergent flux and fit it to the desired value. Thus from equation (2-59) we have

$$F(0) = 2 \int_0^\infty \left(\frac{3}{4}F\tau + c' \right) E_2(\tau) d\tau = 2c'E_3(0) + \frac{3}{4}F \left[\frac{4}{3} - 2E_4(0) \right] \quad (3-33)$$

so that, using the relation $E_n(0) = 1/(n-1)$ and demanding $F(0) \equiv F$, we find $c' = \frac{1}{2}F$. Thus

$$J_E(\tau) = \frac{3}{4}F \left(\tau + \frac{2}{3} \right) \quad (3-34)$$

In Eddington's approximation $q(\tau) \equiv \frac{2}{3}$. Imposing the constraint of radiative equilibrium and the assumption of LTE we have from equation (3-16)

$$T^4 \approx \frac{3}{4} T_{\text{eff}}^4 \left(\tau + \frac{2}{3} \right) \quad (3-35)$$

Equation (3-35) predicts that the ratio of the boundary temperature to the effective temperature is $(T_0/T_{\text{eff}}) = (\frac{1}{2})^{1/4} = 0.841$, which agrees fairly well with the exact value $(T_0/T_{\text{eff}}) = (3^{1/2}/4)^{1/4} = 0.8114$. Assuming $S(\tau) = J_E(\tau)$ we may calculate the angular dependence of the emergent radiation field in the Eddington approximation by substituting equation (3-34) into equation (2-52) to obtain

$$I_E(0, \mu) = \frac{3}{4}F \int_0^\infty \left(\tau + \frac{2}{3} \right) \mu^{-1} \exp(-\tau/\mu) d\tau = \frac{3}{4}F \left(\mu + \frac{2}{3} \right) \quad (3-36)$$

which yields a very specific form for the Eddington-Barbier relation [cf. equation (2-53)]. The *center* of a star's disk, as seen by an external observer, corresponds to $\theta = 0^\circ$, or $\mu = 1$; the *limb* is at $\theta = 90^\circ$, $\mu = 0$. The ratio $I(0, \mu)/I(0, 1)$, which gives the intensity at angle $\theta = \cos^{-1} \mu$ relative to disk-center, is referred to as the *limb-darkening law*. In the Eddington approximation the limb-darkening is

$$I_E(0, \mu)/I_E(0, 1) = \frac{3}{5} \left(\mu + \frac{2}{3} \right) \quad (3-37)$$

This result predicts the limb intensity to be 40 percent of the central intensity. Observations of the sun in the visual regions of the spectrum are actually in good agreement with this value and, in fact, it was precisely this agreement

that led K. Schwarzschild (416, 25) to propose the validity of radiative equilibrium in the outermost layers of the solar photosphere.

Equation (3-35) predicts that $T = T_{\text{eff}}$ when $\tau = \frac{2}{3}$. This result has given rise to the useful conceptual notion that the “effective depth” of continuum formation is $\tau \approx \frac{2}{3}$; in fact, this is often a rather good estimate. In support of this idea we may note that a photon emitted outward from $\tau = \frac{2}{3}$ has a chance of the order of $e^{-0.67} \approx 0.5$ of emerging from the surface; this corresponds in a reasonable way with the place we would intuitively identify with the region of continuum formation.

Exercise 3-2: The Eddington-Barbier relation shows that the intensity $I(0, \mu)$ is characteristic of $S(\tau)$ at $\tau(\mu) \approx \mu$. Show then that the average depth that characterizes the flux is $\langle \tau \rangle = \frac{2}{3}$.

Anticipating the exact solution given in Table 3-2, we can evaluate the accuracy of $J_E(\tau)$; one finds that the worst error occurs at the surface, where $\Delta J/J = (J_E - J_{\text{exact}})/J_{\text{exact}} = 0.155$. Both the size of the error and the fact that it occurs at $\tau = 0$ are unsurprising when we recognize that the basic assumption upon which the derivation is based, namely $J \equiv 3K$, is known to be inaccurate at the surface. We know that $J(\tau)$ must satisfy the integral equation (3-6), and we know further that the Λ -operator has its largest effect at $\tau = 0$ [see equation (2-63) and associated discussion]. This suggests that an improved estimate of $J(\tau)$ can be obtained from

$$J_E^{(2)}(\tau) = \Lambda_t[J_E(t)] = \Lambda_t \left[\frac{3}{4} F \left(t + \frac{2}{3} \right) \right] = \frac{3}{4} F \left[\tau + \frac{2}{3} - \frac{1}{3} E_2(\tau) + \frac{1}{2} E_3(\tau) \right] \quad (3-38)$$

Recalling the properties of $E_n(\tau)$, it is clear that the largest difference between $J_E^{(2)}(\tau)$ and $J_E(\tau)$ occurs at the surface, where we find $J_E^{(2)}(0)/J_E(0) = \frac{7}{6}$. The new estimate of T_0/T_{eff} is thus $(\frac{7}{6})^{1/4} = 0.813$ (exact value is 0.8114) and $q(0)$ drops from $\frac{2}{3}$ to $\frac{7}{12} = 0.583$ (exact value is $1/\sqrt{3} = 0.577$).

It is thus clear that an application of the Λ -operator has produced a dramatic improvement in the solution near the surface. Note, however, that there is no improvement in the solution at $\tau \rightarrow \infty$, where q remains at its original value $\frac{2}{3}$. In principle, successive applications of the Λ -operator should improve the solution, and, eventually, produce the exact solution. In fact, one can show that $\lim_{n \rightarrow \infty} \Lambda^n(1) = 0$ [see (684, 31)] so that an initial error ϵ at any depth can ultimately be reduced to zero by repeated application of the Λ -operator. In practice, however, the convergence is too slow to be of value, for the effective range of the Λ -operator is of order $\Delta\tau = 1$, so errors at large depth are removed only “infinitely slowly.” (We shall encounter this problem with Λ -iteration repeatedly in a wide variety of contexts! See, e.g.,

§6-1, §7-2.) Further, even a second application of the Λ -operator to $J_E^{(2)}(\tau)$ introduces the functions $\Lambda_t[E_n(t)]$, which are cumbersome to compute [see (361), equations (14-50), (14-53), and (37-36) through (37-44)]. Therefore alternative methods for obtaining a solution must be developed.

Exercise 3-3: Using the results of Table 3-2, evaluate the percentage errors of $J_E(\tau)$ and $J_E^{(2)}(\tau)$ and display them in a plot. The required values of $E_n(\tau)$ can be found in (4, 245).

Exercise 3-4: Show that, although $J_E(\tau)$ was derived assuming $F = \text{constant}$, the flux computed from $J_E(\tau)$ via equation (2-59) is not constant; make a plot of the error $\Delta F(\tau)/F$.

Exercise 3-5: Apply the X -operator [cf. equations (2-62) and (2-65)] to $J_E(\tau)$ to obtain $K_E^{(2)}(\tau) = \frac{1}{16} F \left[\frac{3}{2}\tau + \frac{8}{3} - \frac{2}{3}E_4(\tau) + 2E_5(\tau) \right]$. Use this result to write an analytical expression for the variable Eddington factor $f(\tau) \equiv K(\tau)/J(\tau)$. Show that $f(\tau = \infty) = \frac{2}{3}$ and $f(\tau = 0) = \frac{47}{42} = 0.405$. Using the results of Table 3-2, evaluate the fractional error in $f(\tau)$ [recall equation (3-15)] and plot it.

Exercise 3-6: Show that the improved estimate of the emergent intensity obtained by using $J_E^{(2)}(\tau)$ is $I_E^{(2)}(0, \mu) = \frac{2}{3} F \left\{ \frac{7}{12} + \frac{1}{2}\mu + (\frac{1}{2}\mu + \frac{1}{2}\mu^2) \ln[(1 + \mu)/\mu] \right\}$. Compare this result and $I_E(0, \mu)$ given by equation (3-36) with the exact result shown in Table 3-1, and plot a graph of their fractional errors.

ITERATION: THE UNSÖLD PROCEDURE

The primary shortcoming of the Λ -iteration procedure is its failure to yield an improvement in the solution at great depth. Unsöld (638, 141) proposed an ingenious alternative method that overcomes this inadequacy and can be generalized to the nongrey case. The basic idea is to start from an initial estimate for the source function $B(\tau)$, and to derive a perturbation equation for a change $\Delta B(\tau)$ that more nearly satisfies the requirement of radiative equilibrium.

If we calculate the flux from the initial guess $B(\tau)$, we will find that it is a function of depth, $H(\tau)$, and not exactly constant unless $B(\tau)$ happened to be the exact solution of the problem. From the first-order moment equation (3-9) we then have

$$K(\tau) = \int_0^\tau H(\tau') d\tau' + C \quad (3-39)$$

If we make the Eddington approximation $J(\tau) = 3K(\tau)$ and evaluate C by writing $J(0) = 2H(0)$ [cf. equation (3-34)] we obtain

$$J(\tau) \approx 3 \int_0^\tau H(\tau') d\tau' + 2H(0) \quad (3-40)$$

But from the zero-order moment equation (3-8) we have

$$B(\tau) = J(\tau) - [dH(\tau)/d\tau] \quad (3-41)$$

so that

$$B(\tau) \approx 3 \int_0^\tau H(\tau') d\tau' + 2H(0) - [dH(\tau)/d\tau] \quad (3-42)$$

Equation (3-42) cannot be exact because of the approximations made in its derivation, but it can be used with sufficient accuracy to compute perturbations. In particular, suppose $\Delta B(\tau)$ is chosen just so the flux computed from $B(\tau) + \Delta B(\tau)$ is constant; thus

$$B(\tau) + \Delta B(\tau) \approx 3 \int_0^\tau H d\tau' + 2H \quad (3-43)$$

and by subtraction of equation (3-42) from (3-43) we obtain an expression for $\Delta B(\tau)$, namely

$$\Delta B(\tau) = 3 \int_0^\tau \Delta H(\tau') d\tau' + 2\Delta H(0) - [d\Delta H(\tau)/d\tau] \quad (3-44)$$

Thus if we know the flux errors $\Delta H(\tau) \equiv H - H(\tau)$ we can compute the correction $\Delta B(\tau)$; this correction is then applied and new values of the flux are computed, which give new (smaller!) errors ΔH ; the process is iterated until H becomes constant and $\Delta B \rightarrow 0$ at all τ . Equation (3-44) can be generalized for nongrey atmospheres: see equation (7-18). Unsöld's procedure is very powerful compared to Λ -iteration, for it provides a great improvement in the solution at depth as well as at the surface; this result is demonstrated in the following exercise.

Exercise 3-7: Assume a starting solution $B(\tau) = 3H(\tau + c)$; i.e., $q(\tau) \equiv c$. (a) Show that $\Delta H(\tau) \equiv H - H(\tau) = \frac{1}{2}H[E_4(\tau) - cE_3(\tau)]$. Obtain expressions for $\Delta H(0)$ and $d(\Delta H)/d\tau$. (b) Apply Unsöld's procedure and show that

$$\Delta B(\tau) = 3H \left[\frac{17}{24} - c - \frac{1}{2}cE_2(\tau) + \frac{1}{2}E_3(\tau) + \frac{3}{2}cE_4(\tau) - \frac{3}{2}E_5(\tau) \right]$$

(c) Show that, independent of the initial choice of c , the improved solution has $q(0) = \frac{7}{12} = 0.583$ (exact value 0.577) and $q(\infty) = \frac{17}{12} = 0.708$ (exact value = 0.710). (d) Show that, in contrast, the Λ -operator acting on $q \equiv c$ gives $q(0) = \frac{1}{2}c + \frac{1}{4}$, which agrees with Unsöld's value only if $c = \frac{3}{4}$, and $q(\infty) = c$, which shows no improvement whatever at depth.

THE METHOD OF DISCRETE ORDINATES

The method to be described now furnishes a means of obtaining both approximate solutions and the exact solution of the grey problem. More important, it introduces the fundamental mathematical scheme that provides the basis for practically all modern techniques of solving transfer equations. Introducing the definition of J [equation (1-4)] into equation (3-5), the

transfer equation to be solved may be written in the form

$$\mu [\partial I(\tau, \mu)/\partial \tau] = I(\tau, \mu) - \frac{1}{2} \int_{-1}^1 I(\tau, \mu) d\mu \quad (3-45)$$

which is classified as an *integro-differential equation*. The essential difficulty in obtaining the solution arises from the presence of the integral over angle. However, definite integrals such as that in equation (3-45) may be evaluated numerically by means of a *quadrature sum* consisting of the function evaluated at a finite set of points on the interval of integration times appropriate weights. Thus introducing $\{\mu_j\}$ on $[-1, 1]$ we write, for any function $f(\mu)$,

$$\frac{1}{2} \int_{-1}^1 f(\mu) d\mu \approx \frac{1}{2} \sum_{j=-n}^n a_j f(\mu_j) \quad (3-46)$$

The numbers $\{\mu_j\}$ are called the *quadrature points*, $\{a_j\}$ the *quadrature weights*, and $\{f(\mu_j)\}$ the *discrete ordinates*. Having chosen a definite quadrature formula, we replace the integro-differential transfer equation (3-45) with a coupled system of $2n$ ordinary differential equations:

$$\mu_i (\partial I_i / \partial \tau) = I_i - \frac{1}{2} \sum_{j=-n}^n a_j I_j, \quad (i = \pm 1, \dots, \pm n) \quad (3-47)$$

where I_i denotes $I(\tau, \mu_i)$. The radiation field is no longer represented as a *continuous* function, but rather in terms of a set of *pencils* of radiation, each of which represents the value of $I(\mu)$ over a definite interval. On physical grounds it is reasonable to expect the solution to become exact in the limit $n \rightarrow \infty$.

The accuracy of the quadrature depends both upon the number of points, and upon their distribution on the interval. If the points are distributed uniformly on the interval we obtain a *Newton-Cotes* formula, of which *Simpson's rule* with points at $\{\mu_i\} = (-1, 0, 1)$ is a familiar example. A better choice is to use a *Gaussian* formula, in which the $2n$ points on $[-1, 1]$ are chosen to be the roots of the Legendre polynomial of order $2n$. It would take us too far afield to discuss the construction and accuracy of quadrature formulae [see (161, Chap. 2)]; an important result that we shall merely state is this: an m -point Newton-Cotes formula gives exact results for polynomials of order $m - 1$ (for m even) or m (for m odd), but an m -point Gauss formula is exact for polynomials of order $2m - 1$. For solving the transfer equation the *double-Gauss* formula is superior (619) to the ordinary (or "single") Gauss formula. Here one chooses two separate n -point quadratures on the ranges $(-1 \leq \mu \leq 0)$ and $(0 \leq \mu \leq 1)$; on each range the n points are given by the roots of the Legendre polynomial of order n , scaled from $[-1, 1]$ to

the appropriate range. This approach has the advantage that $I(\tau, +\mu)$ and $I(\tau, -\mu)$ are approximated independently, and thus the integration formula can account, without difficulty, for the physical fact that $I(-\mu) = 0$ at $\tau = 0$ while $I(+\mu)$ remains finite. In the single-Gauss formula, the discontinuity in $I(\mu)$ at $\mu = 0$ when $\tau = 0$ introduces significant errors. In all of these formulae the points are chosen symmetrically about zero so that $\mu_{-j} = -\mu_j$, while $a_{-j} = a_j$.

We now wish to solve the system of equations (3-47). Observing that the system is linear and of the first order, we take a trial solution of the form $I_i = g_i \exp(-k\tau)$, where g_i and k are to be specified. Substituting into equation (3-47) we find

$$g_i(1 + k\mu_i) = \frac{1}{2} \sum_{j=-n}^n a_j g_j = c \quad (3-48)$$

so that $g_i = c/(1 + k\mu_i)$. If we use this specific form for g_i and again substitute the trial solution into equation (3-47), we find

$$\frac{1}{2} \sum_{j=-n}^n a_j (1 + k\mu_j)^{-1} = 1 \quad (3-49)$$

This is the *characteristic equation*, which is satisfied only by certain values of k , called the *characteristic roots* (eigenvalues). Recalling that $a_{-j} = a_j$ and $\mu_{-j} = -\mu_j$, equation (3-49) can be used to define the *characteristic function* $T(k^2)$,

$$T(k^2) \equiv 1 - \sum_{j=1}^n a_j (1 - k^2 \mu_j^2)^{-1} \quad (3-50)$$

The roots of T [i.e., those values of k for which $T(k^2) = 0$] are the desired characteristic roots. If we set $f(\mu) \equiv 1$ in equation (3-46) we see that

$$\frac{1}{2} \sum_{j=-n}^n a_j = \sum_{j=1}^n a_j = 1$$

hence it follows that $k^2 = 0$ is a solution of the characteristic equation; i.e., $T(k^2 = 0) = 0$. There are an additional $(n - 1)$ nonzero roots, which may be seen as follows. Note that $k^2 = \mu_j^{-2}$ is a pole of T , which becomes infinite for these values of k^2 . For $k^2 = \mu_j^{-2} - \epsilon$, $T(k^2) < 0$, and by making ϵ arbitrarily small, $T(k^2) \rightarrow -\infty$. Similarly, for $k^2 = \mu_j^{-2} + \epsilon$, $T(k^2) > 0$, and as $\epsilon \rightarrow 0$, $T \rightarrow +\infty$. It is thus clear that T must pass through zero somewhere on the interval between successive poles, hence the $(n - 1)$ nonzero roots must satisfy the relations

$$\mu_1^{-2} < k_1^2 < \mu_2^{-2} < \cdots < k_{n-1}^2 < \mu_n^{-2}$$

where we have ordered $\{\mu_i\}$ such that $\mu_i > \mu_{i+1}$. Note that the largest μ_i must be less than unity, hence the smallest nonzero k^2 must be greater than unity. In all there exist $2n - 2$ nonzero values of the k 's, in pairs of the form $\pm k_i$ ($i = 1, \dots, n - 1$).

The general solution of the system (3-47) is therefore of the form

$$I_i(\tau) = b \left[\sum_{a=1}^{n-1} L_a (1 + k_a \mu_i)^{-1} e^{-k_a \tau} + \sum_{a=1}^{n-1} L_{-a} (1 - k_a \mu_i)^{-1} e^{+k_a \tau} \right] \quad (3-51)$$

We must now seek the special solution corresponding to the root $k^2 = 0$. In view of equation (3-11) which shows that $J(\tau)$ must become linear in τ at depth, we examine trial solutions of the form $I_i = b(\tau + q_i)$. Substituting this expression into equation (3-47) we obtain

$$q_i = \mu_i + \frac{1}{2} \sum_{j=-n}^n a_j q_j \quad (3-52)$$

Now observing that if we set $f(\mu) = \mu$ in equation (3-46) the quadrature sum $\sum a_j \mu_j$ is zero, we see that equation (3-52) is satisfied by the simple choice $q_i = Q + \mu_i$. Hence the particular solution is $I_i(\tau) = b(\tau + Q + \mu_i)$ and the complete solution is

$$I_i(\tau) = b \left(\tau + Q + \mu_i + \sum_{a=1}^{n-1} \frac{L_a e^{-k_a \tau}}{1 + k_a \mu_i} + \sum_{a=1}^{n-1} \frac{L_{-a} e^{+k_a \tau}}{1 - k_a \mu_i} \right) \quad (3-53)$$

We must now specify the $2n$ unknown coefficients b , Q , and $L_{\pm a}$. This is done by application of the boundary conditions.

In the case of a *finite* slab of total optical thickness T , both $I_{-i}^- \equiv I(0, -\mu_i)$ and $I_i^+ \equiv I(T, +\mu_i)$ are given functions of μ . Thus we may write $2n$ equations for the $2n$ unknowns:

$$I(0, -\mu_i) = b \left(Q - \mu_i + \sum_{a=1}^{n-1} \frac{L_a}{1 - k_a \mu_i} + \sum_{a=1}^{n-1} \frac{M_a e^{-k_a T}}{1 + k_a \mu_i} \right) = I_{-i}^- \quad (3-54a)$$

and

$$I(T, +\mu_i) = b \left(Q + T + \mu_i + \sum_{a=1}^{n-1} \frac{L_a e^{-k_a T}}{1 + k_a \mu_i} + \sum_{a=1}^{n-1} \frac{M_a}{1 - k_a \mu_i} \right) = I_i^+ \quad (3-54b)$$

where, to improve the numerical condition of the equations, $M_a \equiv L_{-a} e^{k_a T}$. Equations (3-54) may be solved by standard numerical techniques for linear equations.

In the case of a *semi-infinite* atmosphere in radiative equilibrium we have the boundary conditions $I_{-i} = I(0, -\mu_i) \equiv 0$, and demand that $I(\tau)$ must not diverge exponentially as $\tau \rightarrow \infty$. To satisfy the latter constraint we set

$$L_{-a} \equiv 0 \quad (3-55)$$

and use the upper boundary condition to write the n equations

$$Q - \mu_i + \sum_{a=1}^{n-1} L_a (1 - k_a \mu_i)^{-1} = 0, \quad (i = 1, \dots, n) \quad (3-56)$$

Solution of equations (3-56) yields the n unknowns Q and L_a . In addition, we require that the flux equal the nominal flux F . Thus we demand that

$$2 \int_{-1}^1 I(\mu) \mu \, d\mu = 2 \sum_{j=-n}^n a_j \mu_j I_j = F \quad (3-57)$$

Substituting equations (3-53) (with $L_{-a} \equiv 0$), we have

$$2b \left[(\tau + Q) \sum_{j=-n}^n a_j \mu_j + \sum_{j=-n}^n a_j \mu_j^2 + \sum_{a=1}^{n-1} L_a e^{-k_a \tau} \sum_{j=-n}^n \frac{a_j \mu_j}{1 + k_a \mu_j} \right] = F \quad (3-58)$$

In view of equation (3-46) the first sum is zero, the second equals $\frac{2}{3}$, and from the characteristic equation the fourth is found to be zero.

Exercise 3-8: Verify the statement made above about the values of the sums in equation (3-58).

Thus we find that $b = \frac{2}{3}F$, as would be expected from equation (3-11); note also that the quadrature calculation yields a *constant* flux automatically. Finally, the complete solution for the semi-infinite atmosphere may be written

$$I_i(\tau) = \frac{3}{4} F \left[\tau + Q + \mu_i + \sum_{a=1}^{n-1} L_a e^{-k_a \tau} (1 + k_a \mu_i)^{-1} \right], \quad (i = 1, \dots, n) \quad (3-59)$$

We may compute $J(\tau)$ by substituting equations (3-59) into the quadrature formula; making use of the characteristic equation (3-49), we obtain

$$J(\tau) = \frac{3}{4} F \left(\tau + Q + \sum_{a=1}^{n-1} L_a e^{-k_a \tau} \right) \quad (3-60)$$

and thus the discrete-ordinate representation of $q(\tau)$ is

$$q(\tau) = Q + \sum_{a=1}^{n-1} L_a e^{-k_a \tau} \quad (3-61)$$

Exercise 3-9: Derive equation (3-60).

Numerical results for $q(\tau)$ were obtained for $n = 1, \dots, 4$ by Chandrasekhar (153) using a single-Gauss formula and by Sykes (619) using the superior double-Gauss formula. In every case the *exact* value $q(0) = 1/\sqrt{3}$ is obtained. The maximum percentage (absolute) error in $J(\tau)$ for the single-Gauss solutions is (9.0, 4.1, 2.7, 2.0) for $n = 1, \dots, 4$, respectively, while for the double-Gauss it is (9.0, 1.8, 0.9) for $n = 1, \dots, 3$, respectively. The double-Gauss estimates of $q(\infty)$, namely Q , are 0.71132 and 0.71057 for $n = 2$ and 3; these values compare favorably with the exact value 0.710446. The double-Gauss solution with $n = 3$ gives the emergent intensity $I(0, \mu)/F$ with a root-mean-square error of only 0.1%, and is very accurate (0.02%) for $\mu \geq 0.3$. It should be stressed that the main importance of the discrete ordinate method is that in the limit $n \rightarrow \infty$ it yields the exact solution and that it affords an extremely powerful approximation technique for more complicated problems.

Several very important results that will be useful in later work can be established by analytical manipulation of the characteristic equation and the boundary conditions. To simplify the notation we define $x \equiv 1/k$ and $X \equiv 1/k^2$. The characteristic function defined in equation (3-50) may be rewritten in the equivalent forms

$$T(X) \equiv 1 - X \sum_{j=1}^n \frac{a_j}{X - \mu_j^2} = \sum_{j=1}^n a_j - X \sum_{j=1}^n \frac{a_j}{X - \mu_j^2} = \sum_{j=1}^n \frac{a_j \mu_j^2}{\mu_j^2 - X} \quad (3-62)$$

To clear $T(X)$ of fractions, multiply through by $\prod_{j=1}^n (\mu_j^2 - X)$; this yields

$$P(X) \equiv \prod_{j=1}^n (\mu_j^2 - X) T(X) = \sum_{i=1}^n a_i \mu_i^2 \prod_{j \neq i}^n (\mu_j^2 - X) \quad (3-63)$$

which is clearly a polynomial of order $(n - 1)$ in X . But we know that $T(X)$ has the $(n - 1)$ roots $X_1 = 1/k_1^2, \dots, X_{n-1} = 1/k_{n-1}^2$, so $P(X)$ must have the form $C(X - X_1) \cdots (X - X_{n-1})$. To evaluate the constant, we note that the coefficient of the term in X^{n-1} in equation (3-63) is $(-1)^{n-1} \sum_{i=1}^n a_i \mu_i^2 = (-1)^{n-1} \frac{1}{3}$; this is simply C itself. We thus have

$$P(X) = \frac{1}{3} (X_1 - X) \cdots (X_{n-1} - X)$$

and therefore

$$T(X) = \frac{1}{3} \left[\prod_{j=1}^{n-1} (X_j - X) \right] / \prod_{j=1}^n (\mu_j^2 - X) \quad (3-64)$$

From equation (3-62) we see that $T(X = 0) = 1$, hence setting $X = 0$ in equation (3-64) we obtain the useful (see below) result that

$$\mu_1 \mu_2 \cdots \mu_n k_1 k_2 \cdots k_{n-1} = 1/\sqrt{3} \quad (3-65)$$

Now consider the emergent intensity $I(0, \mu)$. Define a function $S(\mu)$ such that

$$S(\mu_i) \equiv Q - \mu_i + \sum_{\alpha=1}^{n-1} L_\alpha (1 - k_\alpha \mu_i)^{-1} \quad (3-66)$$

The surface boundary conditions in equation (3-56) may then be written

$$I(0, -\mu_i) = \frac{3}{4} F S(\mu_i) = 0 \quad (3-67)$$

We then generalize $S(\mu)$ to apply at all values of μ and write

$$I(0, \mu) = \frac{3}{4} F S(-\mu) \quad (3-68)$$

for $\mu \geq 0$. Note that, with this generalization, $I(0, -\mu)$ is not $\equiv 0$, but will in general have nonzero values for $-\mu \neq -\mu_i$. By working with $S(\mu)$, we can obtain an expression for $I(0, \mu)$ that does not involve the constants L_α and Q explicitly. Clear fractions from equation (3-66) to obtain

$$S(\mu) \prod_{\alpha=1}^{n-1} (1 - k_\alpha \mu) = (Q - \mu) \prod_{\alpha=1}^{n-1} (1 - k_\alpha \mu) + \sum_{\alpha=1}^{n-1} L_\alpha \prod_{i=1}^{n-1} (1 - k_i \mu) \quad (3-69)$$

The righthand expression is obviously a polynomial of order n in μ . But $S(\mu)$ has the n roots μ_1, \dots, μ_n ; hence this polynomial must be of the form $C(\mu - \mu_1) \cdots (\mu - \mu_n)$. To find C we note that the coefficient μ^n on the righthand side of equation (3-69) is $(-1)^n k_1 \cdots k_{n-1}$, which is C itself. Therefore

$$S(\mu) = \frac{(\prod_{i=1}^{n-1} k_i) \prod_{i=1}^n (\mu_i - \mu)}{\prod_{i=1}^{n-1} (1 - k_i \mu)} = \frac{\prod_{i=1}^n (\mu_i - \mu)}{\prod_{i=1}^{n-1} (x_i - \mu)} \quad (3-70)$$

which, when inserted into equation (3-68), yields the desired expression for $I(0, \mu)$. It is customary to define a *limb-darkening function* $H(\mu)$ as

$$H(\mu) \equiv I(0, \mu)/I(0, 0) \quad (3-71)$$

[note that unlike equation (3-37), the reference point here is the limb, not disk-center]. In the discrete-ordinate approximation we find from equations (3-68) and (3-70)

$$H(\mu) = \left[\prod_{i=1}^n (1 + \mu_i^{-1} \mu) \right] / \prod_{i=1}^{n-1} (1 + k_i \mu) \quad (3-72)$$

By further analysis using $S(\mu)$ it is possible to write explicit expressions for the L_α 's and Q in terms of the points $\{\mu_i\}$ and the roots $\{k_\alpha\}$ [see (161, 78–79; 684, 25)].

Before leaving the discrete ordinate method, let us show that $q(0) = 1/\sqrt{3}$ is the exact value. First, note that in the n th discrete approximation

$$J_n(0) = \frac{3}{4} F \left(Q + \sum_{\alpha=1}^{n-1} L_\alpha \right) = \frac{3}{4} F q(0) \quad (3-73)$$

while from equation (3-59) we find

$$I_n(0, 0) = \frac{3}{4} F \left(Q + \sum_{\alpha=1}^{n-1} L_\alpha \right) = J_n(0) \quad (3-74)$$

independent of the order n . Thus we conclude that in the exact solution $J(0) = I(0, 0)$. But from equations (3-68) and (3-70)

$$I_n(0, 0) = \frac{3}{4} F S(0) = \frac{3}{4} F \mu_1 \cdots \mu_n k_1 \cdots k_{n-1} \quad (3-75)$$

Then, combining equations (3-65), (3-75), and (3-73), we deduce that, independent of the order n , $q_n(0) = 1/\sqrt{3}$; hence this result is exact.

3-4 Exact Solution

The exact solution for $q(r)$ and $H(\mu)$ can be obtained by taking the discrete-ordinate method to the limit $n \rightarrow \infty$ (161, Chap. 5; 361, §27), by applying the principle of invariance (161, Chap. 4; 361, §28), or by direct Laplace transform methods (361, §29; 684, Chap. 3). Only certain important results will be quoted here, and the reader should consult the references cited for details.

Several expressions for $H(\mu)$ exist (361, 186–187); a form convenient for numerical computation is

$$H(\mu) = (\mu + 1)^{-1/2} \exp \left[\frac{1}{\pi} \int_0^{\pi/2} \frac{\theta \tan^{-1}(\mu \tan \theta)}{1 - \theta \cot \theta} d\theta \right] \quad (3-76)$$

TABLE 3-1
Exact Limb-Darkening Law for
Grey Atmospheres

μ	$I(0, \mu)/F$	μ	$I(0, \mu)/F$
0.0	0.43301	0.6	0.95009
0.1	0.54012	0.7	1.02796
0.2	0.62802	0.8	1.10535
0.3	0.71123	0.9	1.18238
0.4	0.79210	1.0	1.25912
0.5	0.87156		

Evaluation of this integral (152; 518) yields the results summarized in Table 3-1.

The value of $q(\infty)$ can be obtained by noting from equation (3-15) that $K(0) = Hq(\infty)$, and thus, using equation (3-71),

$$q(\infty) = \left[\int_0^1 H(\mu)\mu^2 d\mu \right] / \int_0^1 H(\mu)\mu d\mu \quad (3-77)$$

From the known expressions for $H(\mu)$ one then obtains

$$q(\infty) = \frac{6}{\pi^2} + \frac{1}{\pi} \int_0^{\pi/2} \left(\frac{3}{\theta^2} - \frac{1}{1 - \theta \cot \theta} \right) d\theta \quad (3-78)$$

which yields $q(\infty) = 0.71044609$ (519). Finally, a closed-form expression can

TABLE 3-2
The Exact Solution for $q(\tau)$

τ	$q(\tau)$	τ	$q(\tau)$
0.00	0.577351	0.8	0.693534
0.01	0.588236	1.0	0.698540
0.03	0.601242	1.5	0.705130
0.05	0.610758	2.0	0.707916
0.10	0.627919	2.5	0.709191
0.20	0.649550	3.0	0.709806
0.30	0.663365	3.5	0.710120
0.40	0.673090	4.0	0.710270
0.50	0.680240	5.0	0.710398
0.60	0.685801	∞	0.710446

be written (407) for $q(\tau)$, namely

$$q(\tau) = q(\infty) - \frac{1}{2\sqrt{3}} \int_0^1 \frac{e^{-\tau/u} du}{H(u)Z(u)} \quad (3-79)$$

where $H(u)$ is as defined above and

$$Z(u) \equiv \left[1 - \frac{1}{2} u \ln \left(\frac{1+u}{1-u} \right) \right]^2 + \frac{1}{4} \pi^2 u^2 \quad (3-80)$$

Results obtained from a numerical evaluation of equation (3-79) are given in Table 3-2.

3-5 Emergent Flux from a Grey Atmosphere

The basic physical assumption made in the grey-atmosphere problem is that the opacity is independent of frequency. In this event, the constraint of radiative equilibrium reduces to $S(\tau) \equiv J(\tau)$, and the problem simplifies to that of obtaining the solution of equation (3-6). If, in addition, it is assumed that LTE prevails, then we may equate $B(\tau) = (\sigma_R T^4)/\pi$ to $J(\tau)$, and thus arrive at equation (3-16) for $T(\tau)$. The radiation field has a dependence upon frequency because the source function, which we assume is $B_v(\tau)$, depends upon frequency. Given the source function, the flux, also frequency-dependent, can be computed at any depth by means of equation (2-59), which now reads

$$F_v(\tau) = 2 \int_{\tau}^{\infty} B_v[T(t)] E_2(t - \tau) dt - 2 \int_0^{\tau} B_v[T(t)] E_2(\tau - t) dt \quad (3-81)$$

The temperature appears in the Planck function only in the combination (hv/kT) ; further, the ratio $T(\tau)/T_{\text{eff}}$ is a unique function of τ [cf. equation (3-16)]—say, $1/p(\tau)$. We may therefore simplify the equation by introducing a parameter $\alpha \equiv (hv/kT_{\text{eff}})$, in terms of which we can write $(hv/kT) = \alpha p(\tau)$. Expressing the flux in the same units by writing $F_a(\tau) \equiv F_v(\tau)(dv/d\alpha)$, and using the relation $F \equiv (\sigma_R T_{\text{eff}}^4)/\pi$, we may rewrite equation (3-81) as

$$\frac{F_a(\tau)}{F} = \left(\frac{4\pi k^4}{h^3 c^2 \sigma_R} \right) \alpha^3 \left\{ \int_{\tau}^{\infty} \frac{E_2(t - \tau) dt}{\exp[\alpha p(t)] - 1} - \int_0^{\tau} \frac{E_2(\tau - t) dt}{\exp[\alpha p(t)] - 1} \right\} \quad (3-82)$$

The expression in the brackets is a function of α and τ only, and may be calculated once and for all. A tabulation of $F_a(\tau)/F$ is given in (161, 295), and a plot of the function is displayed in Figure 3-1. The figure shows clearly the degradation of photon energies as they transfer from depth to the surface; for example, the most common photon energy at $\tau = 0$ is only about

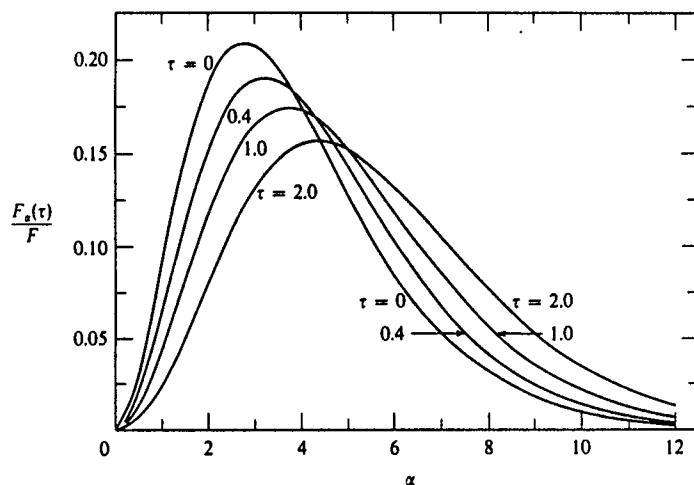


FIGURE 3-1
Frequency distribution of flux at selected depths in a grey atmosphere. From (155), by permission.

75 percent of that at $\tau = 1$. This progressive reddening of photons in the outer layers results from the outward decrease in temperature produced by the requirement of radiative equilibrium.

3-6 Small Departures from Greyness

By use of an appropriate mean opacity, it is possible to account for small departures from greyness, at least approximately, and thus to extend greatly the usefulness of the results obtained for a grey atmosphere. Suppose that the frequency variation of the opacity is the same at all depths so that we can write

$$\chi_v = \bar{\chi}_c(1 + \beta_v) \equiv \bar{\chi}_c\gamma_v \quad (3-83)$$

where

$$\bar{\chi}_c F \equiv \int_0^\infty \chi_v F_v^{(1)} dv \quad (3-84)$$

In equation (3-84), $F_v^{(1)}$ denotes the flux in a grey atmosphere. The mean opacity $\bar{\chi}_c$ defined in equation (3-84) is known as the *Chandrasekhar mean*; as we shall see in what follows, this mean is constructed in a way that makes optimum use of the information contained in the grey solution. Unlike the flux mean [equation (3-21)] the Chandrasekhar mean can be computed straightforwardly for any given frequency dependence (i.e., β_v or γ_v) of the opacity because $F_v^{(1)}$ is a known function.

Let us now consider how we may solve the nongrey transfer problem using a method of successive approximations. The nongrey transfer equation (assuming LTE) is

$$\mu(\partial I_v / \partial \bar{\tau}) = (\chi_v / \bar{\chi})(I_v - B_v) = (1 + \beta_v)(I_v - B_v) \quad (3-85)$$

If we suppose that the departures β_v may be regarded as small, then a first approximation to the solution of equation (3-85) is obtained by setting $\beta_v \equiv 0$ initially. The transfer equation then returns to the equation for the grey problem itself, namely

$$\mu(\partial I_v^{(1)} / \partial \bar{\tau}) = I_v^{(1)} - B_v \quad (3-86)$$

whose solution is already known. To obtain a second approximation we write

$$\begin{aligned} \mu(\partial I_v^{(2)} / \partial \bar{\tau}) &= I_v^{(2)} - B_v + \beta_v(I_v^{(1)} - B_v) \\ &= I_v^{(2)} - B_v + \beta_v \mu(\partial I_v^{(1)} / \partial \bar{\tau}) \end{aligned} \quad (3-87)$$

by substitution from equation (3-86). If we demand that the radiation field resulting from this second approximation should satisfy the constraint of radiative equilibrium, then we must have $(dF^{(2)} / d\bar{\tau}) \equiv 0$, where $F^{(2)}$ is the integrated flux; then from equation (3-87)

$$J^{(2)} - B + \frac{d}{d\bar{\tau}} \left[\int_0^\infty \beta_v F_v^{(1)} dv \right] = 0 \quad (3-88)$$

But note that equations (3-83) and (3-84) imply that

$$\bar{\chi}_c F = \bar{\chi}_c \int_0^\infty (1 + \beta_v) F_v^{(1)} dv = \bar{\chi}_c F + \bar{\chi}_c \int_0^\infty \beta_v F_v^{(1)} dv \quad (3-89)$$

or that

$$\int_0^\infty \beta_v F_v^{(1)} dv \equiv 0 \quad (3-90)$$

Therefore the radiative equilibrium constraint for a nongrey atmosphere treated by the above approximation scheme collapses to $J^{(2)} = B(\bar{\tau})$. This shows that the *grey* solution for $T(\bar{\tau})$ on the Chandrasekhar-mean optical-depth scale will automatically satisfy the condition of radiative equilibrium in the first approximation to the nongrey atmosphere. The method for obtaining higher approximations is described in (161, 296 ff.).

At this first level of approximation we may compute the nongrey emergent intensity as

$$I_v(0, \mu) = \int_0^\infty B_v [T(\bar{\tau})] \exp(-\gamma_v \bar{\tau} / \mu) (\gamma_v / \mu) d\bar{\tau} \quad (3-91)$$

and the flux as

$$F_v(0) = 2 \int_0^\infty B_v[T(\bar{\tau})] E_2(\gamma_v \bar{\tau}) \gamma_v d\bar{\tau} \quad (3-92)$$

If we introduce the parameter $\alpha \equiv (hv/kT_{\text{eff}})$ as was done in §3-5, and write

$$B_v[T(\bar{\tau})] = B_v(T_0) \left[\frac{\exp[\alpha T_{\text{eff}}/T_0] - 1}{\exp[\alpha p(\bar{\tau})] - 1} \right] = B_v(T_0) b_\alpha(\bar{\tau}) \quad (3-93)$$

equations (3-91) and (3-92) reduce to the parametric forms

$$I_v(0, \mu) = B_v(T_0) \int_0^\infty b_\alpha(\bar{\tau}) \exp(-\gamma_v \bar{\tau}/\mu) (\gamma_v/\mu) d\bar{\tau} \equiv B_v(T_0) \mathcal{I}(\alpha, \gamma_v/\mu) \quad (3-94)$$

and

$$F_v(0) = 2B_v(T_0) \int_0^\infty b_\alpha(\bar{\tau}) E_2(\gamma_v \bar{\tau}) \gamma_v d\bar{\tau} \equiv B_v(T_0) \mathcal{F}(\alpha, \gamma_v) \quad (3-95)$$

The function $b_\alpha(\bar{\tau})$ is unique for a given value of α , and hence the functions $\mathcal{I}(\alpha, \beta)$ and $\mathcal{F}(\alpha, \beta)$ may be computed once and for all; tables of these functions are given in (161, 306–307).

The functions $\mathcal{I}(\alpha, \beta)$ and $\mathcal{F}(\alpha, \beta)$ described above at one point played an important role in the development of the theory of stellar atmospheres. By analysing the observational material available for the sun, Münch (473) was able to find those values of γ_v that best reproduced the observed fluxes and limb-darkening. These were shown to be compatible with the frequency variation of the absorption coefficient of the negative hydrogen ion, H^- , as computed by Chandrasekhar. Analyses such as these led to conclusive identification of H^- as the major opacity source in the solar atmosphere. We examine opacities in some detail in the next chapter.

Absorption Cross-Sections

In this chapter we outline the quantum mechanical calculation of atomic absorption cross-sections. The discussion is meant to be self-contained, but limitations of space require that knowledge of the basic principles of quantum mechanics at the level of (392, Chaps. 2–8) be presupposed.

4-1 The Einstein Relations for Bound–Bound Transitions

Let us first consider the absorption and emission of radiation by an atom in a transition between two bound states. Assume that the lower state (i) has statistical weight g_i , and the upper state (j) statistical weight g_j . There are three basic processes involved, which are usually described in terms of rate coefficients first introduced by Einstein (207).

The first process is the direct *absorption* of radiation, leading to an upward transition from level i to level j . The rate at which this process occurs for radiation of specific intensity I_v can be written in terms of the *Einstein coefficient* B_{ij} as

$$n_i(v) R_{ij}(d\omega/4\pi) = n_i(v) B_{ij} I_v(d\omega/4\pi) \quad (4-1)$$

where $n_i(v)$ is the number of atoms per cm^3 in state i that can absorb radiation at frequencies on the range $(v, v + dv)$. In general the spectrum line corresponding to the transition will not be sharp; rather, because of perturbations exerted by nearby atoms and ions, as well as the finite lifetime of the upper state, it will have a spread in frequency that we can describe by an *absorption profile*, ϕ_v , normalized such that $\int \phi_v dv = 1$. Thus if the total number of atoms in state i is n_i , the number capable of absorbing at frequency v is $n_i(v) = n_i \phi_v$. In making the transition from level i to level j , the atom absorbs photons of energy $h\nu_{ij} = E_j - E_i$. Thus the rate at which *energy* is removed from an incident beam of radiation is

$$a_v I_v = n_i(B_{ij}h\nu_{ij}/4\pi)\phi_v I_v \quad (4-2)$$

where a_v denotes a macroscopic absorption coefficient (per unit volume), uncorrected for stimulated emission (see below).

For atoms returning from level j to level i , two processes are possible. The first of these is a spontaneous transition with the emission of a photon. Writing the *probability of spontaneous emission* per unit time as A_{ji} , the rate of emission of energy is

$$\eta_v(\text{spontaneous}) = n_j(A_{ji}h\nu_{ij}/4\pi)\psi_v \quad (4-3)$$

Here the emission profile ψ_v specifies the number of atoms in the upper state that can emit photons on the frequency range $(v, v + dv)$; it is normalized such that $\int \psi_v dv = 1$. The other possible return process is a transition *induced by the radiation field (stimulated emission)*. The rate at which such emission occurs is assumed proportional to the intensity of the incident radiation field. The energy emitted may be written in terms of the Einstein coefficient B_{ji} as

$$\eta_v(\text{induced}) = n_j(B_{ji}h\nu_{ij}/4\pi)\psi_v I_v \quad (4-4)$$

In writing equation (4-4), use has been made of the result that the profile for induced emission is the same as that for spontaneous emission, as can be shown from general quantum mechanical considerations (197, §62). It should be noted that spontaneous emission takes place *isotropically*. Induced emission is proportional to and has the same angular distribution as I_v ; because of this, induced emissions are sometimes considered to be *negative absorptions*, though this is not quite correct, for in general ψ_v will not be identical to ϕ_v .

The coefficients A_{ji} , B_{ji} , and B_{ij} are simply related, as can be shown by calculating rates of absorption and emission in thermodynamic equilibrium. In strict T.E., the radiation field is isotropic, and $I_v \equiv B_v$, the Planck function. Furthermore, in T.E. the occupation numbers of levels i and j are related

by the Boltzmann law [cf. equation (5-5)]

$$(n_j/n_i)^* = (g_j/g_i) \exp(-h\nu_{ij}/kT) \quad (4-5)$$

Moreover, in T.E., $\psi_v = \psi_v^* = \phi_v$ [cf. equation (2-14)]. Now in strict T.E., each upward transition on the range $(v, v + dv)$ must be exactly balanced (detailed balancing) by an emission on that range. Hence, frequency by frequency we must have

$$n_i^* B_{ij} B_v = n_j^* A_{ji} + n_j^* B_{ji} B_v \quad (4-6)$$

Solving for B_v , we find

$$B_v = \frac{n_j^* A_{ji}}{n_i^* B_{ij} - n_j^* B_{ji}} = \left(\frac{A_{ji}}{B_{ji}} \right) \left[\left(\frac{g_i B_{ij}}{g_j B_{ji}} \right) \exp(h\nu_{ij}/kT) - 1 \right]^{-1} \quad (4-7)$$

But the correct expression for the Planck function as obtained from statistical mechanical arguments is $B_v = (2h\nu^3/c^2)[\exp(h\nu/kT) - 1]^{-1}$, and to make this expression correspond to equation (4-7) we conclude that

$$A_{ji} \equiv (2h\nu^3/c^2)B_{ji} \quad (4-8)$$

$$\text{and} \quad g_i B_{ij} \equiv g_j B_{ji} \quad (4-9)$$

We shall use these results repeatedly in later work.

It should be noted that, although the *Einstein relations* in equations (4-8) and (4-9) were derived, for ease, from a thermodynamic equilibrium argument, the Einstein coefficients are really *properties of the atom only*, and must be independent of the nature of the radiation field. Therefore we must conclude that equations (4-8) and (4-9) are true in general. It is of interest that historically a line of argument similar to that presented above led to the realization that the stimulated emission process must occur in nature—a fact not intuitively obvious at first sight.

Exercise 4-1: Show that for a Planckian radiation field at typical stellar temperatures ($\sim 10^4$ °K) spontaneous emissions occur much more rapidly than induced emissions in the ultraviolet where $h\nu/kT \gg 1$, while the reverse is true at far-infrared and radio wavelengths where $h\nu/kT \ll 1$.

The microscopic formulation described above may immediately be incorporated into the equation of transfer. If *only* the bound-bound process occurs, then the appropriate transfer equation is

$$\mu(\partial I_v / \partial z) = [n_j A_{ji} \psi_v - (n_i B_{ij} \phi_v - n_j B_{ji} \psi_v) I_v] (h\nu_{ij}/4\pi) \quad (4-10)$$

Here we have followed the usual practice of grouping together all terms involving I_v . In this way one can define a *line absorption coefficient corrected for stimulated emission*, namely

$$\chi_i(v) = \left(\frac{n_i B_{ij} h v_{ij}}{4\pi} \right) \phi_v \left(1 - \frac{n_j B_{ji} \psi_v}{n_i B_{ij} \phi_v} \right) = \left(\frac{n_i B_{ij} h v_{ij}}{4\pi} \right) \phi_v \left(1 - \frac{n_j g_i \psi_v}{n_i g_j \phi_v} \right) \quad (4-11)$$

and a *line source function*

$$S_i = \frac{n_j A_{ji} \psi_v}{n_i B_{ij} \phi_v - n_j B_{ji} \psi_v} = \left(\frac{2 h v_{ij}^3}{c^2} \right) \left[\frac{n_i g_j \phi_v}{n_j g_i \psi_v} - 1 \right]^{-1} \quad (4-12)$$

The transfer equation then reduces to the standard form [equation (2-36)].

In many cases of astrophysical interest, the simplifying approximation of *complete redistribution* is valid; then $\psi_v \equiv \phi_v$, and equations (4-11) and (4-12) reduce to

$$\chi_i(v) = \left(\frac{n_i B_{ij} h v_{ij}}{4\pi} \right) \phi_v \left(1 - \frac{n_j g_i}{n_i g_j} \right) \quad (4-13)$$

and $S_i = (2 h v_{ij}^3 / c^2) [(n_i g_j / n_j g_i) - 1]^{-1}$ (4-14)

These expressions will be used through most of this book, except in Chapter 13 where a distinction between ψ_v and ϕ_v will be made. In the case of LTE, Boltzmann statistics apply; hence $(n_j/n_i) = (n_j/n_i)^* = (g_j/g_i) \exp(-h v_{ij}/kT)$, and the absorption coefficient becomes

$$\chi_i^*(v) = (n_i B_{ij} h v_{ij} / 4\pi) \phi_v [1 - \exp(-h v_{ij}/kT)] \quad (4-15)$$

The factor $[1 - \exp(-h v_{ij}/kT)]$ is usually referred to as the *correction for stimulated emission*; but as is evident from equations (4-11) and (4-13), this expression for the correction factor is valid in LTE only. Similarly, in LTE the source function becomes

$$S_i^* = (2 h v_{ij}^3 / c^2) [\exp(h v_{ij}/kT) - 1]^{-1} \equiv B_v \quad (4-16)$$

as expected from the Kirchhoff–Planck relation [equation (2-5)].

Equation (4-14) contains implicitly the solution of the statistical equilibrium equations (cf. Chapter 5), inasmuch as it makes reference to the ratio of the populations of the levels involved. Only in the case of LTE can this ratio be expressed in terms of a single thermodynamic variable, T ; in general it will depend upon the temperature, density, and the radiation field (in all transitions of the atom). We shall therefore refer to equation (4-14) as an *implicit form* of the source function. An alternative approach is explicitly to introduce *analytically* the solution of the statistical equilibrium equations

into the source function, yielding what we shall refer to as an *explicit form*. As we shall see in Chapters 7 and 11 through 14, the latter form is by far the more powerful and useful.

4-2 The Calculation of Transition Probabilities

Let us now turn to the calculation of the Einstein coefficients. Specifically, we shall derive the direct absorption probability B_{ij} , as B_{ji} and A_{ji} can be obtained from B_{ij} by use of equations (4-8) and (4-9). The computation may be made on three successively more accurate levels of approximation, as follows.

(1) Classical Atom and Electromagnetic Field. The electron is considered to be a damped harmonic oscillator driven by the electromagnetic field. A *unique* absorption coefficient is derived, which is dimensionally correct and accurate for very strong lines; for weak lines it may be wrong by orders of magnitude.

(2) Quantum Mechanical Atom and Classical Electromagnetic Field. Here the correct values of B_{ij} and B_{ji} can be derived, but A_{ji} does not appear in the formulation (although it is still given correctly by the Einstein relations).

(3) Quantum Mechanical Atom and Quantized Electromagnetic Field. Here the correct results are automatically obtained for all three coefficients, and this approach represents the complete theory.

In this section we shall carry through the calculation by method (1) for historical interest and general background, and by method (2) to obtain the correct expression for B_{ij} . Application of method (3) is more complicated and does not need to be carried through if one is satisfied to use the Einstein relations. A complete discussion of the third method may be found, e.g., in (197, Chap. 10; 293, §§7, 14, 17; and 418, Chap. 22).

THE CLASSICAL OSCILLATOR

Consider first the electromagnetic radiation from a moving charge. Suppose a particle has charge e , velocity v , and acceleration \ddot{v} . Then from classical electromagnetic theory (331, Chap. 9; 343, Chap. 17; 494, Chap. 20) the electric and magnetic fields at a distant position r relative to the charge are found to be

$$\mathbf{E}(r, t) = (e \dot{v} / c^2 r) \sin \theta \hat{\theta} \quad (4-17)$$

and $\mathbf{H}(r, t) = (e \dot{v} / c^2 r) \sin \theta \hat{\phi}$ (4-18)

where θ denotes the angle between the acceleration \ddot{v} and \hat{r} , $\hat{\theta}$ and $\hat{\phi}$ are unit vectors in a spherical system defined by \ddot{v} and \hat{r} , and \dot{v} is evaluated at a

time $t' = t - (r/c)$. The power radiated per cm^2 is given by the Poynting vector [cf. equation (1-35)]

$$\mathbf{S} = (c/4\pi)(\mathbf{E} \times \mathbf{H}) = (e^2 v^2 / 4\pi c^3 r^2) \sin^2 \theta \hat{\mathbf{r}} \quad (4-19)$$

Now integrating over a sphere of radius r by forming $\mathbf{S} \cdot d\mathbf{A}$ where $d\mathbf{A} = (r^2 d\omega) \hat{\mathbf{r}} = (r^2 d\mu d\phi) \hat{\mathbf{r}}$ and writing $\sin^2 \theta = (1 - \mu^2)$, we find the total power radiated in all directions is

$$P(t) = (e^2 v^2 / 4\pi c^3) \int_0^{2\pi} d\phi \int_{-1}^1 (1 - \mu^2) d\mu = (2e^2 v^2 / 3c^3) \quad (4-20)$$

In particular, for a *harmonic oscillator* we can write $x(t) = x_0 \cos \omega t$, $v(t) = -\omega x_0 \sin \omega t$, and $\ddot{v}(t) = -\omega^2 x_0 \cos \omega t$. Substituting into equation (4-20) and averaging over one period of the oscillation by noting that $\langle \cos^2 \omega t \rangle = \frac{1}{2}$, we find

$$\langle P(\omega) \rangle = (e^2 x_0^2 \omega^4 / 3c^3) \quad (4-21)$$

Because the oscillator is radiating away energy, the oscillation will eventually decay. We may describe the decay in terms of a damping force that may be viewed as the force exerted on the moving particle by its own electromagnetic field. To calculate the effective damping force, we assume that the rate of work done by it accounts for the energy loss by the oscillator. Thus from equation (4-20) we write

$$\mathbf{F}_{\text{rad}} \cdot \mathbf{v} + (2e^2 v^2 / 3c^3) = 0 \quad (4-22)$$

Then

$$\int_{t_1}^{t_2} (\mathbf{F}_{\text{rad}} \cdot \mathbf{v}) dt + (2e^2 v^2 / 3c^3) \left(\int_{t_1}^{t_2} \mathbf{v} \cdot \dot{\mathbf{v}} - \int_{t_1}^{t_2} \mathbf{v} \cdot \mathbf{v} dt \right) = 0 \quad (4-23)$$

Over a cycle the integrated term vanishes, therefore on the average

$$\mathbf{F}_{\text{rad}} = (2e^2 v^2 / 3c^3) \mathbf{v} \quad (4-24)$$

To a good order of approximation we may calculate \mathbf{v} from its value for the undamped oscillator, namely $\mathbf{v} = -\omega_0^2 \mathbf{v}$, and thus we can write

$$\mathbf{F}_{\text{rad}} = -m\gamma \mathbf{v} \quad (4-25)$$

where

$$\gamma \equiv (2e^2 \omega_0^2 / 3mc^3) \quad (4-26)$$

The constant γ is called the *classical damping constant* because of the formal resemblance of the radiation reaction term as expressed in equation (4-25) to a viscous damping term.

We now can calculate the scattering coefficient for a classical oscillator in an imposed electromagnetic field. In the classical picture the interaction is a conservative scattering process; hence we can compute the energy scattered out of a beam by calculating the energy radiated by an oscillator driven by the electromagnetic field of the incident radiation. The equation of motion for an oscillator of mass m and charge e driven by a field of amplitude E_0 and frequency ω is

$$m(\ddot{x} + \omega_0^2 x) = eE_0 e^{i\omega t} - my\dot{x} \quad (4-27)$$

Taking a trial solution for x that is proportional to $\exp(i\omega t)$, we find for the steady-state solution

$$x = Re \left[\frac{(e/m)E_0 e^{i\omega t}}{(\omega^2 - \omega_0^2) + iy\omega} \right] \quad (4-28)$$

from which we derive

$$\dot{x} = \dot{v} = Re \left[\frac{-(e\omega^2/m)E_0 e^{i\omega t}}{(\omega^2 - \omega_0^2) + iy\omega} \right] \quad (4-29)$$

Thus, substituting into equation (4-20) and averaging over a period, we have

$$\langle P(\omega) \rangle = \left(\frac{e^4 \omega^4}{3m^2 c^3} \right) \frac{E_0^2}{(\omega^2 - \omega_0^2)^2 + y^2 \omega^2} \quad (4-30)$$

which is to be identified with the total energy scattered out of the beam. To calculate the energy scattered, we suppose that the scattering cross-section is isotropic, and write $I(\mu, \phi) = I_0 \delta(\mu - \mu_0) \delta(\phi - \phi_0)$; in §1-2 we found that to produce a correspondence between the macroscopic and electromagnetic descriptions of radiation, we have $I_0 = (c E_0^2 / 8\pi)$. Thus

$$\begin{aligned} \langle P(\omega) \rangle &= \sigma(\omega) \oint I d\Omega = \sigma(\omega) \left(\frac{c E_0^2}{8\pi} \right) \int_0^{2\pi} d\phi \int_{-1}^1 d\mu \delta(\mu - \mu_0) \delta(\phi - \phi_0) \\ &= (c E_0^2 / 8\pi) \sigma(\omega) \end{aligned} \quad (4-31)$$

Comparing equations (4-30) and (4-31) we see that the scattering coefficient is

$$\sigma(\omega) = (8\pi e^4 \omega^4 / 3m^2 c^4) [(\omega^2 - \omega_0^2)^2 + y^2 \omega^2]^{-1} \quad (4-32)$$

Equation (4-32) can be simplified by noting that, because $y \ll \omega$ for frequencies corresponding to light, $\sigma(\omega)$ is a sharply peaked function in the neighborhood $\omega \approx \omega_0$. To a good approximation we can replace

$$(\omega^2 - \omega_0^2) = (\omega + \omega_0)(\omega - \omega_0) \approx 2\omega_0(\omega - \omega_0)$$

and substitute equation (4-26) for γ into equation (4-32) to find

$$\sigma(\omega) = \left(\frac{\pi e^2}{mc} \right) \left[\frac{\gamma}{(\omega - \omega_0)^2 + (\gamma/2)^2} \right] \quad (4-33)$$

The total cross-section can be found by integrating equation (4-33) over all frequencies, namely

$$\sigma_{\text{tot}} = \frac{\pi e^2}{mc} \int_0^\infty \frac{(\gamma/4\pi^2) dv}{(v - v_0)^2 + (\gamma/4\pi)^2} = \frac{\pi e^2}{mc} \frac{1}{\pi} \int_{-\infty}^\infty \frac{dx}{1 + x^2} = \frac{\pi e^2}{mc} \quad (4-34)$$

where we have written $x = 4\pi(v - v_0)/\gamma$ and observed that, for all practical purposes, $-4\pi v_0/\gamma = -\infty$. The total cross-section gives a measure of the efficiency with which energy is removed from the beam. The factor in square brackets in equation (4-33) is thus a normalized profile function that is known as the *Lorentz profile* (or *damping profile*). For our present purposes, attention will be confined to the total cross-section alone; the profile function will be discussed in detail in Chapter 9.

The classical result derived above predicts a unique scattering efficiency for all transitions; this is not surprising insofar as the theory makes no reference to the actual atomic structure or to the nature of the levels between which the transition occurs. The quantum mechanical treatment shows that cross-sections for different transitions may differ by orders of magnitude. A customary way of writing the quantum mechanical result for the total cross-section is

$$\sigma_{\text{tot}} = (\pi e^2 / mc) f_{ij} \quad (4-35)$$

where f_{ij} is called the *oscillator strength* of the transition. In pictorial terms, f_{ij} may be thought of as giving the "effective number" of classical oscillators involved in the transition; only for the strongest lines does f_{ij} approach unity. The oscillator strength is related to the Einstein coefficient B_{ij} by the expression

$$\sigma_{\text{tot}} = (\pi e^2 / mc) f_{ij} = B_{ij} (hv_{ij} / 4\pi) \quad (4-36)$$

QUANTUM MECHANICAL CALCULATION

Let us now consider the calculation of B_{ij} when the atom is treated according to quantum mechanics and the radiation field according to classical electrodynamics. The atomic structure is described by a *wave function* $\psi(r_1, r_2, \dots, r_N, t)$ where r_1 , etc., are the positions of the bound electrons. The quantity $\psi^* dr_1 \cdots dr_N$ is interpreted to be the probability of finding the atom with the electrons in the volume element $(r_1, r_1 + dr_1)$, etc. The

wave functions are solutions of *Schrödinger's equation*

$$H\psi = i\hbar(\partial\psi/\partial t) \quad (4-37)$$

where H is the total *Hamiltonian* of the system in operator form [see, e.g., (418, Chaps. 8–10) for a discussion of mathematical expressions for the Hamiltonian]. The Hamiltonian operator is constructed from the classical Hamiltonian according to the rule

$$H(q_i, p_i) \rightarrow H[q_i, (\hbar/i)(\partial/\partial q_i)] \quad (4-38)$$

where q_i and p_i are space coordinates and momenta, respectively. The atom has certain *stationary states* (or *eigenstates*) in which its energy is constant. For simplicity we shall assume that these states are *nondegenerate*. Thus if H_A is the Hamiltonian of an atom which is in a stationary state j of energy E_j , then

$$H_A\psi_j = (i\hbar)(\partial\psi_j/\partial t) \equiv E_j\psi_j \quad (4-39)$$

which implies

$$\psi_j(t) = \psi_j(0) \exp(-iE_j t/\hbar) \quad (4-40)$$

We may therefore write the general solution in the form

$$\psi_j(r, t) = \phi_j(r) \exp(-iE_j t/\hbar) \quad (4-41)$$

where the *time-independent* solutions ϕ_j satisfy the equation

$$H_A\phi_j = E_j\phi_j \quad (4-42)$$

and are *orthogonal* so that

$$\int \phi_i^* \phi_j d\tau \equiv \langle \phi_i^* | \phi_j \rangle = \delta_{ij} \quad (4-43)$$

A general state of the system at time $t = 0$ can be expanded in terms of the eigenstates (which form a complete set) by writing

$$\psi(0) = \sum_j a_j \phi_j \quad (4-44)$$

where $a_j = \langle \phi_j^* | \psi(0) \rangle$. For a system in a general state with wavefunction $\psi(0)$, the probability of finding the system in a specific state j by a measurement process is $a_j^* a_j = |a_j|^2$. At an arbitrary time t , we can write the general state as

$$\psi(t) = \sum_j a_j(t) \phi_j \exp(-iE_j t/\hbar) = \sum_j a_j(t) \phi_j \quad (4-45)$$

and again the probability of finding the system in a specific state j is $|a_j(t)|^2$.

If the atom is *unperturbed* (i.e., $H \equiv H_A$), then the a_j 's are *constant*. If, however, the atom is *perturbed* by some potential V , then the a 's will change with time; this is interpreted as the atom undergoing *transitions* from one state to another. An example of such a perturbation is that exerted by an external electromagnetic field upon the atomic electrons. In the lowest order of approximation we can assume the atom is in a uniform, time-varying electromagnetic field, $\mathbf{E} = (E_0 \cos \omega t)\mathbf{i}$. The assumption of uniformity is reasonable for light waves, which have wavelengths ($\lambda \sim 10^{-5}$ cm) that are large compared to a typical atomic dimension characterized by the *Bohr radius* ($a_0 = 5 \times 10^{-9}$ cm). The potential of the atomic electrons in the field is

$$V = e \sum_{i=1}^N \mathbf{E} \cdot \mathbf{r}_i \equiv \mathbf{E} \cdot \mathbf{d} = (E_0 \cos \omega t)(\mathbf{i} \cdot \mathbf{d}) \quad (4-46)$$

where \mathbf{d} is the *dipole moment* of the atom. With a perturbing potential, Schrödinger's equation becomes

$$(H_A + V)\psi = i\hbar(\partial\psi/\partial t) \quad (4-47)$$

Substituting equation (4-45) for ψ we have

$$(H_A + V) \sum_n a_n(t) \psi_n(t) = i\hbar \sum_n d_n \psi_n + i\hbar \sum_n a_n (\partial \psi_n / \partial t) \quad (4-48)$$

In view of equation (4-39), equation (4-48) reduces to

$$i\hbar \sum_n d_n \psi_n = \sum_n a_n V \psi_n \quad (4-49)$$

We may isolate a particular coefficient d_m by using the orthogonality of the ϕ 's. Thus, multiply equation (4-49) by ϕ_m^* and integrate over all space. We then have

$$i\hbar \sum_n d_n \exp[i(E_m - E_n)t/\hbar] \langle \phi_m^* | \phi_n \rangle = \sum_n a_n(t) \exp[i(E_m - E_n)t/\hbar] \langle \phi_m^* | V | \phi_n \rangle \quad (4-50)$$

Now writing $\omega_{mn} \equiv (E_m - E_n)/\hbar$ and $V_{mn} \equiv \langle \phi_m^* | V | \phi_n \rangle$, and using equation (4-43), equation (4-50) reduces to

$$d_m(t) = (i\hbar)^{-1} \sum_n a_n(t) V_{mn} e^{i\omega_{mn} t} \quad (4-51)$$

For the perturbing potential given by equation (4-46), we see that

$$\begin{aligned} V_{mn} &= (E_0 \cos \omega t) \mathbf{i} \cdot \langle \phi_m^* | \mathbf{d} | \phi_n \rangle = (E_0 \cos \omega t) (\mathbf{i} \cdot \mathbf{d}_{mn}) \\ &\equiv 2h_{mn} \cos \omega t = h_{mn}(e^{i\omega t} + e^{-i\omega t}) \end{aligned} \quad (4-52)$$

The quantities d_{mn} are called the *dipole moment matrix elements*. Substituting equation (4-52) into equation (4-51) we have

$$d_m(t) = (i\hbar)^{-1} \sum_n a_n(t) h_{mn} e^{i\omega_{mn} t} (e^{i\omega t} + e^{-i\omega t}) \quad (4-53)$$

We now make the simplifying assumption that, at time $t = 0$, the atom is in a definite eigenstate k , and we consider a time interval T so short that this state is not appreciably depopulated. That is, at $t = 0$, we assume $a_k(0) = 1$ and $a_n(0) = 0$ for all $n \neq k$. Moreover, we choose T such that $a_k(t) \approx 1$ for all $t \leq T$. Then the sum in equation (4-53) may be replaced by a single term

$$d_m(t) = (i\hbar)^{-1} h_{mk} e^{i\omega_{mk} t} (e^{i\omega t} + e^{-i\omega t}) \quad (4-54)$$

Integrating equation (4-54) with respect to time we obtain

$$a_m(t) = \frac{h_{mk}}{i\hbar} \left\{ \frac{\exp[i(\omega_{mk} - \omega)t] - 1}{(\omega_{mk} - \omega)} + \frac{\exp[i(\omega_{mk} + \omega)t] - 1}{(\omega_{mk} + \omega)} \right\} \quad (4-55)$$

As we are interested in absorption processes we choose $E_m > E_k$, so that $\omega_{mk} > 0$. From the denominator of the first term in the braces, we see that the dominant contribution to $a_m(t)$ will come when $\omega \approx \omega_{mk}$ (i.e., radiation near the line frequency is most effective in producing transitions). It is clear that the second term can be neglected in comparison with the first. Then, writing $x = (\omega - \omega_{mk})$, and forming $|a_m|^2 = a_m^* a_m$, we have

$$|a_m(t)|^2 = 4\hbar^{-2} h_{mk}^2 x^{-2} \sin^2\left(\frac{1}{2}xt\right) = \hbar^{-2} E_0^2 |\mathbf{i} \cdot \mathbf{d}_{mk}|^2 x^{-2} \sin^2\left(\frac{1}{2}xt\right) \quad (4-56)$$

Equation (4-56) gives the number of $k \rightarrow m$ transitions (per atom in the initial state k) produced in time t by radiation of frequency $v = \omega/2\pi$. To calculate the total number of transitions, we must sum over all frequencies that can contribute. Suppose that the line has a profile ϕ , that falls sharply to zero over some characteristic frequency interval Δv , and that over this range (at least) the intensity of radiation (and hence E_0^2) is constant with a value J_v . Then integrate over $dv = d\omega/2\pi = dx/2\pi$, and define $u \equiv \frac{1}{2}xt$, to obtain

$$\mathcal{N}_{km} = (E_0^2/4\pi\hbar^2) |\mathbf{i} \cdot \mathbf{d}_{mk}|^2 t \int_{-U}^U u^{-2} \sin^2 u du \quad (4-57)$$

Now for thermal radiation, a characteristic frequency interval $\Delta\omega$ over which the intensity will be constant is of the order $(kT/h) \sim 10^{15}$, while transition times $t \sim 10^{-8}$ sec; hence the limits $\pm U$ on the integral may be extended formally to $\pm \infty$. The value of the integral is then found in standard tables to be π . Further, as was shown in §1-2, $E_R = (4\pi J_v/c) = (E_0^2/8\pi)$, therefore

$$\mathcal{N}_{km} = (8\pi^2/\hbar^2 c) |\mathbf{i} \cdot \mathbf{d}_{mk}|^2 J_v t \quad (4-58)$$

Now in terms of the Einstein coefficient B_{km} ,

$$\mathcal{N}_{km} = B_{km} J_v t \quad (4-59)$$

hence

$$B_{km} = (8\pi^2/\hbar^2 c)|\mathbf{i} \cdot \mathbf{d}_{mk}|^2 \quad (4-60)$$

In general we shall be interested in the absorptivity of bulk material. If we assume the atoms are oriented at random with respect to a beam of radiation, then $\langle |\mathbf{i} \cdot \mathbf{d}_{mk}|^2 \rangle = d_{mk}^{-2} \langle \cos^2 \theta \rangle = \frac{1}{3} d_{mk}^{-2}$, so we may write, finally

$$B_{km} = (8\pi^2 d_{mk}^{-2}/3\hbar^2 c) \quad (4-61)$$

The spontaneous emission rate follows from equations (4-8) and (4-9), which give

$$A_{mk} = (64\pi^4 v^3/3hc^3)S(i, j) \quad (4-62)$$

In many cases the upper and lower states of a line will be degenerate (or we may wish to group several levels belonging to a multiplet). It is then customary to sum over all substates k of the lower state i and substates m of the upper state j , and to define a *line strength* S such that

$$S(i, j) \equiv \sum_{mk} d_{mk}^{-2} \quad (4-63)$$

Then we may write

$$g_j A_{ji} = (64\pi^4 v^3/3hc^3)S(i, j) \quad (4-64)$$

or, equivalently,

$$g_i B_{ij} = (32\pi^4/3\hbar^2 c)S(i, j) \quad (4-65)$$

and from equation (4-63)

$$g_i f_{ij} = (8\pi^2 mv/3\hbar e^2)S(i, j) \quad (4-66)$$

Finally, noting that $S(i, j)$ is a sum over all upper and lower substates, equation (4-66) can be used to express the total oscillator strength of a "line" connecting two degenerate levels (or of the entire multiplet connecting two sets of closely-spaced levels). Let n' be the principal quantum number of the lower level, and label each sublevel with l' ; let n and l correspond to the upper level. Then

$$g_{n'} f(n', n) = \sum_{l', l} g_{n'l'} f(n', l'; n, l) \quad (4-67)$$

APPLICATION TO HYDROGEN

Hydrogen, the most abundant element in the Universe, has the simplest atomic structure, and it is possible to obtain exact analytical expressions for

its wave functions and oscillator strengths. There are four quantum numbers that specify a distinct state of hydrogen: n , the principal quantum number, which characterizes energy; l , the azimuthal quantum number, which characterizes the orbital angular momentum; m , the magnetic quantum number, which gives the projection of the orbital angular momentum along a preferred axis (taken to be the z -axis); and s , the spin quantum number of the electron, equal to $\pm \frac{1}{2}$.

In most atomic systems, the energies of different (n, l) states are distinct, but for hydrogen they depend upon the principal quantum number n only, and

$$E_n = -R/n^2 \quad (4-68)$$

where R is the *Rydberg constant*

$$R = (2\pi^2 \mu_H e^4/\hbar^2) \quad (4-69)$$

Here μ_H is the *reduced mass*, given in terms of the masses of a proton, m_p , and electron, m_e , by

$$\mu_H^{-1} \equiv m_p^{-1} + m_e^{-1} \quad (4-70)$$

The wave function has the form [cf. (392, Chap. 5; 418, Chaps. 9 and 10)]

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_l^m(\theta, \phi) \quad (4-71)$$

where Y_l^m is the *spherical harmonic function* expressible in terms of associated Legendre functions, and R_{nl} is the radial function, which can be expressed in terms of associated Laguerre polynomials and exponentials. These functions are normalized such that

$$\int_0^\infty R_{nl}^2(r)r^2 dr = 1 \quad (4-72a)$$

$$\text{and } \int_0^{2\pi} d\phi \int_0^\pi d\theta [Y_l^m(\theta, \phi)]^* Y_{l'}^{m'}(\theta, \phi) \sin \theta = \delta_{ll'} \delta_{mm'} \quad (4-72b)$$

In equation (4-72a), r is measured in units of the *Bohr radius*

$$a_0 = \hbar^2/(4\pi^2 e^2 \mu_H) \quad (4-73)$$

It is often convenient to work with the function $P_{nl}(r) \equiv rR_{nl}(r)$ which is defined such that P_{nl}^2 measures the charge density of the electronic wave function.

Because all states with a given n are degenerate, we require the statistical weight g_n and normally will work with the oscillator strength $f(n', n)$ for all transitions $(n' \rightarrow n)$. The statistical weight is

$$g_n = 2n^2 \quad (4-74)$$

which follows from the fact that the allowed values of l are $0 \leq l \leq n - 1$; those of m are $-l \leq m \leq l$; and each nlm state has two possible spin orientations $s = \pm \frac{1}{2}$.

Exercise 4-2: Derive equation (4-74).

Because the wave functions are known analytically, explicit expressions can be derived for the oscillator strengths:

$$f(n', l'; n, l) = \frac{1}{3} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \frac{\max(l, l')}{(2l' + 1)} \sigma^2(n', l'; n, l) \quad (4-75)$$

and

$$\begin{aligned} f(n', n) &= \frac{1}{3n'^2} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right) \left[\sum_{l'=1}^{n'-1} l' \sigma^2(n', l'; n, l' - 1) \right. \\ &\quad \left. + \sum_{l'=0}^{n'-1} (l' + 1) \sigma^2(n', l'; n, l' + 1) \right] \end{aligned} \quad (4-76)$$

where $\sigma^2(n', l'; n, l) \equiv \left(\int_0^\infty P_{n'l'}(r) P_{nl}(r) r dr \right)^2$ (4-77)

An explicit expression for σ^2 was first derived by Gordon (254) and an explicit form for $f(n', n)$ was derived by Menzel and Pekeris (417). Extensive tables of $f(n', n)$ can be found in (417) and (257). A very convenient form for hydrogen oscillator strengths is obtained by expressing them in terms of the semi-classical value derived by Kramers (363), namely

$$f_K(n', n) = \frac{32}{3\pi\sqrt{3}} \left(\frac{1}{n'^2} - \frac{1}{n^2} \right)^{-3} \left(\frac{1}{n^3 n'^5} \right) \quad (4-78)$$

which shows the principal dependences of f upon n' and n . It is then customary to express the exact f -value in terms of Kramers' approximation f_K by writing

$$f(n', n) = g_I(n', n) f_K(n', n) \quad (4-79)$$

where $g_I(n', n)$ is called the *Gaunt factor*. The Gaunt factors are all numbers of order unity; an extensive tabulation of $g_I(n', n)$ can be found in (60).

Exercise 4-3: Using the analytical expressions for hydrogen wave functions given in texts on quantum mechanics [e.g., (392, 183)], calculate the f -values for $Lx(n' = 1 \rightarrow n = 2)$ and $Ha(n' = 2 \rightarrow n = 3)$. Obtain values for each $f(n', l'; n, l)$ and combine these to find $f(n', n)$. Compare your values with those given in tables [e.g., (9, 70)].

TRANSITION PROBABILITIES FOR LIGHT ELEMENTS

(a) *Hartree-Fock Method.* When the atom has more than one electron, the wave equation can no longer be solved in closed form, and approximations must be made. The actual Hamiltonian for an N -electron atom is

$$H = -(\hbar^2/2m) \sum_{i=1}^N \nabla_i^2 - \sum_{i=1}^N (Ze^2/r_i) + \sum_{\substack{\text{all pairs} \\ (i, j)}} (e^2/|\mathbf{r}_i - \mathbf{r}_j|) \quad (4-80)$$

The first term represents the kinetic energy of the electrons, the second their electrostatic potential with the nucleus of charge Z , and the third their mutual Coulomb repulsion. It is the last term that causes the principal difficulties.

One of the most important methods of deriving approximate wave functions is *Hartree's self-consistent field method*. In this approach, the sum over electron pairs is replaced for each electron by its spherical average. An excellent description of how this average is computed is given in (576, Chaps. 3 and 9). Each electron then moves in a potential that depends only upon its distance from the nucleus, and we make the replacement

$$\sum_{\substack{\text{all pairs} \\ (i, j)}} (e^2/|\mathbf{r}_i - \mathbf{r}_j|) \rightarrow \sum_i V_i(r_i) \quad (4-81)$$

This results in the approximation of the actual potential by a *central field*. With a central field potential, the angular factors in the Schrödinger equation can be separated out in exactly the same way as for hydrogen, and for each electron the wave function has the form

$$U_i(r, \theta, \phi; n, l, m, s) = r^{-1} P_{nl}(r) Y_l^m(\theta, \phi) X(s) \quad (4-82)$$

where the normalizations given in equation (4-72) still apply. The functions U_i are called *electron orbitals*. The radial equation for each orbital is of the form (r in units of a_0 , E in Rydbergs)

$$(d^2 P_{nl}/dr^2) + [E_{nl} + 2r^{-1} Z_{eff}(r) - l(l+1)r^{-2}] P_{nl} = 0 \quad (4-83)$$

Here $Z_{eff}(r)$ is the "effective nuclear charge" sensed by an electron after allowance is made for shielding by other electrons [using the central fields of equation (4-81)]. The atom is now considered to be made up of N such orbitals, and these are used to construct the wave function for the entire configuration.

Because of the *Pauli exclusion principle*, the set of four quantum numbers (n, l, m, s) for each orbital cannot be identical for any two orbitals. Also, the

wave function of the atom must be constructed so that it is *antisymmetric* under the interchange of the coordinates of any two electrons. In practice these conditions may be met by writing the wave function as a *Slater determinant* (576, Chap. 12),

$$\phi(r_1, \dots, r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} U_1(\alpha) & U_1(\beta) & \cdots & U_1(v) \\ U_2(\alpha) & U_2(\beta) & \cdots & U_2(v) \\ \vdots & \vdots & & \vdots \\ U_N(\alpha) & U_N(\beta) & \cdots & U_N(v) \end{vmatrix} \quad (4-84)$$

where the numbers $1, 2, \dots, N$ denote the orbitals of electrons 1, 2, etc., while α, β, \dots, v stand for the space and spin coordinates of electrons α, \dots, v , respectively.

The solution for the wave function is carried out iteratively. Thus $Z_{\text{eff}}(r)$ depends in an involved way on integrals over the electron orbitals, but in turn it determines those orbitals. Therefore, we start with an approximate set of orbitals, compute Z_{eff} , solve for the P_{nl} 's, recompute Z_{eff} , and iterate until the procedure converges. The calculations are time-consuming and laborious, but are within the capabilities of modern computers, and a large number of wave functions for a wide variety of atomic configurations are now available.

A specific term in an atomic spectrum can be characterized by certain quantum numbers describing the atom as a whole. In light atoms these describe the total orbital angular momentum L (the vector sum of the individual l 's), the total spin angular momentum S (the vector sum of the s_i 's), and the total angular momentum J , which is the vector sum of L and S . This type of coupling of the individual momenta is called ($L-S$) or *Russell-Saunders coupling*. As a given L , S , and J may result from more than one arrangement of the individual l 's, m 's, and s 's of the orbitals, the complete wave function will, in general, consist of a *sum* of Slater determinants, and thus may be very complicated.

In calculating transition probabilities, it is generally assumed that only one orbital is different between the initial and final state—i.e., only one electron undergoes a transition. In this case the matrix element r_{ij} can be split into factors, one coming from the initial and final *radial* wave functions, and another depending on the *angular* and *spin* wave functions. It is customary, therefore, to write the expression for the line strength in the form

$$S(n', L', S'; n, L, S, J) = a_0^2 e^2 \sigma^2(n', l'; n, l) \mathcal{S}(M) \mathcal{S}(L) \quad (4-85)$$

Here

$$\sigma^2 \equiv (4l_{\max}^2 - 1)^{-1} \left(\int_0^\infty P_{n'l'} P_{nl} r dr \right)^2 \quad (4-86)$$

where $l_{\max} = \max(l, l')$. The factor $\mathcal{S}(M)$ is the *strength of the multiplet*, depending on nLS and $n'L'S'$, and the factor $\mathcal{S}(L)$ is the *strength of the line within the multiplet*. Extensive tables of $\mathcal{S}(M)$ and $\mathcal{S}(L)$ can be found in (11, Chap. 8 and Appendix; 9, §§26–28; 250; 251), and general formulae for computing these factors are given in (534; 535; 572, §§10.8–10.10; and 191). Generally, the most difficult part of the calculation is the determination of σ^2 , but serious complications also occur when there are deviations from $L-S$ coupling.

(b) *The Coulomb Approximation.* Because of the labor involved in obtaining σ^2 from Hartree-Fock calculations, it is desirable to have an approximate method that can be applied easily. Such an approach was developed by Bates and Damgaard (74), who pointed out that often the largest contribution to the radial integral comes from large values of r , where the electron moves in a nearly Coulomb potential. In this event, the integral can be approximated using hydrogenic wave functions, provided the principal quantum numbers are chosen to give the observed energy of the level. If Z is the charge in the asymptotic potential, then the appropriate effective quantum number is $n_i^* = Z/\varepsilon_{nl}^{1/2}$ where ε_{nl} is the energy of the level below the continuum, measured in Rydbergs; in general, n_i^* is not an integer. Bates and Damgaard then show that one can write

$$\sigma(n_{i-1}^*, l-1; n_i^*, l) = \mathcal{F}(n_i^*, l) \mathcal{I}(n_{i-1}^*, n_i^*, l)/Z \quad (4-87)$$

Extensive tables of the functions \mathcal{F} and \mathcal{I} can be found in (74) and (483); an extension of the theory is given in (389). Because of the simplicity of the method, it has been widely applied in astrophysical analyses; an extensive tabulation of Coulomb approximation f -values is given in (264, 363–441).

(c) *Experimental Methods.* In many cases the Coulomb approximation is inaccurate, while a more accurate quantum mechanical calculation is simply too complicated to carry out. In these cases the f -values must be determined by experiments, which in addition, provide a direct comparison standard to test the accuracy of various theoretical computations. A wide variety of experimental techniques exist; brief descriptions of some of the more useful methods are given in (11, 300–310; 261, 146–149; 264, Chap. 15).

There is a huge literature containing both experimental and theoretical determinations of f -values or transition probabilities; a complete bibliography of this work is given in (454; 230; and 231). Compilations of critically evaluated (i.e., “best values”) transition probabilities for many of the elements of astrophysical interest are given in (453; 584; 670; 672; and 673).

Exercise 4-4: Calculate f -values for the He I $\lambda 5876$ ($2p^3P-3d^3D$), He I $\lambda 6678$ ($2p^1P-3d^1D$), and He I $\lambda 4471$ ($2p^3P-4d^3D$) lines using equations (4-66) and (4-85) with Coulomb approximation values of σ^2 and multiplet- and line-strengths from tables. Compare with standard values in (672).

4-3 The Einstein-Milne Relations for the Continuum

The Einstein relations were generalized to bound-free processes by Milne (461) in a paper of considerable interest and importance. We consider photoionization processes that start with atoms (or ions) in a definite bound state (not necessarily the ground state) and produce an ion in a definite state (perhaps excited) of the next highest ionization stage plus a free electron moving with velocity v . The inverse process is a recombination of a free electron by a collision with an ion (in the particular state mentioned above) to form an atom (in the proper state). The recombination process can occur spontaneously or can be induced by incident radiation. Let n_0 be the number density of the atoms, n_1 the density of the ions, and n_e the density of free electrons. The electrons have a Maxwellian velocity distribution, and we write $n_e(v) dv$ for the number with speeds on the range $(v, v+dv)$. Let p_v be the probability of photoionization of an atom by a photon in the frequency range $(v, v+dv)$; then the number of photoionizations in time dt on this frequency range is $n_0 p_v I_v dv dt$. The usual energy absorption coefficient α_v is related to p_v by the expression $\alpha_v \equiv p_v h\nu$. Further, let $F(v)$ be the spontaneous recapture probability and $G(v)$ be the induced recapture probability for electrons in the velocity range $(v, v+dv)$ by the ions; then the number of recombinations by electrons of velocity v in time dt is

$$n_1 n_e(v) [F(v) + G(v) I_v] v dv dt$$

The energy of the photon required to ionize the atom (and thus of the photon emitted in the recombination process) is

$$h\nu = \chi_I + \frac{1}{2} mv^2 \quad (4-88)$$

where χ_I is the ionization potential from the atomic to the ionic state (i.e., the energy difference between these states).

Now in thermodynamic equilibrium, the number of photoionizations must exactly equal the number of recombinations. In T.E., $I_v \equiv B_v$, hence

$$n_0^* p_v B_v = n_1^* n_e(v) [F(v) + G(v) B_v] (h/m) \quad (4-89)$$

where the asterisks denote T.E. occupation numbers, and equation (4-88) has been used to write $h dv = mv dv$. Solving for B_v , we find

$$B_v = [F(v)/G(v)] \{ [n_0^* p_v m / n_1^* n_e(v) h G(v)] - 1 \}^{-1} \quad (4-90)$$

This expression is to be compared with the standard expression for the Planck function, namely $B_v(T) = (2h\nu^3/c^2)[e^{h\nu/kT} - 1]^{-1}$. For a Maxwellian vel-

city distribution [cf. equation (5-2)]

$$n_e(v) dv = n_e(m/2\pi kT)^{\frac{3}{2}} \exp(-mv^2/2kT) 4\pi v^2 dv \quad (4-91)$$

Anticipating the results of Chapter 5 [cf. equation (5-14)], the T.E. relation between n_0^* and n_1^* is

$$(n_0/n_1)^* = n_e(g_0/2g_1)(h^2/2\pi mkT)^{\frac{1}{2}} \exp(\chi_I/kT) \quad (4-92)$$

Using equations (4-88), (4-91) and (4-92) we find that

$$n_0^* p_v m / n_1^* n_e(v) h G(v) = (h^2 g_0 / 8\pi m^2 g_1 v^2) [p_v / G(v)] e^{h\nu/kT} \quad (4-93)$$

Thus to reduce equation (4-90) to the Planck function we must have

$$F(v) = (2h\nu^3/c^2) G(v) \quad (4-94)$$

$$\text{and } p_v = (8\pi m^2 v^2 g_1 / h^2 g_0) G(v) = (4\pi c^2 m^2 v^2 g_1 / h^3 g_0 v^3) F(v) \quad (4-95)$$

These are the continuum analogues of equations (4-8) and (4-9). Again we recognize that, although these relations have been derived from thermodynamic equilibrium arguments, the quantities p_v , $F(v)$, and $G(v)$ must really depend only on the properties of the atom; hence equations (4-94) and (4-95) are true in general.

The great importance of the results just derived becomes more clearly manifest when we write the transfer equation assuming that at the frequency under consideration only the particular photoionization and recombination processes considered above occur. The generalization to a multilevel, multi-atom case with several overlapping opacities and emissivities is trivial because each term adds linearly and the conclusions we shall derive apply to the sum. The transfer equation is

$$\mu(\partial I_v / \partial z) = -n_0 p_v h\nu I_v + n_1 n_e(v) [F(v) + G(v) I_v] (h^2 v / m) \quad (4-96)$$

Neither n_0 nor n_1 necessarily has its LTE value in the above equation. If we are to write the transfer equation in standard form, then it is clear that the absorption coefficient corrected for stimulated emission must be

$$\kappa_v = \{n_0 - n_1 n_e(v) [h G(v) / m p_v]\} (p_v h\nu) \quad (4-97)$$

Using equations (4-88), (4-91), (4-92) and (4-95), and recalling that $\alpha_v = p_v h\nu$, we find

$$\kappa_v = (n_0 - n_0^* e^{-h\nu/kT}) \alpha_v \quad (4-98)$$

In equation (4-98), n_0^* denotes the LTE value of n_0 computed from equation (4-92) using the actual values of n_1 and n_e (i.e., the LTE population relative

to the actual ion density). In the particular case of LTE where $n_0 \equiv n_0^*$,

$$\kappa_v^* = n_0^* \alpha_v (1 - e^{-hv/kT}) \quad (4-99)$$

As was true for bound-bound transitions, the term $(1 - e^{-hv/kT})$ is usually called the correction factor for stimulated emission; but it is clear that this expression is correct *only* for LTE. Indeed we see from equation (4-98) that the stimulated emission *always* occurs at the LTE rate (if we understand n_0^* to have the meaning given above); this *must* be true because the recombination process is a *collisional* process involving particles with an *equilibrium* (i.e., Maxwellian) velocity distribution. Note the contrast here with the result given in equation (4-13) for bound-bound transitions, where in general the stimulated emission term does *not* have its equilibrium value. When departures from LTE affect the bound-free opacity, they change the *direct* absorption term involving n_0 (which in general will not equal n_0^*). We shall use these results both in calculating the stimulated emission rates in the equations of statistical equilibrium [cf. equation (5-63)] and in writing a general expression for the opacity [cf. equation (7-1)].

Returning to equation (4-96) and examining the term involving $F(v)$, it is clear that the *emissivity* is

$$\eta_v = [hn_1 n_e(v)F(v)/mp_v] \alpha_v \quad (4-100)$$

which, with the help of equations (4-88), (4-91), (4-92), and (4-95), can be written

$$\eta_v = (2hv^3/c^2)n_0^* \alpha_v e^{-hv/kT} = n_0^* \alpha_v (1 - e^{-hv/kT}) B_v = \kappa_v^* B_v(T) \quad (4-101)$$

Thus the continuum emissivity always occurs at the LTE rate (if n_0^* is defined as above), which is what we would expect, for the recombination process is collisional. Notice that this derivation recovers the Kirchhoff-Planck law, equation (2-6), and extends its validity somewhat. Again, notice the contrast with the bound-bound spontaneous emission where departures from LTE enter directly if n_j is not identical to n_j^* . These results will be exploited in calculating spontaneous emission rates in the statistical equilibrium equations [cf. equation (5-61)] and in writing a general expression for the emissivity [cf. equation (7-2)].

Exercise 4-5: Verify equations (4-93), (4-98), and (4-101).

4-4 Continuum Absorption Cross-Sections

Cross-sections for bound-free absorption can be calculated quantum mechanically by essentially the same methods as used in §4-2 for bound-

bound transitions. Consider absorptions from a bound state n , of statistical weight g_n , to the continuum in a frequency interval Δv . The free states have wave functions characterized by E , the energy of the free electron, and are normalized such that

$$\langle E'|E \rangle = \delta(E' - E) \quad (4-102)$$

so that there are ΔE states in the energy interval ΔE . Thus by analogy with equation (4-65) and in view of (4-36) we can write

$$g_n \alpha_v \Delta v = (8\pi^2/3\hbar^2 c) \Delta E \langle E | d | n \rangle^2 (hv/4\pi) \quad (4-103)$$

$$\text{or } \alpha_v = (8\pi^3 v/3c g_n) \langle E | d | n \rangle^2 \quad (4-104)$$

The calculation of free-state wave functions will not be considered in this book; the reader should refer to standard texts on quantum mechanics—e.g., (197) or (418)—for information on this subject. Further, we shall not consider the details of calculations based on equation (4-104), though results of such work will be quoted. An approximate method for the evaluation of α_v by means of equation (4-104), the quantum defect method, is described below.

An alternative formula for α_v can be written if we suppose each continuum state k to have an effective oscillator strength f_{nk} for absorptions from the bound state n . If there are Δk free states in the frequency interval Δv , then

$$\alpha_v = (\pi e^2/mc) f_{nk} (\Delta k / \Delta v) \quad (4-105)$$

This formulation is useful for calculating the cross-sections of hydrogen.

The *quantum defect method*, developed by Seaton and Burgess (566; 120), is the continuum analogue of the Coulomb approximation. This method exploits the fact that the dominant contribution to the matrix element $\langle E | d | n \rangle^2$ often occurs in regions where the wave functions can be represented by Coulomb wave functions in the appropriate potential. Consider absorptions from a bound state (n, l) to the continua $(E, l \pm 1)$ where E is the energy of the free electron. Let I_{nl} be the ionization energy of this state, expressed in Rydbergs, and let Z be the charge on the ion after the electron is removed. Then define the effective quantum number v_{nl} such that $I_{nl} = Z^2/v_{nl}^2$. In general, v_{nl} will not be equal to the principal quantum number n of the shell to which the electron belongs, and we can define a *quantum defect* $\mu(v, l) \equiv n - v_{nl}$. The quantum defect can be found for each level $(nlSL)$ of a given spectroscopic type, defined by (ISL) (e.g., 3P or 4D), in a series. Defining $\varepsilon_{nl} \equiv -1/v_{nl}^2$, we can determine the behavior of $\mu(\varepsilon_{nl}, l)$ versus ε_{nl} ; in favorable cases μ is a simple function of ε (say, constant, or linear in ε). It is then assumed that this variation of μ with ε can be extrapolated into the continuum (i.e., for $\varepsilon > 0$) to give $\mu'(\varepsilon)$. This establishes the properties of the

continuum wave functions. The radial matrix element can then be evaluated using hydrogenic wave functions, and the cross-section when the energy of the ejected electron is $k^2 = Z^2\epsilon$ (in Rydbergs) can be written

$$\alpha(nl, k^2) = 8.56 \times 10^{-19} [(I_{nl} + k^2)/I_{nl}^2] \sum_{l' = l \pm 1} C_{l'} |g(vl; \epsilon l')|^2 \text{ cm}^2 \quad (4-106)$$

$$\text{Here } g(vl; \epsilon l') = [\zeta(v, l)]^{-\frac{1}{2}} G(vl; \epsilon l') \cos\{\pi[v + \mu(\epsilon) + \chi(vl; \epsilon l')]\} \quad (4-107)$$

$$\zeta(v, l) \equiv 1 + 2v^{-3} [\partial\mu(\epsilon)/\partial\epsilon] \quad (4-108)$$

and $G(vl; \epsilon l')$ and $\chi(vl; \epsilon l')$ are tabulated functions (503) [NOTE: the notation in the reference cited differs from that in (120), which is used here]. The coefficients $C_{l'}$ are algebraic factors obtained from the integrations over angular and spin coordinates and are tabulated in (120) for several important cases; they are analogues of the factor $\mathcal{S}(\mathcal{M})\mathcal{S}(\mathcal{L})$ appearing in equation (4-85) for bound-bound oscillator strengths.

The quantum defect method, despite its simplicity, often gives very good cross-sections [see (120; 503)] and has been widely employed in astrophysical work. A number of quantum defects $\mu(\epsilon)$ are given in (503) where they are used to calculate cross-sections and opacities for abundant elements in stellar atmospheres [see also (502)]. For brevity, only absorption by hydrogen and helium, and their ions, will be discussed in this chapter; these are the most abundant elements in stellar material, and usually dominate the opacity. References to other opacity sources will be given in §7-2.

HYDROGEN

A simple way of obtaining bound-free and free-free absorption cross-sections for hydrogen was suggested by Menzel and Pekeris (417). They introduced the formalism of representing *bound* states by *real* (integer) quantum numbers, and *free* states by *imaginary* quantum numbers. The bound-state energies relative to the continuum are given by equation (4-68), and it follows that the energy of the transition ($n' \rightarrow n$) is

$$hv_{n'n} = \mathcal{R}[(1/n')^2 - (1/n)^2] \quad (4-109)$$

If a free state has the imaginary quantum number ik , then by analogy

$$hv_{n'k} = \mathcal{R}[(1/n')^2 + (1/k)^2] = (\mathcal{R}/n'^2) + \frac{1}{2}mv^2 \quad (4-110)$$

where the first term clearly represents the ionization potential from bound state n' , and the second the energy of the free electron. Note that $k \rightarrow \infty$ at the ionization limit and becomes small high in the continuum.

The formula for the continuum oscillator strength follows from a generalization of equations (4-78) and (4-79) to

$$f_{n'k} = \left(\frac{32}{3\pi\sqrt{3}} \right) \left(\frac{1}{n'^5 k^3} \right) \left(\frac{1}{n'^2} + \frac{1}{k^2} \right)^{-3} g_{II}(n', k) \quad (4-111)$$

where g_{II} is the bound-free Gaunt factor. Formulae for the Gaunt factor are given in (417) and an extensive numerical tabulation is given in (352); g_{II} is a number of order unity at the ionization threshold, shows a slow rise to about 1.10 (in the limit as $n' \rightarrow \infty$) at about 1 Rydberg above threshold, and then decreases to small values in the X-ray region. The absorption cross-section can now be derived by substituting equation (4-111) into (4-105), noting from equation (4-110) that for n' fixed,

$$(dk/dv) = -(hk^3/2\mathcal{R}) \quad (4-112)$$

We then find

$$\alpha_v = \left(\frac{\pi e^2}{mc} \right) \left(\frac{hk^3}{2\mathcal{R}} \right) \left(\frac{32}{3\pi\sqrt{3}} \right) \left(\frac{1}{n'^5 k^3} \right) \frac{g_{II}(n', k)}{(hv/\mathcal{R})^3} \quad (4-113)$$

which, in view of equation (4-69), reduces to

$$\alpha_v = \left(\frac{64\pi^4 me^{10}}{3\sqrt{3} ch^6} \right) \frac{1}{n'^5 v^3} g_{II}(n', v) = \mathcal{K} \frac{g_{II}(n', v)}{n'^5 v^3} \quad (4-114)$$

where $\mathcal{K} = 2.815 \times 10^{29}$. Thus bound-free absorption from level n commences abruptly at the threshold frequency $v_n = (\mathcal{R}/hn^2)$ and falls off at higher frequencies as v^{-3} (neglecting the weak variation of the Gaunt factor).

The threshold cross-section is given by

$$\alpha(v_n, n) = 7.91 \times 10^{-18} n g_{II}(n, v_n) \text{ cm}^2$$

The opacity per cm^3 of the stellar material can be computed by multiplying the cross-section for level n by the number of hydrogen atoms (per cm^3) in that level, and summing over all levels that can absorb at a given frequency v (i.e., all n such that $v_n \leq v$). The bound-free opacity of hydrogen calculated in this way has a jagged character, as shown in Figure 4-1. Except for the hottest stars, most of the hydrogen is in the ground state, and the absorption edge at $\lambda 912 \text{ \AA}$ (one Rydberg) is extremely strong. For $912 \text{ \AA} \leq \lambda \leq 3647 \text{ \AA}$, absorptions from the ground state can no longer occur, and the dominant opacity source is photoionization from the $n = 2$ level (Balmer continuum). Similarly, for $3647 \text{ \AA} \leq \lambda \leq 8206 \text{ \AA}$, both $n = 1$ and $n = 2$ cannot absorb, and the dominant continuum is from $n = 3$ (Paschen continuum); and so on. Actually the opacity variation shown in Figure 4-1 is idealized in that there

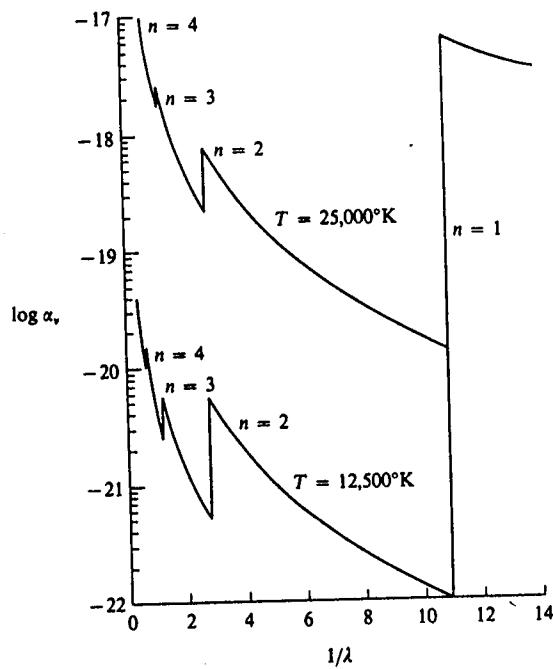


FIGURE 4-1
Opacity from neutral hydrogen at $T = 12,500^\circ\text{K}$ and $T = 25,000^\circ\text{K}$, in LTE; photoionization edges are labeled with the quantum number of state from which they arise. Ordinate: sum of bound-free and free-free opacity in cm^2/atom ; abscissa: $1/\lambda$ where λ is in microns.

exists a series of lines converging on each photoionization threshold at the series limit. Near the limit the lines blend together smoothly and merge into the continuum. Bound-free absorption from hydrogen is the dominant continuum opacity source in stars of spectral types A and B.

Let us now consider the free-free opacity of hydrogen. In this process, a free electron passing near a proton causes a transitory dipole moment, and absorptions and emissions of photons (with a consequent change in the electron's energy) become possible. By analogy with the calculation of bound-free absorption, we introduce imaginary quantum numbers for both the initial and final states, say ik and il , such that, if v is the initial velocity of the free electron, and v is the frequency of the radiation absorbed, then

$$\mathcal{R}k^{-2} = \frac{1}{2}mv^2 \quad (4-115)$$

and

$$\mathcal{R}k^{-2} + hv = \mathcal{R}l^{-2} \quad (4-116)$$

Assume that absorptions take place from a band of states dk into a band of states $dl = (dl/dv)\Delta v$; then in equation (4-105) we replace f_{nk} with $f_{kl} dk$, and Δk with dl to obtain

$$\alpha(v, v) = (\pi e^2/mc)f_{kl} dk (dl/dv) \quad (4-117)$$

as the absorption coefficient per ion and per electron moving with velocity v . The appropriate generalization of equations (4-78) and (4-79) is

$$f_{kl} = \frac{64}{3\pi\sqrt{3}} \frac{1}{g_k} \left(\frac{1}{k^2} - \frac{1}{l^2} \right)^{-3} \frac{g_{\text{III}}(k, l)}{k^3 l^3} \quad (4-118)$$

where g_k is the statistical weight of a free electron, given by quantum statistics as

$$g_k = (2h^{-3})(4\pi m^3 v^2 dv) = (16\pi\mathcal{R}m^2 v/h^3 k^3) dk \quad (4-119)$$

the second equality following from equation (4-115). Substituting into equation (4-117) we find

$$\alpha(v, v) = \left(\frac{\pi e^2}{mc} \right) \left(\frac{64}{3\pi\sqrt{3}} \right) \left(\frac{h^3 k^3}{16\pi\mathcal{R}m^2 v} \right) \left(\frac{\mathcal{R}}{hv} \right)^3 \frac{g_{\text{III}}(v, v)}{k^3 l^3} \left(\frac{dl}{dv} \right) \quad (4-120)$$

and making use of the relation that for k (or v) fixed, $(dl/dv) = (hv^3/2\mathcal{R})$ from equation (4-116), we obtain

$$\alpha(v, v) = \left(\frac{2\mathcal{R}he^2}{3\pi\sqrt{3}m^3 c} \right) \left(\frac{g_{\text{III}}(v, v)}{v^3 v} \right) \quad (4-121)$$

The total absorption cross-section per ion and per electron is obtained by summing over all incident electron velocities, assuming a Maxwellian velocity distribution as given by equation (4-91). The result is

$$\alpha(v, T) = \left(\frac{4e^6}{3ch} \right) \left(\frac{2\pi}{3km^3} \right)^{\frac{1}{2}} T^{-\frac{1}{2}} v^{-3} \bar{g}_{\text{III}}(v, T) \quad (4-122)$$

where use has been made of equation (4-69), and \bar{g}_{III} is the thermal average of the Gaunt factor

$$\bar{g}_{\text{III}}(v, T) \equiv \int_0^\infty g_{\text{III}}(v, u) e^{-u} du \quad (4-123)$$

where $u \equiv (mv^2/2kT)$.

Exercise 4-6: Verify equations (4-122) and (4-123).

Inserting numerical values for the atomic constants, multiplying by the electron and proton densities, and correcting for stimulated emission (notice that because the process is collisional it is always in LTE, at the *actual* electron and ion densities), we obtain the opacity coefficient

$$\kappa_v(\text{free-free}) = 3.69 \times 10^8 \bar{g}_{\text{III}}(v, T) v^{-3} T^{-\frac{1}{2}} n_e n_p (1 - e^{-hv/kT}) \quad (4-124)$$

Formulae for \bar{g}_{III} are given in (417) and extensive tables can be found in (85) and (352). The free-free opacity plays an ever more important role at low frequencies compared to the bound-free, because of the decreasing number of photoionization edges that contribute as $v \rightarrow 0$. Further, the free-free becomes more important at high temperatures, for as can be seen from equation (4-92), in the limit $(kT/\chi_{\text{ion}}) \gg 1$, the bound state populations vary as $n_i \propto n_e n_p T^{-\frac{1}{2}}$; hence the ratio of free-free to bound-free opacity rises $\propto T$ in the high-temperature limit. The free-free process is the dominant true absorption mechanism in, e.g., the O-stars.

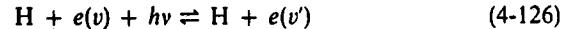
THE NEGATIVE HYDROGEN ION

Hydrogen, because of its large polarizability, can form a *negative ion* consisting of a proton and two electrons. This ion has a single bound state with a binding energy of 0.754 eV. Because of its low binding energy, H^- does not exist at high temperatures (it is destroyed by ionization) but is prevalent mainly in the atmospheres of solar-type and cooler stars. It was recognized by Pannekoek and Wildt that H^- could be an important opacity source in such stars. As it turns out, the absorption cross-section of H^- is large and, although only a small fraction of the hydrogen exists in this form, the opacity from H^- is the *dominant* one in the atmospheres of cooler stars.

The negative hydrogen ion can absorb and emit radiation via both bound-free and free-free processes; i.e.,



where $\frac{1}{2}mv'^2 = hv = 0.754$ eV, and



where $\frac{1}{2}mv'^2 = \frac{1}{2}mv^2 + hv$. In the free-free process, an electron passing near to a neutral hydrogen atom induces, by polarization, a temporary dipole moment that can interact with the radiation field, leading to absorptions and emissions. The bound-free absorption process has its threshold at about 16500 Å (1.65 μ), corresponding to the detachment energy. It reaches a maximum cross-section of about 4×10^{-17} cm² at 8500 Å and decreases toward shorter wavelengths. The free-free cross-section is about equal to the

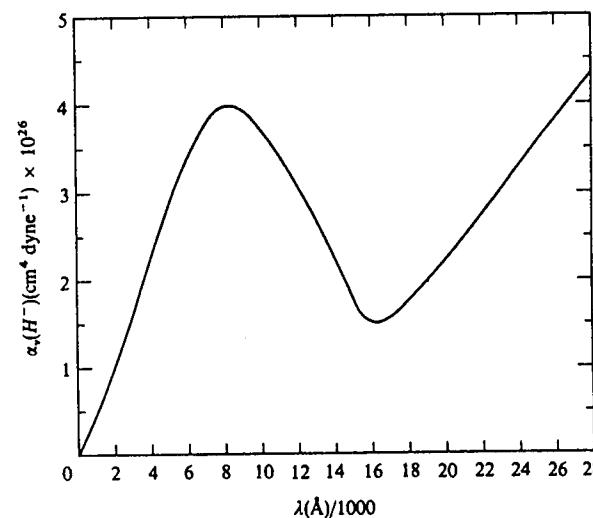


FIGURE 4-2
Bound-free and free-free opacity from H^- at $T = 6300^\circ\text{K}$. Ordinate: cross-section ($\times 10^{26}$) per neutral H atom and per unit electron pressure $p_e = n_e kT$; abscissa: $\lambda/1000$ where λ is in Å.

bound free near 15000 Å (1.5 μ) and increases towards longer wavelengths. The summed absorption coefficient (see Figure 4-2) has a minimum at about 1.6 μ ; although other absorption processes act to wash out the minimum, the opacity for cool stars is smallest near this wavelength.

The determination of cross-sections for the two processes mentioned above is difficult and has been attempted both theoretically and experimentally. Very elaborate wave functions are required to give the desired accuracy. Pioneer calculations that gave fairly accurate values were carried out by Chandrasekhar and Breen (162). These were shown to be in accord with empirically deduced values for the absorption coefficient in the sun, and led to the firm identification of H^- as the major opacity source in the solar atmosphere (see §3-6). More accurate values are now available for both the bound-free (242) and free-free (604) cross-sections; these are in good agreement with experimental values.

In LTE, the number of H^- ions per cm³ is given by a Saha formula [see equation (5-14)] that is of the form $n^*(H^-) = n(H)p_e\Phi(T)$ where $n(H)$ is the number of hydrogen atoms per cm³, $p_e = n_e kT$, and $\Phi(T)$ contains the temperature dependence of the ionization equilibrium. The LTE opacity can thus be written $\kappa_v^*(H^-) = \alpha_v(H^-)n(H)p_e\Phi(T)(1 - e^{-hv/kT})$; departures from LTE may enter both in the calculation of $n(H^-)$ and in the stimulated emission

correction factor. Because $\kappa^*(H^-)$ is proportional to p_e , it is clear that it will be a more important opacity source in dwarfs than in giants. Also, because the electron density in G-type and cooler stars depends upon the abundance of the metals, H^- will be a much weaker opacity source in Population II stars (which have low heavy-element abundances).

OTHER IONS OF HYDROGEN

Hydrogen exists in two other forms that can contribute significantly to the opacity in stellar atmospheres, namely H_2^+ and H_2^- . The positive ion H_2^+ consists of a single electron shared by two protons; absorption cross-sections are given in (72) and (117). As the number density of H_2^+ is proportional to $n(H)n_p$, H_2^+ contributes significantly to the total opacity only for the temperature-pressure range where both neutral and ionized H-atoms exist simultaneously in appreciable numbers; i.e., where the hydrogen is about half-ionized. This range is characteristic of the A-stars, and H_2^+ makes about a 10 percent contribution to the opacity in the visible part of the spectrum (the H_2^+ absorption peak at $\lambda 1100 \text{ \AA}$ is swamped by the Balmer continuum of hydrogen).

The negative molecular ion H_2^- exists only at relatively low temperatures, characteristic of the M-stars, and its free-free continuum makes a significant contribution at long wavelengths (the bound-free process is negligible). In this process, an electron passing near an H_2 molecule temporarily induces a dipole moment by polarization effects, and this moment can interact with the radiation field. The H_2^- continuum tends to fill in the opacity minimum of H^- at 1.6μ . The free-free cross-section is given in (592).

HELIUM

Helium is observed in stellar spectra in both its neutral and singly-ionized states. Because the ionization potential of neutral helium is 24.58 eV, it persists to temperatures characteristic of the B-stars, where hydrogen is already strongly ionized; in the O-stars, He II becomes a major opacity source. The threshold for absorption from the ground state of He I is at $\lambda 504 \text{ \AA}$; the ultraviolet spectrum for $\lambda < 504 \text{ \AA}$ is dominated by He I absorption for stars of types B0 and cooler. The excited states of helium fall into two groups, singlets and triplets, and each (n, l, s) state has a different ionization energy. Roughly speaking, the ionization energies lie close to the hydrogenic value at the same n ; thus helium contributes several absorption edges near each hydrogen edge (for $n \geq 2$). Because the excitation energy of even the lowest excited state is so large (19.72 eV), helium adds to the opacity in the visible regions of stellar spectra only in hot (B-type) stars. Generally, helium

is appreciably ionized before the excited states contribute to the opacity significantly. In a few stars the helium to hydrogen ratio is anomalous, and approaches or exceeds unity; here helium can dominate the opacity.

Helium is a three-body system, and exact wave functions cannot be obtained. A number of special methods can be applied to obtain accurate approximate wave functions [see (87, §§24–32; 577, §§18.1 – 18.3)]; variational techniques applied to the ground state have been refined to the point of yielding very precise wave functions. The ground-state absorption coefficient calculated from an accurate Hartree-Fock wave function is given in (603); this agrees well with experimental values (311). Absorption cross-sections from the $2^3S, 2^3P, 2^1S, 2^1P$ levels have been calculated using accurate variational bound-state wave functions and close-coupling free-state wave functions (332). For higher excited states, precise cross-sections have not been published, and here one may use the quantum defect method.

Ionized helium is a hydrogenic ion with $Z = 2$. As energies in such ions scale as Z^2 , the frequencies of the ionization edges, v_n , are larger by a factor of four, and the ground-state edge occurs at $\lambda 227 \text{ \AA}$. This edge dominates the far ultraviolet spectrum of O-stars, except at the very highest temperatures where the helium becomes doubly ionized. The $n = 2$ edge of He II coincides with the hydrogen Lyman continuum; higher edges from states with even quantum numbers coincide with hydrogen edges from states with $n = n(\text{He II})/2$, while those from states with odd quantum numbers fall between the hydrogen edges.

Hydrogenic cross-sections can be used for He II, but the bound-free cross sections are a factor of Z^4 larger, and the free-free are a factor of Z^2 larger. The hydrogenic Gaunt factors apply if one evaluates them as functions of (v/v_n) . He II affects the visible spectrum only in stars of types B0 and hotter.

Finally, helium can give rise to a free-free opacity in cool stars. Cross-sections for this process are given in (593; 340).

Exercise 4-7: Calculate the photoionization cross-sections of HeI from the four $n = 2$ states by the quantum defect method and compare these results with the more accurate values cited above.

4-5 Continuum Scattering Cross-Sections

As mentioned in Chapter 2, continuum radiation may be scattered as well as absorbed. In the latter case, photons are destroyed, and their energy contributed at least partially to the thermal content of the gas. In a scattering event, the photon is not destroyed, but merely redistributed in angle, and perhaps shifted slightly in frequency. Cross-sections for the two most important scattering processes in stellar atmospheres are derived in this section:

THOMSON SCATTERING

The scattering of light by free electrons is referred to as *Thomson scattering*. The classical formula for this process can be obtained directly from equation (4-32) by noting that for an unbound electron both the resonant frequency ω_0 and the damping parameter are zero. Thus we find

$$\sigma_e = (8\pi e^4/3m^2c^4) = 6.65 \times 10^{-25} \text{ cm}^2 \quad (4-127)$$

Note that this cross-section is *independent of frequency*. The Thomson cross-section has been verified by quantum mechanical calculations in the limit of low photon energies; i.e., $h\nu \ll mc^2$. At high photon energies ($\lambda < 1 \text{ \AA}$, in the X-ray region) one must employ the *Klein-Nishina* formula (293, §22; 392, 433), which predicts a smaller cross-section; in practice the departure of σ from σ_e can be ignored in stellar atmospheres work (except for X-ray binaries).

In the derivation of equation (4-32) an angle averaging was performed, and thus the angular dependence of the scattering coefficient was suppressed; the correct angular dependence is given by the dipole phase function in equation (2-19). In stellar atmospheres applications, this angular dependence can almost always be ignored and the process considered to be isotropic. Frequency redistribution in the laboratory frame caused by Doppler shifts from the electrons' motions have also been neglected; these will be considered in Chapter 13 (see Exercises 13-5 and 13-6). In the continuum, the frequency redistribution just mentioned can be ignored; near a spectral line, it may be necessary to take it into account. Electron scattering is one of the most important opacity sources in hot stars (e.g., the O-stars).

RAYLEIGH SCATTERING

The term *Rayleigh scattering* refers to the scattering of radiation by bound systems, such as atoms or molecules, at frequencies much lower than characteristic transition frequencies of the system. Again using equation (4-32), the process can be described by representing real transitions of the scatterer with equivalent classical oscillators of appropriate strengths f_{ij} , and resonant frequencies ω_{ij} equal to the actual transition frequencies. Then for $\omega \ll \omega_{ij}$, equation (4-32) simplifies to yield

$$\sigma(\omega) = (8\pi e^4/3m^2c^4)f_{ij}\omega^4/(\omega_{ij}^2 - \omega^2)^2 = \sigma_e f_{ij}\omega^4/(\omega_{ij}^2 - \omega^2)^2 \quad (4-128)$$

Far from the resonant frequency, $\sigma(\omega)$ varies as ω^4 or λ^{-4} , which leads to a strong color dependence of the scattered radiation; a well-known example of this dependence is the blue color of the sky, resulting from sunlight scattered by molecules of air.

Rayleigh scattering can be important in the atmospheres of stars of moderate temperature (spectral types G and K). Here most of the hydrogen is neutral and in the ground state. The resonant frequencies corresponding to the Lyman lines ($1 \rightarrow n$) lie far in the ultraviolet, and visible photons interact with these transitions by the Rayleigh scattering mechanism. The macroscopic scattering coefficient is obtained by summing over all lines and multiplying by the density of hydrogen in the ground state. Rayleigh scattering from neutral hydrogen can dominate the total opacity at relatively low temperatures and high frequencies; see the graphs in (97) and (651). Moreover, in stars with low metal abundances (Population II stars), the number of free electrons (coming mainly from the metals) is greatly reduced; accordingly the opacity from H^- is diminished, and thus the importance of Rayleigh scattering is much enhanced. Molecular hydrogen, H_2 , may also scatter radiation in an analogous fashion. The cross-section per molecule (189) is comparable to the cross-section per atom for atomic hydrogen. At low temperatures (e.g., in M-stars), H_2 is much more prevalent than atomic H, and thus molecular Rayleigh scattering dominates.

It should be noted that in a continuum scattering process there is no analogue of the stimulated emission that occurs in absorption processes. Thus in the macroscopic scattering coefficient there is no correction factor for stimulated emission such as appears in equations (4-98) and (4-99).

The Equations of Statistical Equilibrium

Stellar atmospheres are regions of high temperature and low density. Therefore the gas consists mainly of single atoms, ions, and free electrons; in cooler stars molecules also form. Because of the low densities, the material always behaves as a perfect gas. The *state* of the gas is specified when we know the distribution of the particles over all available bound and free energy levels—i.e., when we know the *occupation numbers* of these levels. We then have the information required to compute the gas pressure, mass density, opacity, emissivity, etc. of the material.

To specify occupation numbers, we must deal with the phenomena of excitation and ionization of each chemical species in the gas. One approach is to *assume* that we may apply the equilibrium relations of statistical mechanics and thermodynamics at local values of the temperature and density; this is the *local thermodynamic equilibrium* (LTE) approach. As we shall see, LTE provides an extremely convenient method for computing the particle distribution functions. One of the fundamental properties of stellar atmospheres, however, is the presence of an intense radiation field whose character is very different from the equilibrium Planck distribution. This radiation field interacts strongly with the material via radiative excitations and photo-

ionizations (and their inverses), and thus acts to help determine the occupation numbers of the gas; we shall show in fact, that *radiative transitions dominate* the state of the gas. In this case the occupation numbers must be determined from *equations of statistical equilibrium*, which specify all of the microprocesses that produce transitions from one atomic state to another.

The fact that the state of the material depends upon the radiation field introduces the essential difficulty of stellar atmospheres theory for, as we mentioned in Chapter 2, the radiation field, in turn, depends on the occupation numbers via the absorptivity and emissivity and their effects upon the transfer of radiation through the atmosphere. Thus what is required is a completely *self-consistent simultaneous solution of both the radiative transfer and statistical equilibrium equations*. This is a difficult problem in general, and its solution occupies the bulk of Chapters 7, 11, and 12 of this book. For the present we shall only show that there are strong expectations that the state of the material will depart from that predicted by LTE, which is therefore at best a computational expedient. If in any particular case the occupation numbers obtained from the general analysis happen to agree with those predicted by LTE, then one may legitimately use the LTE assumption; but for a wide range of problems (line-formation in particular), such agreement is not generally attained (nor can we accurately predict a priori when it will be for most cases of interest!).

5-1 Local Thermodynamic Equilibrium

In thermodynamic equilibrium, the state of the gas (i.e., the distribution of atoms over bound and free states) is specified uniquely by two thermodynamic variables (we shall choose the absolute temperature T and the total particle density N) via the well-known equilibrium relations of statistical mechanics. These relations will not all be derived in this chapter, as they are easily found in standard texts [see, e.g., (565, Chaps. 12, 14, and 15; 11, Chap. 3)] but will be summarized in forms useful for further developments in this book. The assumption of LTE asserts that we may employ these same relations in a stellar atmosphere at the *local* values $T(r)$ and $N(r)$ despite the gradients that exist in the atmosphere. This simple assumption is actually a very strong one, for it implies that we propose to calculate the above-mentioned distribution functions without reference to the physical ensemble in which the given element of material is found. Thus it is assumed that it is irrelevant whether the material is contained within an equilibrium cavity (the classical *hohlraum*), an atmosphere with a strong radiation field, or in the exhaust of a space vehicle, despite the obvious dissimilarities of these situations! In LTE, we have a purely *local* theory, which makes no allowance for coupling of the state of one element of gas with that of another,

say by radiative exchange (except as may be imposed by certain global constraints on the atmosphere—e.g., hydrostatic or radiative equilibrium). Moreover, in LTE the absolute temperature T has a quite general significance. The same T applies in the calculation of the velocity distribution functions of atoms, ions, and electrons; the distribution of atoms and ions over all states (Boltzmann–Saha equations); and the distribution of thermal emission (Planck function). In short, the full implications of the LTE assumption are quite sweeping. It is this very fact which makes it so effective in reducing the complexity of the equations, and at the same time so difficult to justify physically and so vulnerable to error.

THE MAXWELLIAN VELOCITY DISTRIBUTION

The probability, in thermodynamic equilibrium, that a particle of mass m at temperature T has a velocity on the range $(v, v + dv)$ is given by the *Maxwellian velocity distribution*

$$f(v) dv_x dv_y dv_z = \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \exp[-m(v_x^2 + v_y^2 + v_z^2)/2kT] dv_x dv_y dv_z \quad (5-1)$$

or, in terms of speeds on the range $(v, v + dv)$

$$f(v) dv = \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} \exp(-mv^2/2kT) 4\pi v^2 dv \quad (5-2)$$

These distributions may be characterized in terms of the *most probable speed*

$$v_0 = (2kT/m)^{\frac{1}{2}} = 12.85(T/10^4 A)^{\frac{1}{2}} \text{ km/sec} \quad (5-3)$$

where A is the atomic weight of the particle. Related parameters are the root-mean-square speed $\langle v^2 \rangle^{\frac{1}{2}} = (3kT/m)^{\frac{1}{2}}$, and the root-mean-square velocity in one component (e.g., along the line of sight) $\langle v_x^2 \rangle^{\frac{1}{2}} = (kT/m)^{\frac{1}{2}}$.

THE BOLTZMANN EXCITATION EQUATION

In thermodynamic equilibrium at temperature T , atoms are distributed over their bound levels according to the *Boltzmann excitation equation*. Let n_{ijk} denote the number density of atoms in excited level i of ionization state j of chemical species k . Let $j = 0$ denote neutral atoms, $j = 1$ singly ionized atoms, etc. Measure the excitation energy χ_{ijk} relative to the ground state of the atom. Let g_{ijk} denote the statistical weight assigned to the level to account for degenerate sublevels (e.g., the $2J + 1$ m -states in the absence of a magnetic field). Then, according to the Boltzmann law the population of

any excited level is

$$(n_{ijk}/n_{0jk})^* = (g_{ijk}/g_{0jk}) \exp(-\chi_{ijk}/kT) \quad (5-4)$$

where the subscript 0 denotes the ground level and the superscript * denotes LTE. For any two excited levels l and m ,

$$\begin{aligned} (n_{mj_k}/n_{lj_k})^* &= (g_{mj_k}/g_{lj_k}) \exp[-(\chi_{mj_k} - \chi_{lj_k})/kT] \\ &= (g_{mj_k}/g_{lj_k}) \exp(-hv_{lm}/kT) \end{aligned} \quad (5-5)$$

where hv_{lm} is the energy of a photon that equals the energy difference between the levels. In calculations of ionization equilibria, we typically wish to know the *total number of atoms in a particular ionization state*, which can be written as

$$\begin{aligned} N_{jk}^* &= \sum_i n_{ijk}^* = (n_{0jk}^*/g_{0jk}) \sum_i g_{ijk} \exp(-\chi_{ijk}/kT) \\ &= (n_{0jk}^*/g_{0jk}) U_{jk}(T) \end{aligned} \quad (5-6)$$

$$\text{where } U_{jk}(T) \equiv \sum_i g_{ijk} \exp(-\chi_{ijk}/kT) \quad (5-7)$$

is called the *partition function*. A form of equation (5-4) customarily used in classical curve-of-growth analyses of spectra (see §§10-3 and 10-4) is

$$(n_{ijk}/N_{jk})^* = g_{ijk} \exp(-\chi_{ijk}/kT)/U_{jk}(T) \quad (5-8)$$

The partition function is tedious to compute, and for some atoms and ions (e.g., of the rare earths) our knowledge of the term structure is so incomplete that we lack the needed data. Tabulations of partition functions (11, 115–117) and convenient analytical fits with approximation formulae (103; 220) are available. Often a fair estimate is just g_{0jk} or a sum over a few low-lying states. Note that formally the partition function in equation (5-7) diverges if the sum extends over all (an infinite number) of bound states, for a lower bound to each term of the sum is $\exp(-\chi_{ijk}/kT)$ (where χ_{ijk} is the ionization potential), which is nonzero. This problem is not a physical one, for in reality the highest levels cannot remain bound because they are strongly perturbed by neighboring atoms and ions. To estimate the effect we might suppose that the only levels that are bound are those contained within the average volume available to ions. For a particle density N , the mean interatomic distance is $r_0 = (3/4\pi N)^{\frac{1}{3}}$, and for a hydrogenic ion of charge Z the radius of the state of principal quantum number n is $r_n = n^2 a_0/Z$ where a_0 is the Bohr radius = 5.3×10^{-9} cm. If we set $r_n = r_0$ and choose

a typical value of $N \sim 10^{15}$ we find $n \approx 30Z^{\frac{1}{2}}$, so clearly the sum is finite. A more accurate calculation (see §9-4) shows that in a plasma with charge density n_e and temperature T , an ion of charge Z suffers a lowering of the ionization potential by an amount $\Delta\chi \approx 3 \times 10^{-8} Z n_e^{\frac{1}{2}} T^{-\frac{1}{2}}$ eV. For hydrogenic energy levels this implies $n_{\max}^2 \approx 4 \times 10^8 Z n_e^{-\frac{1}{2}} T^{\frac{1}{2}}$ or $n_{\max} \sim 60Z^{\frac{1}{2}}$ for $n_e \sim 10^{14}$ and $T \sim 10^4$.

THE SAHA IONIZATION EQUATION

Above the discrete bound eigenstates of an atom there exists a continuum of levels in which the electron is unbound and has a nonzero kinetic energy. The energy above the ground level at which this continuum begins is called the *ionization potential* χ_I . The relative numbers of atoms and ions in successive stages of ionization can be computed from the *Saha ionization equation*, which we shall derive as an extension of the Boltzmann formula to free states.

Consider a process in which an atom of species k is ionized from its ground level, resulting in an ion in the ground level plus a free electron in the continuum moving with speed v . The energy required to carry out this process is $\chi_{I,0,k} + \frac{1}{2}mv^2$ (where we have used notation parallel to that used in our discussion of the Boltzmann formula). The statistical weight of the initial state is $g_{0,0,k}$, and the statistical weight of the final state (ion + electron) may be written $g(v) = g_{0,1,k} \times g_{\text{electron}}$. If we use $n_{0,1,k}(v)$ to denote the number of ions in the ground level with accompanying free electron with speed in the range $(v, v + dv)$, we may apply equation (5-4) to write

$$[n_{0,1,k}(v)/n_{0,0,k}]^* = [g(v)/g_{0,0,k}] \exp[-(\chi_{I,0,k} + \frac{1}{2}mv^2)/kT] \quad (5-9)$$

We identify g_{electron} with the number of phase space elements available to the free electron, which, according to quantum statistics, is

$$g_{\text{electron}} = 2(dx dy dz dp_x dp_y dp_z)/h^3$$

where the factor of 2 accounts for the two possible orientations of the electron spin. We choose the space-volume element to contain exactly one free electron, and make the substitution $dx dy dz = n_e^{-1}$. We rewrite the momentum volume element in terms of the electron's speed,

$$dp_x dp_y dp_z = 4\pi p^2 dp = 4\pi m^3 v^2 dv$$

Then equation (5-9) becomes

$$\begin{aligned} & [n_{0,1,k}(v)/n_{0,0,k}]^* \\ &= 8\pi m^3 h^{-3} (g_{0,1,k}/g_{0,0,k}) n_e^{-1} \exp[-(\chi_{I,0,k} + \frac{1}{2}mv^2)/kT] v^2 dv \end{aligned} \quad (5-10)$$

Now, summing over all final states by integrating over the electron velocity distribution we obtain

$$\begin{aligned} & (n_{0,1,k} n_e / n_{0,0,k})^* \\ &= 8\pi m^3 h^{-3} (g_{0,1,k}/g_{0,0,k}) (2kT/m)^{\frac{1}{2}} \exp(-\chi_{I,0,k}/kT) \int_0^\infty e^{-x^2} x^2 dx \end{aligned} \quad (5-11)$$

or, evaluating the integral,

$$n_{0,0,k}^* = n_{0,1,k}^* n_e^* \frac{1}{2} (h^2/2\pi mkT)^{\frac{1}{2}} (g_{0,0,k}/g_{0,1,k}) \exp(\chi_{I,0,k}/kT) \quad (5-12)$$

which is a basic form of *Saha's equation*. Note that in the derivation we made no explicit reference to the ionization state of the initial "atom," hence we may extend equation (5-12) to apply between any two successive stages of ionization

$$n_{0,jk}^* = n_{0,j+1,k}^* n_e^* \frac{1}{2} (h^2/2\pi mkT)^{\frac{1}{2}} (g_{0,jk}/g_{0,j+1,k}) \exp(\chi_{I,jk}/kT) \quad (5-13)$$

If, further, we apply Boltzmann's formula, equation (5-4), we obtain an expression for the occupation number of any state of ion j in terms of the temperature, electron density, and ground state population of ion $j+1$, namely

$$\begin{aligned} n_{ijk}^* &= n_{0,j+1,k} n_e (g_{ijk}/g_{0,j+1,k}) C_I T^{-\frac{1}{2}} \exp[(\chi_{Ijk} - \chi_{ijk})/kT] \\ &\equiv n_{0,j+1,k} n_e \Phi_{ijk}(T) \end{aligned} \quad (5-14)$$

Equation (5-14) is the most useful form of Saha's equation for the formalism we shall employ, and will be used to *define* LTE populations in the full non-LTE equations of statistical equilibrium (for this reason the superscript * on $n_{0,j+1,k}$ and n_e has been omitted). The constant has the value $C_I = 2.07 \times 10^{-16}$ in cgs units.

By applying equation (5-6), we may rewrite equation (5-14) as

$$n_{ijk}^* = N_{j+1,k}^* n_e [g_{0,j+1,k}/U_{j+1,k}(T)] \Phi_{ijk}(T) \equiv N_{j+1,k}^* n_e \tilde{\Phi}_{ijk}(T) \quad (5-15)$$

Further, by summing over all bound levels of the lower ionization stage and again using equation (5-6), we obtain an equation for the ratio of the total number of atoms in successive stages of ionization:

$$(N_{jk}/N_{j+1,k})^* = n_e [U_{jk}(T)/U_{j+1,k}(T)] C_I T^{-\frac{1}{2}} \exp(\chi_{Ijk}/kT) \equiv n_e \tilde{\Phi}_{jk}(T) \quad (5-16)$$

By recursive application of equation (5-15) between successive stages of ionization, we can obtain an expression for the fraction of atoms of chemical

species k in ionization stage j relative to the total number of atoms of that species:

$$\begin{aligned} f_{jk}(n_e, T) &\equiv (N_{jk}/N_k)^* \\ &= \frac{(N_{j-1,k}/N_{jk})^* \cdots (N_{j_k}/N_{j+1,k})^*}{1 + (N_{j-1,k}/N_{jk})^* + (N_{j-1,k}/N_{jk})^*(N_{j-2,k}/N_{j-1,k})^* + \cdots + (N_{j-1,k}/N_{jk})^* \cdots (N_{0k}/N_{1k})^*} \\ &= \prod_{l=j}^{j_k-1} [n_e \tilde{\Phi}_{lk}(T)] / \sum_{m=0}^{j_k} \prod_{l=m}^{j_k-1} [n_e \tilde{\Phi}_{lk}(T)] \\ &\equiv P_{jk}(n_e, T)/S_k(n_e, T), \quad (j = 1, \dots, J_k) \end{aligned} \quad (5-17)$$

where J_k is the last ionization stage of species k considered. We observe the convention that the product term for $l = J_k$ (which formally becomes void) is replaced by unity in both the numerator and denominator.

Consideration of the above results shows that, if we know (n_e, T) , then we may determine, for any chemical species k , the fraction in any chosen ionization stage from equation (5-17), and in any particular excitation state from equation (5-15). If, in addition, we know the total number density of atoms of this species, we can obtain absolute occupation numbers n_{ijk} . In practice this procedure is useful in LTE calculations of line spectra where we are given a model atmosphere that specifies $n_e(z)$ and $T(z)$. In computation of the model itself, however, we generally do not know $n_e(z)$, but rather the total particle density $N(z)$; we must then determine n_e , and as can be seen from equation (5-17), this implies we must solve a nonlinear set of equations. Let us therefore now consider methods of solving the nonlinear problem.

5-2 The LTE Equation of State for Ionizing Material

The Saha–Boltzmann relations allow a computation of the fraction of each chemical species in various stages of ionization, and the number of free electrons that each contributes to the plasma. Stellar atmospheres consist of a mixture of elements with widely differing ionization potentials; in general some of the species may be neutral while others are singly or multiply ionized. Usually the transition from one ionic stage to the next occurs fairly abruptly with increasing temperature, and normally a particular chemical species exists essentially entirely in two successive ionization stages. This provides a sensitive diagnostic tool to infer the temperature structure of a stellar atmosphere, for it implies that ratios of line strengths of two successive ionic spectra (e.g., He I and He II, or Ca I and Ca II) will vary

rapidly as a function of temperature. In fact, this was the basis upon which the first understanding of the spectral sequence as a temperature sequence was built by Saha (546; 547), Pannekoek (495), Cecilia Payne (501), and Fowler and Milne (222; 223). In normal stellar atmospheres hydrogen is by far the most abundant constituent, and helium is next most abundant with $N(\text{He})/N(\text{H}) \approx 0.1$. The heavier elements have much smaller abundances relative to hydrogen [see, e.g., (252) for element abundances in the solar atmosphere]. At typical temperatures in the solar atmosphere (6000°K) hydrogen is essentially neutral, and the electrons are contributed mainly by the “metals” such as Na, Mg, Al, Si, Ca, and Fe. At higher temperatures, characteristic of the A-stars (10,000°K), hydrogen ionizes and becomes the dominant source of electrons. At very high temperatures, characteristic of the O- and early B-stars, helium ionizes and makes an appreciable contribution of electrons.

CHARGE AND PARTICLE CONSERVATION

In calculations of stellar atmospheres we specify the gas pressure from the equation of hydrostatic equilibrium. Thus, given p_g and T , we know the total number density N from the relation

$$p_g = N k T = (N_{\text{atoms}} + N_{\text{ions}} + n_e) k T = (N_N + n_e) k T \quad (5-18)$$

Here N_N denotes the density of “nuclei”; i.e., atoms and ions of all types. In equation (5-18) and subsequent equations of this section we suppress the “*” that denotes LTE for notational simplicity. We define the abundance α_k of chemical species k to be such that $N_k = \alpha_k N_N$ where $\sum_k \alpha_k \equiv 1$. Then

$$N_k = \alpha_k (N - n_e) \quad (5-19)$$

summarises the constraint of *particle conservation* (i.e., $\sum N_k = N_N$). In addition we require the plasma to be electrically neutral; then the number of free electrons equals the total ionic charge, and the condition of *charge conservation* reads

$$n_e = \sum_k \sum_{j=1}^{J_k} j N_{jk} = \sum_k N_k \sum_{j=1}^{J_k} j f_{jk}(n_e, T) = (N - n_e) \sum_k \alpha_k \sum_{j=1}^{J_k} j f_{jk}(n_e, T) \quad (5-20)$$

As mentioned above, if we know (n_e, T) we may calculate N and the f_{jk} directly. But if we know (N, T) , we must find n_e from a nonlinear equation. Before the availability of electronic computers this problem was solved by constructing tables of $\log p_g(T, \log p_e)$ (here $p_e \equiv n_e k T$), in which interpolations could be made to find $\log p_e(T, \log p_g)$. Examples of such tables are

given in (11, 130) and (638, 104). We shall develop a different procedure, along lines suggested by L. H. Auer, that is better suited for machine computation, and that fits into the overall approach of Chapter 7 for the computation of model atmospheres. But first consider an instructive example that yields physical insight in limiting cases.

Suppose that the gas consists only of hydrogen ($\chi_H = 13.6 \text{ eV}$) and one metal "M" with a single ionization stage of much lower ionization potential (say $\chi_M = 4$ or 5 eV) and an abundance relative to hydrogen $\alpha_M \ll 1$. At high temperatures where the hydrogen is appreciably ionized, it will contribute most of the electrons; at lower temperatures the hydrogen is neutral, and n_e is determined by f_M , the ionization fraction of the metal. The number of particles of all types is

$$N = n_H(1 + f_H) + \alpha_M n_H(1 + f_M) \quad (5-21)$$

while the number of electrons is

$$n_e = n_p + n_{M+} = n_H(f_H + \alpha_M f_M) \quad (5-22)$$

$$\text{Then } p_e/p_g = (f_H + \alpha_M f_M)/[1 + f_H + \alpha_M(1 + f_M)] \quad (5-23)$$

At high enough temperatures, $f_H \rightarrow 1$, and as $\alpha_M \ll 1$, $(p_e/p_g) \rightarrow \frac{1}{2}$. At intermediate temperatures, where $\alpha_M \ll f_H \ll 1$, and at the same time $f_M \approx 1$, $(p_e/p_g) \approx f_H$. At low temperatures, $f_H \rightarrow 0$ while $f_M/f_H \gg 1$, hence $(p_e/p_g) \rightarrow \alpha_M f_M$. We thus see that at high temperatures the metals are essentially irrelevant to the determination of p_e/p_g , while at low temperatures they play a crucial role. In particular, note that the metal abundance enters directly in fixing p_e in cool stars; this is important because the dominant opacity source in cooler atmospheres is absorption by the H^- ion, and $n(H^-)/n(H)$ is proportional to n_e . Thus in these stars the metal abundance fixes the opacity as well.

For a pure hydrogen gas, equations (5-16), (5-19), and (5-20) may be solved analytically to obtain

$$n_e(H) = \tilde{\Phi}_H^{-1}[(N\tilde{\Phi}_H + 1)^{\frac{1}{2}} - 1] \quad (5-24)$$

which shows that at low degrees of ionization, $n_e \sim N^{\frac{1}{2}}$ for a given T .

Exercise 5-1: Derive equation (5-24).

If only the metal in our two-component gas described above is ionized ($f_H \ll \alpha_M$) then we have

$$n_e(M) \approx \tilde{\Phi}_M^{-1} \left\{ \left[\alpha_M N \tilde{\Phi}_M + \frac{1}{4}(1 + 2\alpha_M) \right]^{\frac{1}{2}} - \frac{1}{2}(1 + \alpha_M) \right\} \quad (5-25)$$

A fairly good estimate of n_e can be obtained from equations (5-24) and (5-25) if $\alpha_M \ll 1$ and $\chi_M \ll \chi_H$ by writing $n_e \approx n_e(H) + n_e(M)$.

SOLUTION BY LINEARIZATION

Let us now turn to the problem of determining n_e for a given value of (N, T) by means of an iterative linearization procedure (generalized Newton-Raphson method). We shall describe the procedure in fair detail because it is a simple example of the approach we shall use in more complicated cases (e.g., the non-LTE rate equations and the transfer equation). The only equation to be solved (contrast this with the non-LTE case, cf. §5.5!) is equation (5-20) where $f_{jk}(n_e, T)$ is given by equation (5-17). Suppose that we have an initial estimate of the electron density, n_e^0 ; suppose also we find that using n_e^0 to evaluate the righthand side of equation (5-20) yields a density $n_e^1 \neq n_e^0$. It is then clear that the true density differs from n_e^0 , so we write $n_e = n_e^0 + \delta n_e$ where δn_e is to be determined in such a way as to satisfy equation (5-20) exactly. Because the equation is nonlinear, we cannot determine this δn_e exactly, but on the supposition that $\delta n_e/n_e^0 \ll 1$, we can estimate δn_e by expanding all terms to first order and solving for δn_e . Then we have

$$n_e^0 + \delta n_e \approx [(N - n_e^0 - \delta n_e) \cdot \tilde{\Sigma}(n_e^0, T)] + (N - n_e^0)[\partial \tilde{\Sigma}(n_e, T)/\partial n_e]_{n_e^0} \delta n_e \quad (5-26)$$

$$\text{or } \delta n_e \approx [(N - n_e^0)\tilde{\Sigma} - n_e^0][1 + \tilde{\Sigma} - (N - n_e^0)(\partial \tilde{\Sigma}/\partial n_e)]^{-1} \quad (5-27)$$

$$\text{where } \tilde{\Sigma}(n_e, T) \equiv \sum_k \alpha_k S_k^{-1}(n_e, T) \sum_{j=1}^{J_k} j P_{jk}(n_e, T) \quad (5-28)$$

Note that we may rewrite the functions $P(n_e, T)$ and $S(n_e, T)$ as

$$P_{jk}(n_e, T) \equiv \prod_{l=j}^{J_k-1} [n_e \Phi_{lk}(T)] = n_e^{(J_k-j)} \prod_{j=1}^{J_k} (T) \quad (5-29)$$

$$\text{and } S_k(n_e, T) \equiv \sum_{j=0}^{J_k} P_{jk}(n_e, T) = \sum_{j=0}^{J_k} n_e^{(J_k-j)} \prod_{j=1}^{J_k} (T) \quad (5-30)$$

The value of δn_e given by equation (5-27) will not be exact, so we iterate the procedure by using a new estimate $n_e^0(\text{new}) = n_e^0(\text{old}) + \delta n_e$ to re-evaluate $\tilde{\Sigma}$ and $\partial \tilde{\Sigma}/\partial n_e$, and to compute yet another value of δn_e .

The convergence of this procedure is quadratic (if our original estimate lies within the range of convergence) so, if the first fractional error $\delta n_e/n_e$ is ε , subsequent iterations will produce corrections of order $\varepsilon^2, \varepsilon^4, \varepsilon^8$, etc.,

which implies that one can obtain the result to the desired accuracy quickly. It is also worth noting that the derivative $\partial\Sigma/\partial n_e$ can be evaluated analytically:

$$(\partial\Sigma/\partial n_e) = \sum_k \alpha_k \left[S_k^{-1} \sum_j j(\partial P_{jk}/\partial n_e) - S_k^{-2} (\partial S_k/\partial n_e) \sum_j j P_{jk} \right] \quad (5-31)$$

where $(\partial P_{jk}/\partial n_e)$ and $(\partial S_k/\partial n_e)$ follow immediately from equations (5-29) and (5-30) and produce a compact expression for (5-31). In general, the derivatives appearing in linearization procedures can be estimated numerically; however, we shall usually be able to obtain analytical derivatives, and experience has shown that in this way we obtain better control of the calculation.

Finally, having obtained a satisfactory value for n_e , and, as a byproduct the f_{jk} , we may calculate any particular occupation number from equation (5-15)

$$n_{ijk} = N_{j+1,k} n_e \Phi_{ijk}(T) = \alpha_k (N - n_e) n_e f_{j+1,k}(n_e, T) \Phi_{ijk}(T) \quad (5-32)$$

this completes the computation of the LTE equation of state.

The procedure outlined above has a larger significance than indicated thus far. We have assumed that N and T are given. But these quantities follow from constraints of pressure and energy balance, and in general are known only approximately at any particular stage of calculation of a model. As we shall see in Chapter 7, we may apply the linearization procedure to all the variables involved, and hence we shall need to evaluate the response of the occupation numbers to the perturbations δN and δT . Perturbing equation (5-20) we obtain

$$\begin{aligned} n_e + \delta n_e &= (N + \delta N - n_e - \delta n_e) \Sigma \\ &+ (N - n_e)[(\partial\Sigma/\partial n_e) \delta n_e + (\partial\Sigma/\partial T) \delta T] \end{aligned} \quad (5-33)$$

or, assuming that n_e is a solution of equation (5-20) at the current values of (N, T) ,

$$\begin{aligned} \delta n_e &= [1 + \Sigma - (N - n_e)(\partial\Sigma/\partial n_e)]^{-1} [\Sigma \delta N + (N - n_e)(\partial\Sigma/\partial T) \delta T] \\ &\equiv (\partial n_e/\partial N)_T \delta N + (\partial n_e/\partial T)_N \delta T \end{aligned} \quad (5-34)$$

where again $\partial\Sigma/\partial T$ may be evaluated analytically. Further, from equation (5-32) we may develop an expression for δn_{ijk} of the form $\delta n_{ijk} = \Delta_1 \delta N + \Delta_2 \delta T + \Delta_3 \delta n_e$, which can be collapsed down by use of equation (5-34) to an expression of the form

$$\delta n_{ijk} = (\partial n_{ijk}/\partial N)_T \delta N + (\partial n_{ijk}/\partial T)_N \delta T \quad (5-35)$$

Exercise 5-2: Obtain expressions for the coefficients in equation (5-35) in terms of P_{jk} , S_k , and Φ_{ijk} , and their derivatives.

Equations (5-34) and (5-35) provide the information we shall require in §7-2 to find the response of the opacity and emissivity ($\delta\chi$, $\delta\eta$) to changes in the model structure (δN , δT).

Exercise 5-3: Show that δN_{jk} , for the last ionization stage of element k , has a particularly simple form because f_{jk} involves only S_k . Then show that expressions for δN_{jk} of lower ions can be evaluated recursively from equation (5-16), and that these lead from equation (5-15) to simple expressions of the form of equation (5-35) for δn_{ijk} .

5-3 The Microscopic Requirements of LTE

Before we develop the equations of statistical equilibrium, it is worthwhile to discuss qualitatively the microscopic requirements of LTE. An interesting commentary on these requirements by K. H. Böhm may be found in (261, Chap. 3); we shall summarize and discuss this analysis here along with other material of relevance.

DETAILED BALANCE

In thermodynamic equilibrium, the rate at which each process occurs is exactly balanced by the rate at which its inverse occurs, for all processes; i.e., each process is in *detailed balance*. This is a very strong requirement, and it proves to be very useful in constructing relations among rate coefficients (recall the use of this procedure in Chapter 4). We may classify processes that produce transitions from one state to another (bound or free) into two broad categories: radiative and collisional. Collisional processes are the processes invoked in statistical mechanics to establish equilibrium, and can be expected to be in detailed balance whenever the velocity distribution of the colliding particles is the equilibrium (i.e., Maxwellian) distribution. We shall show below that this can be expected to be the case in stellar atmospheres. Furthermore, we may make the same statement about processes which are essentially collisional in character, even though a photon is emitted (e.g., free-bound radiative recombination and free-free emission); we can therefore use detailed balancing arguments to calculate the rates of these processes when convenient to do so. In contrast, radiative processes (e.g., photoexcitation, photoionization) depend directly upon the character of the radiation field, and will be in detailed balance only if the radiation field is isotropic and has a Planck distribution. We shall show below that this is not the case in stellar atmospheres.

If some processes are in detailed balance while others are not, the final occupation numbers will be determined by a competition among them and may depart more or less strongly from an equilibrium distribution. LTE will be valid in the deepest layers of stellar atmospheres where densities are high and the collision rates become large, and the optical depth is so large that no photon escapes from the atmosphere before being thermalized, so that the radiation field approaches the Planck function. But in the observable layers, precisely the opposite regime is found.

THE NATURE OF THE RADIATION FIELD

A stellar atmosphere is not in any sense a closed system in equilibrium at a uniform temperature. Indeed the opposite situation prevails: radiation flows freely from the surface layers of the star into essentially empty space, which implies that the radiation field is decidedly anisotropic, and that the atmosphere has a large temperature gradient. The radiation field at any point is the integrated result of emissions and absorptions over the entire (possibly large) volume within which a photon can travel from its point of emission to the test point. This volume may include the boundary surface and empty space beyond, with a consequent reduction of intensity, as well as layers of higher temperatures and densities from which intense radiation originates. The radiation field therefore is distinctly nonlocal in nature, and has an absolute intensity, directional distribution, and frequency spectrum that may have no resemblance whatever to the local equilibrium distribution $B_v(T)$. Radiative rates may therefore be far from their equilibrium values, and thus tend to drive the material away from LTE.

The radiation field is plainly anisotropic because the radiating surface subtends a solid angle less than 4π , and essentially no radiation enters from the surrounding void. We may describe this geometrical effect by introducing a *dilution factor* W defined to be $\omega_*/4\pi$ where ω_* is the solid angle subtended by the stellar disk.

Exercise 5-4: Show that

$$W = \frac{1}{2} \{1 - [1 - (r_*/r)^2]^\frac{1}{2}\} \quad (5-36)$$

where r_* is the radius of the radiating surface and r denotes the position of the observer. Show that for $r_*/r \ll 1$, $W = \frac{1}{2}(r_*/r)^2$

As defined, W clearly measures the factor by which the energy density in the radiation field is reduced as the source of radiation moves to a large distance. At the "surface" of a star, it is obvious that $W = \frac{1}{2}$ (actually a little

less because of limb-darkening) but in an extended stellar envelope $W \ll 1$ (and in a planetary nebula, $W \sim 10^{-14}$). Thermodynamic equilibrium requires that $W \equiv 1$, so it is clear that detailed balancing in radiative transitions cannot in general occur in a stellar atmosphere.

In addition to being dilute, the stellar radiation field has a markedly non-Planckian frequency distribution. As we know from the Eddington-Barbier relation, the emergent specific intensity at frequency v is approximately equal to the source function S_v at $\tau_v = 1$. Even if S_v were B_v , the fact that the material is vastly more opaque at some frequencies than at others (line to continuum ratios are often 10^3 and may reach much larger values) implies that the radiation will emerge from greatly differing depths at substantially different temperatures; the radiation field is therefore a composite of widely differing radiation temperatures. The effects of the temperature gradient become extreme when $hv/kT > 1$, for then the Planck function varies as $\exp(-hv/kT)$ and becomes very sensitive to small changes in T . If we were to parameterize the radiation field by introducing a radiation temperature $T_R(\mu, v)$ such that for $\mu \geq 0$, $I(r_*, \mu, v) = WB_v[T_R(\mu, v)]$, we would find marked variations of T_R with both v and μ . For example, in the solar spectrum, T_R ranges from 4800°K in the visible to $\sim 25,000^\circ\text{K}$ in the ultraviolet in the ground-state continuum of He^+ . In sum, the radiation field displays an extremely complex behavior, and the conditions required to assure LTE a priori are simply not met.

THE ELECTRON VELOCITY DISTRIBUTION

In stellar atmospheres, the free electrons are produced by photoionization and collisional ionization. The inverse processes are radiative recombination and three-body collisions, which lead to recaptures of electrons into bound states. While in the continuum, an electron may undergo elastic collisions with other electrons and inelastic collisions (leading to excitation or ionization of bound electrons) with atoms and ions. The elastic collisions redistribute energy among the electrons and tend to lead to an equilibrium partitioning—hence a Maxwellian velocity distribution. If a Maxwellian velocity distribution is in fact attained, we may define the local temperature to be the kinetic temperature of the electrons. On the other hand, inelastic collisions and recombinations disturb the achievement of a Maxwellian velocity distribution, for the inelastic collisions involve electrons only in certain velocity ranges and tend systematically to shift them to much lower velocities, while recombinations remove electrons from the continuum and prevent further elastic collisions. Whether or not the Maxwellian velocity distribution is established hinges upon how rapidly thermalization by elastic collisions occurs compared to the perturbing processes: if it occurs much more rapidly, the velocity distribution will be very nearly Maxwellian.

The thermalization rate can be measured in terms of the *relaxation time* of the system, which, for particles interacting with themselves, is

$$t_c = m^{\frac{1}{2}}(3kT)^{\frac{1}{2}}/[17.9n_e e^4 Z^4 \ln(D/p_0)] \text{ sec} \quad (5-37)$$

(see 598, Chap. 5). Here D is the *Debye radius* (see §9-4) $D = (kT/8\pi e^2 n_e)^{\frac{1}{2}}$ and $p_0 = e^2/mv^2$ is the impact parameter for a 90° collision. Now consider recombinations; if σ is the average cross-section for the process then the mean time between recombinations is

$$t_r = (N\sigma\langle v \rangle)^{-1} = N^{-1}\sigma^{-1}(\pi m/8kT)^{\frac{1}{2}} \text{ sec} \quad (5-38)$$

where N is the density of the particles with which recombination occurs. Two astrophysically important processes are (a) $H + e \rightarrow H^-$ and (b) $H^+ + e \rightarrow H$. At $T \sim 6000^\circ K$ (a typical solar temperature) $\sigma_{H^-} \sim 3 \times 10^{-22}$ cm^2 and $n_e/N_H \sim 10^{-4}$. At $T \sim 10000^\circ K$, $\sigma_H \sim 6 \times 10^{-21}$ cm^2 and $n_e/n_p \sim 1$. Substituting these values into equations (5-37) and (5-38), we find $t_r/t_c \sim 10^5$ for process (a) and $t_r/t_c \sim 10^7$ for process (b). We conclude, therefore, that under representative conditions in stellar atmospheres a free electron will undergo an enormous number of elastic scatterings between recombinations, and that the latter will not seriously hinder equilibration to a Maxwellian distribution.

Let us now consider inelastic collisions. Collisions of electrons with the most abundant element, hydrogen, occur frequently, but the excitation energy of hydrogen is 10 eV while the thermal energy of the electrons is 1 eV. Thus only 3×10^{-5} of the electrons have sufficient energy to induce the excitation, and only a fraction of these will be effective. Using typical excitation cross-sections one finds that (at $10,000^\circ K$) the rate of inelastic excitations is of the same order as the recombination rate—i.e., very small compared to the elastic collision rate. One must also consider collisions with other elements, which may be grouped as follows: (a) the alkalis, which have large cross-sections but low abundances (10^{-6}); (b) Fe, which has numerous low-lying levels and moderate abundance (4×10^{-5}); and (c) C, N, and O, which have small cross-sections but large abundance (10^{-3}). Most of the levels for groups (b) and (c) are metastable, so that most of the inelastic excitations are subsequently cancelled by collisional de-excitation; ignoring this effect we overestimate the number of inelastic excitations. Taking the various factors into account and ignoring compensating de-excitation, Böhm estimates (elastic collisions/inelastic collisions) $\sim 10^3$ and hence concludes that a Maxwellian velocity distribution that defines T_e is established. Recent work (573) suggests that departures from a Maxwellian distribution in a pure hydrogen gas can occur in the high-energy tail if (a) the ionization level is very low ($n_e/n_H \lesssim 0.01$) and (b) the ground-state

population is far from its equilibrium value; these conditions can occur in the solar chromosphere.

Finally, one may ask if the atoms and ions in the atmosphere also have a Maxwellian velocity distribution, and if their kinetic temperature $T_k = T_e$. An analysis of this question (88) for a pure hydrogen atmosphere of atoms, ions, electrons, and radiation, demanding a steady-state solution, while allowing for energy exchange among the four components of the medium, shows that if $n_e > 10^{10}$ (a condition easily met in the bulk of the atmosphere) and $5 \times 10^3 < T_e < 10^5$, then $|T_k - T_e| \lesssim 10^{-3} T_e$. It thus appears safe to conclude that a unique local kinetic temperature applies to all the particles in most atmospheric regions.

THE IONIZATION EQUILIBRIUM

The degree of ionization of stellar material is determined by the balance of photoionizations and collisional ionizations against radiative recombinations and three-body collisional recombinations. Let us first examine the relative rates of photoionization and collisional ionization; it suffices to obtain only an order-of-magnitude estimate.

The energy absorbed by an atom in bound state i at frequency v in interval dv is $4\pi J_v \alpha_i(v) dv$; each photon has energy hv , hence the total number of photoionizations is

$$n_i R_{ik} = n_i 4\pi h^{-1} \int_{v_0}^{\infty} \alpha_i(v) J_v v^{-1} dv \quad (5-39)$$

To estimate R_{ik} , we adopt a hydrogenic cross-section

$$\alpha_v = (\pi e^2/mc) f_c (2v_0^{-2}/v^3)$$

where f_c is the integrated oscillator strength for the continuum. Further, we write

$$J_v = WB_v(T_R) = W(2hv^3/c^2) \sum_{n=1}^{\infty} \exp(-nhv/kT_R) \quad (5-40)$$

$$\text{Then } R_{ik} = (16\pi^2 e^2 v_0^{-2}/mc^3) f_c W \sum_{n=1}^{\infty} E_1(nhv_0/kT_R)$$

The rate of collisional ionizations can be computed from $\sigma(v)$, the collisional ionization cross-section for electrons of velocity v :

$$n_i C_{ik} = n_i n_e \int_{v_0}^{\infty} \sigma(v) f(v) v dv \quad (5-41)$$

TABLE 5-1
Ratio of Radiative to Collisional Ionization Rates

Star	$\chi_{\text{ion}} = 8 \text{ eV}$	$\chi_{\text{ion}} = 1 \text{ eV}$
Sun	10^3	2
O-star	20	0.2

SOURCE: From data by K. H. Böhm, in *Stellar Atmospheres*, ed. J. L. Greenstein, Chicago: University of Chicago Press, 1960, by permission.

To obtain an estimate, we adopt the semiclassical Thomson formula [cf. (684, 120)]

$$\sigma(v) = 3f_c \pi e^4 E^{-1} [(hv_0)^{-1} - E^{-1}] \quad (5-42)$$

where $E = \frac{1}{2}mv^2$ is the energy of the incident electron. Substituting equations (5-2) and (5-42) into (5-41) and integrating we obtain

$$C_{ik} = n_e [12\pi^{\frac{1}{2}} e^4 f_c / (2mk^3 T_e^3)^{\frac{1}{2}}] u_0^{-1} E_2(u_0) \quad (5-43)$$

where $u_0 \equiv hv_0/kT_e$. In the limit that $hv_0 \gg kT_R$ and $hv_0 \gg kT_e$ we retain only the first term of equation (5-40), and use the asymptotic result that for $x \gg 1$, $E_2(x) \rightarrow E_1(x) \rightarrow e^{-x}/x$ to obtain

$$\frac{R_{ik}}{C_{ik}} \approx \frac{4(2\pi^3 k)^{\frac{1}{2}} h v_0^3}{3m^{\frac{1}{2}} e^2 c^3} \left(\frac{W T_R}{n_e T_e^{\frac{1}{2}}} \right) \exp \left[hv_0 \left(\frac{1}{kT_e} - \frac{1}{kT_R} \right) \right] \quad (5-44)$$

For photospheric layers we could adopt $W \approx \frac{1}{2}$, $T_R \approx T_e$. Böhm calculates estimates of R_{ik}/C_{ik} for representative cases of levels with ionization potentials of 1 eV and 8 eV for conditions characteristic of the outer layers ($\tau \sim 0.05$) of the sun and an O-star. In particular, for the sun he adopts $n_e \approx 3 \times 10^{12}$, and $T \approx 5 \times 10^3 \text{ }^\circ\text{K}$ while for the O-star he uses $n_e \approx 3 \times 10^{14}$, $T \approx 3.2 \times 10^4 \text{ }^\circ\text{K}$ and finds the values for R_{ik}/C_{ik} listed in Table 5-1. It is clear that in stellar photospheres, the radiative rates dominate, except for high-lying levels at high temperature and densities. In fact, for O-stars the important levels have even larger values of χ_{ion} than those listed in Table 5-1 (e.g., the ground state of H at 13.6 eV and the ground state of He I at 24.5 eV), and are even more markedly radiatively dominated. Thus the ionization equilibrium is vulnerable to departures from LTE if J_v departs from B_v . Note in passing that in the corona of a star where $T_e \sim 2 \times 10^6 \text{ }^\circ\text{K}$ and $T_R \sim 6 \times 10^3 \text{ }^\circ\text{K}$ (for the sun), while the relevant values of hv_0 are around 300 eV, the exponential factor in equation (5-44) becomes very small and collisional ionizations dominate.

We may carry out similar estimates for the rates of radiative recombination and three-body collisional recombination; these processes are both essentially collisional and hence per ion occur at the LTE rate. We can then use detailed balancing arguments to compute the rates in terms of the equilibrium values of the upward rates. We may still use equation (5-44), except that for the radiative recombinations the appropriate temperature is now T_e not T_R , and $W \equiv 1$. We then find that radiative recombinations always outweigh collisional recombination, both in the photosphere and corona (in the corona, yet another mechanism—dielectronic recombination—outweighs radiative recombination).

The ionization balance is thus determined by photoionizations and radiative recombination; to establish the equilibrium the numbers of ionizations and recombinations are equal: $n_i R_{ik} = n_k R_{ki} = n_i^* R_{ik}^*$ where the last equality follows by a detailed-balance argument. Hence for the ground state,

$$\begin{aligned} (n_{0j}^*/n_{0j}) &= 4\pi W \int_{v_0}^{\infty} (hv)^{-1} \alpha_v B_v(T_R) dv / 4\pi \int_{v_0}^{\infty} (hv)^{-1} \alpha_v B_v(T_e) dv \\ &= W \int_{hv_0/kT_R}^{\infty} e^{-x} x^{-1} dx / \int_{hv_0/kT_e}^{\infty} e^{-x} x^{-1} dx \\ &= WE_1(hv_0/kT_R)/E_1(hv_0/kT_e) \\ &\approx W(T_R/T_e)[\exp(-hv_0/kT_R)/\exp(-hv_0/kT_e)] \end{aligned} \quad (5-45)$$

where we have again used hydrogenic cross-sections. If we substitute for n_{0j}^* from the Saha equation (5-13) we may obtain the approximate ionization equation

$$\begin{aligned} (n_e n_{0,j+1} / n_{0,j}) \\ = W \cdot (2g_{0,j+1}/g_{0,j})(2\pi m k T_R/h^2)^{\frac{1}{2}} \cdot (T_e/T_R)^{\frac{1}{2}} \cdot \exp(-\chi_{ij}/kT_R) \end{aligned} \quad (5-46)$$

which has been extensively applied—e.g., in analyses of gaseous nebulae.

To analyze the ionization balance in stellar atmospheres we now must decide (a) how to choose J_v , and (b) which levels dominate. Böhm suggested comparing the values of $4\pi \int (hv)^{-1} \kappa_v J_v dv$ with $4\pi \int (hv)^{-1} \kappa_v B_v dv$, where κ_v is the total opacity from all overlapping continua and J_v is the mean intensity obtained from LTE model-atmosphere calculations. If these numbers are equal the claim is made that LTE is self consistent. Böhm examines the Fe I \leftrightarrow Fe II equilibrium in a model solar atmosphere and finds that the rates mentioned above have a ratio of 2.9 at $\bar{\tau} = 0.01$, 1.3 at $\bar{\tau} = 0.05$, and essentially unity at $\bar{\tau} \geq 0.1$; from this one is tempted to conclude that the Saha ionization formula is valid below $\bar{\tau} = 0.1$.

There are, however, flaws in this argument. First, it is clear that integrated rates summed over all continua of an atom may be subject to cancellations

and compensations, and it is not at all clear what a given departure between the two integrals implies for any particular level (i.e., some levels may be overpopulated and others underpopulated and the integrals could balance). Second, and far more important, the reasoning is circular if from the outset we use B_v as S_v to calculate J_v , for we know that

$$J_v(\tau_v) = \Lambda_{\tau_v} [B_v(\tau_v)] = B_v(\tau_v) + 0(e^{-\tau_v})$$

i.e., J_v is forced to B_v at $\tau_v \geq 1$, and the two integrals automatically become equal artificially.

As we shall show below (cf. §7-5 and Chapters 11 and 12) the characteristic feature of non-LTE transfer is that the source function contains a dominant *scattering term* that is only weakly coupled to local thermal parameters. In such cases, S_v may differ greatly from B_v over *large* ranges of optical depth (essentially to the depth from which a photon cannot escape without being thermalized despite the high probability of scattering and low probability of destruction). Furthermore, if we attempt to find S_v by starting with B_v , computing J_v , using this to re-evaluate S_v and iterating, it is found (cf. §6-1) that the convergence rate is *extremely slow*; with a single iteration one inevitably obtains an estimate of S_v that is very close to LTE, but that is *false*. Further iterations (perhaps thousands!) are required to propagate information about the existence of a boundary to the deeper layers by the inefficient iteration procedure; each iteration will show a continuing, progressive departure from LTE, and when strict consistency between S_v and J_v is obtained, the departures are much larger and extend far deeper than the first iteration indicates. In short, experience has shown that estimates of the kind outlined above, based upon a single iteration away from LTE are worthless. The fact that the seemingly plausible arguments based on such estimates are false was not realized in much of the classical work on stellar atmospheres, and erroneous conclusions about the validity of LTE were drawn; we shall return to this crucially important point in Chapters 7, 11, and 12—further discussion has also been given by Thomas (626, 141–147).

In summary, we have shown that in the ionization process radiative rates dominate collisional, and given the nonequilibrium character of the radiation field we must expect that LTE will *not* be valid, and therefore from the outset we must perform a simultaneous solution of both the statistical equilibrium and transfer equations. Only when a strictly self-consistent solution is obtained is it possible to decide in which regions LTE actually prevails.

THE EXCITATION EQUILIBRIUM

As in the case of ionizations, we again ask whether any particular transition is dominated by collisional or radiative processes. The radiative excitation rate is given by $B_{ij} \int \phi_v J_v dv$, which we shall estimate by replacing

TABLE 5-2
Ratio of Collisional to Radiative Excitation Rates

Star	$\lambda(\text{\AA}) = 3000$	4000	5000	6000	7000	8000	9000
Sun	0.003	0.007	0.017	0.035	0.061	0.099	0.15
O-Star	0.19	0.44	0.85	1.4	2.2	3.1	4.2

SOURCE: K. H. Böhm, in *Stellar Atmospheres*, ed. J. L. Greenstein, Chicago: University of Chicago Press, 1960, by permission.

J_v with WB_v . We again use equation (5-43) to calculate the collision rate with f_c replaced by $f_{ij} = B_{ij}hvmc/4\pi^2e^2$. We then find

$$\frac{C_{ij}}{R_{ij}} = \left[\frac{3e^2 m^{\frac{1}{2}} \lambda^3}{2h(2\pi^3 kT)^{\frac{1}{2}}} \right] \left(\frac{n_e}{W} \right) E_2(x)(e^x - 1) \quad (5-47)$$

where $x \equiv hv_{ij}/kT$. Böhm estimates this ratio for typical conditions in the solar atmosphere and the atmosphere of an O-star (using $W \equiv 1$) and obtains the results shown in Table 5-2. We see that the radiative rates dominate except in the red and infrared of hot stars. The same remarks made above about the non-Planckian nature of the radiation field apply (even more strongly!) in the lines; hence again we conclude that the statistical equilibrium and transfer equations must be solved self-consistently. One might be tempted to conclude that LTE must prevail in the long-wavelength line spectrum on the basis of the dominance of collision rates. But as we shall see in §12-4 this is not true, and, in fact, these lines often show the largest effects of departures from LTE!

5-4 The Non-LTE Rate Equations

Let us now consider the *equations of statistical equilibrium* (or *rate equations*) by which we calculate the actual occupation numbers of bound and free states of atoms in stellar atmospheres. We shall make the simplifying assumption of *complete redistribution* in the lines (i.e., the emission and absorption profiles are taken to be identical); the equations developed on this basis will be used in our discussion of line formation through Chapter 12, and consideration of partial redistribution effects will be deferred until Chapter 13.

GENERAL FORM

Consider a volume element in a moving medium. The number density of particles of a given (bound or free) state i of chemical species k will change in time according to the *net flux* of particles through the volume and the

net rate at which particles are brought from other states, j , by radiative and collisional processes; that is,

$$(\partial n_{ik}/\partial t) = -\nabla \cdot (n_{ik}\mathbf{v}) + \sum_{j \neq i} (n_{jk}P_{ji} - n_{ik}P_{ij}) \quad (5-48)$$

Here P_{ij} denotes the total rate from level i to j . The first term on the right-hand side can be shown, by use of the divergence theorem, to be the net number of particles streaming into and out of the unit volume. If we sum over all states of species k and write $N_k = \sum_i n_{ik}$, then we have a *continuity equation* for this species

$$(\partial N_k/\partial t) + \nabla \cdot (N_k\mathbf{v}) = 0 \quad (5-49)$$

Multiplying equation (5-49) by m_k , the mass of species k , and summing over all chemical species we obtain the standard hydrodynamical continuity equation

$$(\partial \rho/\partial t) + \nabla \cdot (\rho\mathbf{v}) = 0 \quad (5-50)$$

where $\rho = \sum_k m_k N_k$. For a *steady state*, equation (5-48) simplifies to

$$n_{ik} \sum_{j \neq i} P_{ij} - \sum_{j \neq i} n_{jk}P_{ji} = -\nabla \cdot (n_{ik}\mathbf{v}) \quad (5-51)$$

and for a *static atmosphere* we have (suppressing the subscript k)

$$n_i \sum_{j \neq i} P_{ij} - \sum_{j \neq i} n_j P_{ji} = 0 \quad (5-52)$$

As we consider only static media through Chapter 13, we shall deal almost exclusively with equation (5-52). We shall show how to handle moving media in Chapter 14, and will mention some implications of the righthand side of equation (5-51) in Chapter 15. The total rate P_{ij} in general contains both radiative and collisional terms; let us now write these out in detail.

RADIATIVE RATES

(a) *Bound-Bound Transitions*. We shall develop two notations (which have *identical* physical content) by writing bound-bound rates in terms of Einstein transition probabilities or in terms of energy-absorption cross-sections; the former is useful for analytical manipulation with simplified atomic models, while the latter allows bound-bound and bound-free rates to be written in an identical form well-adapted to model-atmosphere computation. Consider transitions from bound level i to a higher bound level j , in a line with absorption (and emission) profile ϕ_v . The number of transitions produced by incident intensity I_v in the frequency interval dv and solid angle $d\omega$ is $n_i B_{ij} \phi_v I_v dv d\omega/4\pi$ or $n_i (\alpha_{ij}/hv) \phi_v I_v dv d\omega$. In a *static* medium, ϕ_v is

isotropic, so integrating over all angles and frequencies we have the *number of absorptions* in the line

$$\begin{aligned} n_i R_{ji} &= n_i B_{ij} \int \phi_v J_v dv \equiv n_i B_{ij} J_{ij} = n_i 4\pi \alpha_{ij} J_{ij}/hv_{ij} \\ &= n_i 4\pi \int \alpha_{ij}(v)(hv)^{-1} J_v dv \end{aligned} \quad (5-53)$$

In *moving* media (Chapter 14) we may consider either the *comoving frame*, in which case equation (5-53) remains valid if J_v is the mean intensity as measured by an observer at rest with respect to the moving fluid, or the *observer's frame*, in which case ϕ_v now has an angular dependence, and a double integration over angles and frequencies must be carried out explicitly. Similar remarks apply to other radiative rates given below.

The number of *stimulated emissions* is

$$n_j B_{ji} \int \phi_v J_v dv = n_j B_{ji} J_{ij} = n_j (g_i B_{ij}/g_j) J_{ij} = n_j (4\pi/hv_{ij})(g_i \alpha_{ij}/g_j) J_{ij} \quad (5-54)$$

The *number of spontaneous emissions* is

$$n_j A_{ji} \int \phi_v dv = n_j (2hv_{ij}^3/c^2) B_{ji} = n_j (2hv_{ij}^3/c^2) (4\pi/hv_{ij})(g_i \alpha_{ij}/g_j) \quad (5-55)$$

The *total downward rate* is the sum of the spontaneous and stimulated rates:

$$n_j R'_{ji} = n_j (A_{ji} + B_{ji} J_{ij}) = n_j (4\pi/hv_{ij})(g_i \alpha_{ij}/g_j) [(2hv_{ij}^3/c^2) + J_{ij}] \quad (5-56)$$

A prime has been added to R'_{ji} so as to reserve the unadorned symbol for a different use below. We may rewrite equation (5-56) by factoring out the term $(n_i/n_j)^* = g_i \exp(hv_{ij}/kT)/g_j$ from the righthand side, and express the total downward rate as

$$n_j R'_{ji} \equiv n_j \left(\frac{n_i}{n_j} \right)^* R_{ji} = n_j \left(\frac{n_i}{n_j} \right)^* \left[4\pi \int \frac{\alpha_{ij}(v)}{hv} \left(\frac{2hv^3}{c^2} + J_v \right) e^{-hv/kT} dv \right] \quad (5-57)$$

At first sight equation (5-57) appears very cumbersome, for clearly the terms $(hv)^{-1}$, v^3 , and $\exp(-hv/kT)$ can all be taken outside the integral owing to the swift decrease of ϕ_v away from v_{ij} . We have written the downward rate in this particular way because it is then of exactly the same form as the downward rate in the continuum; moreover, the downward collision rates will also have a factor of $(n_i/n_j)^*$ appearing explicitly. In the end we achieve notational economy in the full rate equations by using equation (5-57) rather than the simpler Einstein probability form.

Finally, it is sometimes useful to work with the *net rate* from level j to level i ,

$$n_j (A_{ji} + B_{ji} J_{ij}) - n_i B_{ij} J_{ij} \equiv n_j A_{ji} Z_{ji} \quad (5-58)$$

where the term Z_{ji} is called the *net radiative bracket* (NRB). Net radiative brackets are useful notational devices that we shall employ in Chapters 11 and 12. Further, Z_{ji} can be rewritten as

$$Z_{ji} = 1 - J_{ij}(n_i B_{ij} - n_j B_{ji})/(n_j A_{ji}) \equiv 1 - (J_{ij}/S_{ij}) \quad (5-59)$$

where S_{ij} is the frequency-independent line source function. Because the NRB contains only the ratio of J to S , it is often true that it is known to much higher accuracy in an iterative procedure than either S or J themselves. Under favorable conditions, use of NRB's can significantly enhance the convergence of certain types of solutions of multilevel line-formation problems. If a particular line $i \rightarrow j$ is in *radiative detailed balance*, then $Z_{ji} \equiv 0$, and we may cancel the corresponding terms out of the rate equations *analytically* (i.e., omit R_{ij} and R_{ji}); this situation occurs when a particular line thermalizes, and the cancellation procedure is of great use in simplifying the rate equations (cf. §7-5).

(b) *Bound-Free Transitions.* Let us now calculate the radiative rates from a bound level i to the continuum κ . Let $\alpha_{ik}(v)$ be the photoionization cross-section at frequency v ; then the number of photoionizations is calculated by dividing the energy absorbed in interval dv by the appropriate photon energy hv , and summing over all frequencies. Thus the *number of photoionizations* is

$$n_i R_{ik} = n_i 4\pi \int_{v_0}^{\infty} \alpha_{ik}(v)(hv)^{-1} J_v dv \quad (5-60)$$

We may calculate the *number of spontaneous recombinations* by use of a detailed-balancing argument. In *thermodynamic equilibrium*, the number of spontaneous recombinations must equal the number of photoionizations calculated from equation (5-60) when (a) J_v has its equilibrium value (i.e., B_v) and (b) we correct for stimulated emissions at the T.E. value by multiplying by a factor of $(1 - e^{-hv/kT})$ (c.f. §4-3). Thus if n_κ denotes the ion density,

$$(n_\kappa R'_{ki})_{\text{spont}}^* = n_i^* 4\pi \int_{v_0}^{\infty} \alpha_{ik}(v)(hv)^{-1} B_v (1 - e^{-hv/kT}) dv \quad (5-61)$$

The recombination process is a collisional process involving electrons and ions, and therefore is proportional to $n_\kappa \cdot n_e$. For a given electron density and a given T_e , which by definition describes the electron velocity distribution, the rate just calculated above must still apply *per ion*, even out of T.E. Hence to obtain the non-LTE spontaneous recombination rate we need correct equation (5-61) only by using the actual ion density n_κ . Then

$$\begin{aligned} (n_\kappa R'_{ki})_{\text{spont}} &= n_\kappa (n_i/n_\kappa)^* \cdot 4\pi \int_{v_0}^{\infty} \alpha_{ik}(v)(hv)^{-1} B_v (1 - e^{-hv/kT}) dv \\ &= n_\kappa (n_i/n_\kappa)^* 4\pi \int_{v_0}^{\infty} \alpha_{ik}(v)(hv)^{-1} (2hv^3/c^2) e^{-hv/kT} dv \end{aligned} \quad (5-62)$$

Recall from equation (5-14) that $(n_i/n_\kappa)^* = n_e \Phi_{ik}(T)$, which shows that the spontaneous recombination rate depends on the product of the electron and ion densities and a function of the temperature (which itself depends on atomic properties through the cross-section).

The number of stimulated recombinations may be calculated by a similar procedure; in T.E.,

$$(n_\kappa R'_{ki})_{\text{stim}} = n_i^* \cdot 4\pi \int_{v_0}^{\infty} \alpha_{ik}(v)(hv)^{-1} B_v e^{-hv/kT} dv \quad (5-63)$$

To generalize this result for the non-LTE case, we (a) replace the equilibrium radiation field B_v by the actual value J_v , and (b) use the actual ion density n_κ :

$$(n_\kappa R'_{ki})_{\text{stim}} = n_\kappa (n_i/n_\kappa)^* 4\pi \int_{v_0}^{\infty} \alpha_{ik}(v)(hv)^{-1} J_v e^{-hv/kT} dv \quad (5-64)$$

The total number of recombinations is, therefore,

$$\begin{aligned} n_\kappa (R'_{ki, \text{spont}} + R'_{ki, \text{stim}}) &\equiv n_\kappa (n_i/n_\kappa)^* R_{ki} \\ &= n_\kappa \left(\frac{n_i}{n_\kappa} \right)^* 4\pi \int_{v_0}^{\infty} \frac{\alpha_{ik}(v)}{hv} \left(\frac{2hv^3}{c^2} + J_v \right) e^{-hv/kT} dv \end{aligned} \quad (5-65)$$

The number of recombinations is sometimes expressed in terms of a *recombination coefficient* $\alpha_{RR}(T)$ defined such that total recombination rate as given by equation (5-65) is $n_\kappa n_e \alpha_{RR}(T)$.

By comparison of equations (5-53) and (5-60) we see that in writing complete rate equations we can systematize our notation and write *all upward radiative rates* ($i \rightarrow j$), *for j bound or free*, as $n_i R_{ij}$ where

$$R_{ij} \equiv 4\pi \int_{v_0}^{\infty} \alpha_{ij}(v)(hv)^{-1} J_v dv \quad (5-66)$$

and, by comparison of equations (5-57) and (5-65), *all downward radiative rates* ($j \rightarrow i$) as $n_j (n_i/n_j)^* R_{ji}$ where

$$R_{ji} \equiv 4\pi \int_{v_0}^{\infty} \alpha_{ij}(v)(hv)^{-1} [(2hv^3/c^2) + J_v] e^{-hv/kT} dv \quad (5-67)$$

Note that in equilibrium, $R_{ij}^* = R_{ji}^*$.

COLLISIONAL RATES

The gas in stellar atmospheres is a plasma consisting of atoms, ions, and electrons, among which a wide variety of collisions may occur and produce excitations and ionizations. In cool stars, where the material is primarily

neutral, collisions with neutral hydrogen atoms are numerous and important. As the material becomes appreciably ionized, however, collisions with charged particles predominate owing to the long-range nature of Coulomb interactions. Moreover, because the collision frequency is proportional to the flux of impinging particles, and hence to their velocity, we normally need to consider only collisions with electrons, for in thermal equilibrium their velocities are a factor of $(m_H A/m_e)^{1/2} \approx 43A^{1/2}$ larger than those of ions of atomic weight A .

If we denote the cross-section for producing the transition ($i \rightarrow j$) (where j may be bound or free) by collisions with electrons of velocity v as $\sigma_{ij}(v)$, then the total number of transitions is

$$n_i C_{ij} = n_i n_e \int_{v_0}^{\infty} \sigma_{ij}(v) f(v) v dv \equiv n_i n_e q_{ij}(T) \quad (5-68)$$

where v_0 is the velocity corresponding to E_0 , the threshold energy of the process—i.e., $\frac{1}{2}m_e v_0^2 = E_0$. The downward rate ($j \rightarrow i$) can be obtained immediately on the basis of detailed-balancing arguments, for the electron velocity distribution is the equilibrium (i.e., Maxwellian) function; thus we must have

$$n_i^* C_{ij} \equiv n_j^* C_{ji} \quad (5-69)$$

from which it follows that the number of downward transitions is

$$n_j C_{ji} = n_j (n_i/n_j)^* C_{ij} = n_j (n_i/n_j)^* n_e q_{ij}(T) \quad (5-70)$$

As was the case for radiative transitions, it is sometimes useful to introduce the *net collisional bracket* Y_{ij} and write the net rate for collisions $i \rightarrow j$ ($E_i < E_j$) as

$$n_i C_{ij} Y_{ij} \equiv n_i C_{ij} - n_j C_{ji} = n_i C_{ij} [1 - (n_j/n_j^*)(n_i^*/n_i)] \quad (5-71)$$

The actual cross-sections σ_{ij} required to compute rates are found either experimentally or by rather complicated quantum-mechanical calculations; it would take us too far afield to describe these methods here, so we merely refer the interested reader to (410). There exists a vast literature containing results (theoretical and experimental) for a variety of transitions of astrophysical interest; bibliographies of this literature are issued from time to time by the Information Center of the Joint Institute for Laboratory Astrophysics of the University of Colorado and the National Bureau of Standards. (This center also maintains current literature references in an on-line computer.) As indicated by equation (5-68) we are more directly interested in rates for a given cross-section, so let us examine q_{ij} in a bit more detail. Usually cross-sections are measured in units of πa_0^2 , where a_0 is the Bohr radius; i.e., we write $\sigma_{ij} = \pi a_0^2 Q_{ij}$. Also, Q_{ij} is usually tabulated in terms of the energy of the exciting particle, so writing $\frac{1}{2}mv^2 = E$, and substituting

equation (5-2) into (5-68), we find

$$q_{ij}(T) = C_0 T^{\frac{1}{2}} \int_{u_0}^{\infty} Q_{ij}(ukT) u e^{-u} du \quad (5-72)$$

where $u \equiv E/kT$, and $C_0 = \pi a_0^2 (8k/m\pi)^{\frac{1}{2}} = 5.5 \times 10^{-11}$. Writing $x = (u - u_0)$, where $u_0 = E_0/kT$, we obtain

$$q_{ij}(T) = C_0 T^{\frac{1}{2}} \exp(-E_0/kT) \Gamma_{ij}(T) \quad (5-73)$$

$$\text{where } \Gamma_{ij}(T) \equiv \int_0^{\infty} Q_{ij}(E_0 + xkT)(x + u_0)e^{-x} dx \quad (5-74)$$

Exercise 5-5: Verify equations (5-72) through (5-74).

The advantage of writing the collision rate as in equation (5-73) is that the principal sensitivity to the temperature has been factored out in the product $T^{\frac{1}{2}} \exp(-E_0/kT)$ while $\Gamma_{ij}(T)$ is a slowly-varying function of T .

Of course the main problem in application is to obtain reliable values of Q_{ij} . A characteristic difficulty for astrophysical work is that for many transitions of interest, $kT \ll E_0$, so that the rate depends extremely sensitively upon values of Q_{ij} near threshold. Unfortunately, for $E \approx E_0$ a great computational effort is required to obtain accurate cross-sections because the simplifying approximations that are valid for $E \gg E_0$ break down, and because complicated variations of Q_{ij} result from resonances in the collision process. When values for Q_{ij} can be obtained, one typically fits them by numerical procedures to simple analytical approximants, against which the integration in equation (5-74) can be performed analytically.

For the astrophysically important spectra of H, He I, and He II, accurate experimental cross-sections exist for excitation and ionization from the ground state. For transitions arising from excited states one must rely upon theoretical calculations. For many atoms and ions of interest there may be no detailed estimates whatever available, and one must have recourse to rough methods to estimate rates. A very useful (though quite approximate) expression for excitation rates in radiatively permitted transitions can be written (639) in terms of the oscillator strength f_{ij} , namely

$$C_{ij} = C_0 n_e T^{\frac{1}{2}} [14.5 f_{ij} (I_H/E_0)^2] u_0 \exp(-u_0) \Gamma_e(u_0) \quad (5-75)$$

where $u_0 \equiv E_0/kT$, I_H is the ionization energy of hydrogen, and for ions

$$\Gamma_e(u_0) \equiv \max[\bar{g}, 0.276 \exp(u_0) E_1(u_0)] \quad (5-76)$$

The parameter \bar{g} is about 0.7 for transitions of the form $nl \rightarrow nl'$, and about 0.2 for transitions of the form $nl \rightarrow n'l'$, $n' \neq n$ (95). For neutral atoms $\Gamma_e(u_0)$ has a different form [see (47)]. It is worth stressing that equations

(5-75) and (5-76) provide, at best, *rough* values and should be applied with caution. In particular, collisions are *not* restricted by the dipole transition selection rules $\Delta l = \pm 1$, and cross-sections for other values of Δl may be as large as for $\Delta l = \pm 1$ despite f_{ij} being zero in the dipole approximation. For collisional ionizations there exists a semi-empirical formula (402)

$$\sigma_{ik}(E) = \pi a_0^2 [2.5\zeta(I_H/E_0)^2] \ln(E/E_0) \{1 - b \exp[-c(E - E_0)/E_0]\} / (E/E_0) \quad (5-77)$$

which yields a rate

$$C_{ik} = C_0 n_e T^4 [2.5\zeta(I_H/E_0)^2] u_0 [E_1(u_0) - b e^c u_0 E_1(u_1)/u_1] \quad (5-78)$$

where ζ , b , and c are empirical quantities fitted to individual atoms, and $u_1 \equiv u_0 + c$. An alternative approximate formula can be obtained by expressing the collisional ionization cross-section in terms of the photoionization cross-section (73, 374) which yields a rate (334, 121)

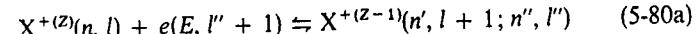
$$C_{ik} = 1.55 \times 10^{13} n_e T^{-4} \bar{g}_i \alpha(v_0) \exp(-u_0)/u_0 \quad (5-79)$$

where $\alpha(v_0)$ is the threshold photoionization cross-section, and \bar{g}_i is of order 0.1, 0.2, and 0.3 for $Z = 1, 2$, and > 2 , respectively (here Z is the charge on the ion). The same caveats expressed about equation (5-75) apply to equations (5-78) and (5-79) as well.

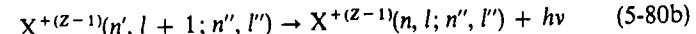
AUTOIONIZATION AND DIELECTRONIC RECOMBINATION

In complex atoms with several electrons, the ionization potential is determined by the *lowest* energy to which a sequence of bound states with only *one* excited electron converge (to the *ground state* of the ion plus a free electron). If two electrons are excited within the atom, they will, in general, give rise to states with energies both below and above the ionization potential defined above. Subject to certain selection rules [(172, 371; 297, 173)] the states above the ionization limit may *autoionize* to the ground state of the ion plus a free electron. The inverse process is also possible and, if an ion in the ground state suffers a collision with an electron of sufficiently great energy, then a doubly excited state of the atom may be formed. In general, this process will be of little interest because the compound state will immediately autoionize again (typical autoionization transition probabilities A_a are in the range 10^{13} – 10^{14} !), and its equilibrium population will be small. In some cases, however, a stabilizing transition occurs in which one of the two excited electrons (usually the one in the lower quantum level) decays radiatively to the lowest available quantum state, leaving a bound atom with a single excited electron. This process can provide an efficient recombination mechanism referred to as *dielectronic recombination*.

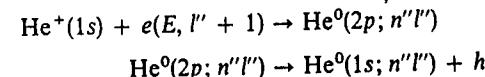
In particular, for an ion of chemical species X and charge Z , we consider processes of the type



followed by the stabilizing transition



which leaves the ion ($Z - 1$) in a bound excited state. As an example, for He^+ we might have



If we denote the doubly excited state by d , the final bound state of the ion ($Z - 1$) by b , and the ground state of the ion Z as κ , then the number of dielectronic recombinations to state b from d can be written as $n_\kappa R_{db} = n_d A_s$, where A_s is the spontaneous transition probability for the stabilizing emission; to a good approximation (particularly for large n'') $A_s = A(n', l + 1; n, l)$ for the Z ion. In the limit of low radiation fields, the reverse process in equation (5-80b) can be ignored, and if A_a measures the transition probability for *autoionization*, n_d can be written (73, 258) in terms of its equilibrium population n_d^*

$$n_d = n_d^* A_a / (A_a + A_s) \quad (5-81)$$

$$\text{where } n_d^* = n_\kappa n_e (g_d/g_\kappa) C_1 T^{-3} \exp(-\chi_{d\kappa}/kT) \equiv n_\kappa n_e \Phi_{kd}(T) \quad (5-82)$$

Here $\chi_{d\kappa}$ is the energy of state d above the ionization limit.

Exercise 5-6: Derive equation (5-82) by applying the Saha equation (5-14) between the continuum κ and bound state b , and the Boltzmann equation (5-5) between states b and d .

Thus from *each* state d to *each* state b we have the number of dielectronic recombinations

$$n_\kappa R_{db} = n_\kappa n_e \Phi_{kd}(T) A_s A_a / (A_s + A_a) \quad (5-83)$$

As in the case of radiative recombinations, it is often useful to define a dielectronic recombination coefficient α_{DR} such that $n_\kappa R_{db} = n_\kappa n_e \alpha_{DR}$. Note that the ratio of numbers of dielectronic to radiative recombinations depends only on the ratio α_{DR}/α_{RR} , and hence is independent of density and is a function of temperature only.

Dielectronic recombination plays an important role in stellar atmospheres in two contexts. First, we can calculate a *total* rate for dielectronic recombination by summing over all states (n, l) and (n', l') ; as was shown in a classic paper by Burgess (118), this process becomes extremely important at high temperatures. For example, at temperatures $T \gtrsim 10^6$ °K, the dielectronic recombination rate for He^+ exceeds the radiative recombination rate by a factor of 10^2 but drops below radiative recombination for $T \lesssim 10^5$ °K. Burgess convincingly demonstrated that dielectronic recombination is the dominant recombination process in the solar corona (where $T \approx 2 \times 10^6$ °K and $n_e \sim 10^8$), and that *this mechanism establishes the coronal ionization balance*. In calculations for the total rate one must sum over vast numbers of states, and the most important contributions come from states with $n'' \gg n'$ and $l'' \gg l + 1$. It is because these high states have large values of χ_{dk} that high temperatures are required to overcome the exponential factor in equation (5-82) and produce significant dielectronic recombination [i.e., a large value of kT is required for the electrons to have sufficient energy for the reaction in equation (5-80a) to occur]. In the sum one encounters a divergence problem at large n'' , similar to that found for partition functions, unless one includes both probabilities A_s and A_a in equation (5-83) and takes into account the fact that A_s will dominate A_a for sufficiently large n'' . The calculations of total rates require the estimation of large numbers of stabilization transition probabilities and collision cross-sections (to calculate A_a by detailed balancing arguments), and are at best difficult; an approximate general formula that provides tolerably accurate values for most ions of interest has been developed (119).

A further study (121) has shown that in the corona the effects of inverse transitions in equation (5-80b) produced by incident photospheric radiation are small, and that the doubly excited states can be destroyed by collisional ionization if densities are sufficiently high, from which one concludes that dielectronic recombination does not play an important role in the deeper layers of the atmosphere (e.g., in the solar chromosphere and photosphere).

A second situation where dielectronic recombinations are important arises for some ions (e.g., C III and N III) that have *low-lying* double-excitation states ($\chi_{dk} < kT$) that feed free electrons into selected bound states. A striking example is afforded by the $2s2p(^1P^0)$ $3d$ state of N III, which lies only 1.6 eV above the ionization potential to N IV $2s^2$ 1S , and which feeds electrons directly into the N III $2s^2$ $3d$ levels and thereby produces the famous N III $\lambda 4634-40$ ($3d \rightarrow 3p$) emission lines in O-type stars (115; 429; 440). In such cases one finds that $A_a \gg A_s$, so that n_d is given by its equilibrium value (relative to *actual* ion densities), equation (5-82); furthermore one need sum over only a few states. On the other hand, these processes occur deep enough in the atmosphere that one must account for the inverse transitions

produced by the radiation field in the stabilizing transition. If state d is characterized as (n', l', L') and state b as (n, l, L) we have the total dielectronic recombination rate

$$n_\kappa R_{db} = n_\kappa n_e \sum_{n', l', L', L} \Phi_{n'l'L'}(T) A(n', l', L'; n, l, L) [1 + (2hv^3/c^2)^{-1} J_{n'l'L'}] \quad (5-84)$$

where J is the mean intensity in the stabilizing transition. Often the double excitation state is so broad (because of the very short lifetime against autoionization) that the radiation field used to compute J can be fixed at the continuum value. If the L' dependence of $\chi_{n', l', L'}$ is small, then one can define $A^*(n', l'; n, l) \equiv g_{l'}^{-1} \sum_{L', L} g(L') A(n', l, L'; n, l, L)$ and replace $\Phi_{n'l'L'}$ with $\Phi_{n'l'}$ to obtain

$$n_\kappa R_{db} = n_\kappa n_e \sum_{n', l'} \Phi_{n'l'}(T) A^*(n', l'; n, l) [1 + (2hv^3/c^2)^{-1} J_{n'l'}] \quad (5-85)$$

while the inverse (upward) rate $b \rightarrow d$ becomes

$$n_b R_{bd} = n_b \sum_{n', l'} B^*(n, l; n', l') J_{n'l'} \quad (5-86)$$

where $B^*(n, l; n', l') \equiv A^*(n', l'; n, l) (g_{l'} c^2 / 2hv^3 g_l)$.

COMPLETE RATE EQUATIONS

Having examined all of the processes of interest, we may now assemble the individual rates into a single complete equation of the form of equation (5-52) for each bound state i of each ionization stage of each chemical species in the material. We shall (a) ignore explicit mention of dielectronic recombination because the rate has the same form as for radiative recombination, and we shall assume that both are included; and (b) assume that all ionizations from bound states of ion j go to the ground state only of ion $j + 1$ (generalization is easy but complicates the notation and discussion). We then may write

$$-\sum_{i'' < i} n_{i''} (R_{i''i} + C_{i''i}) + n_i \left[\sum_{i'' < i} (n_{i''}/n_i)^* (R_{ii''} + C_{i''i}) + \sum_{i' > i} (R_{ii'} + C_{ii'}) \right] \\ - \sum_{i' > i} n_{i'} (n_i/n_{i'})^* (R_{i'i} + C_{ii'}) = 0 \quad (5-87)$$

where the radiative rates are defined by equations (5-66) and (5-67), the collision rates by equation (5-68), and the LTE population ratios by equations (5-5) and (5-14) for bound states, and bound and free states, respectively. One such equation may be written for each bound state. We have one more variable (the ion density n_k) than we have equations. If we wrote down an ionization equation

$$\sum_{i < k} n_i (R_{ik} + C_{ik}) - n_k \sum_{i < k} (n_i/n_k) * (R_{ki} + C_{ki}) = 0 \quad (5-88)$$

we would find it to be *redundant* with the set (5-87).

Exercise 5-7: Show that equation (5-88) results from summing equation (5-87) over all bound states.

We therefore invoke an additional physical constraint to complete the system. For an impurity species (i.e., $\alpha_k/\alpha_H \ll 1$), we close the system by demanding that the total number of atoms and ions (of all kinds) of the species equal the correct fraction of the number of all hydrogen atoms (including protons); i.e.,

$$\sum_{i,j,k} n_{ijk} - (\alpha_k/\alpha_H) \left(\sum_i n_{i,H} + n_p \right) = 0 \quad (5-89)$$

Alternatively, we can close the system by invoking charge conservation (saving the total number conservation for use elsewhere) and write

$$\sum_k \sum_j j N_{jk} + n_p = n_e \quad (5-90)$$

where $N_{jk} = \sum_i n_{ijk}$. The final system, for all levels of all ions of all species is written in the general form

$$\mathcal{A}\mathbf{n} = \mathcal{B} \quad (5-91)$$

where \mathbf{n} denotes a vector that lists *all* occupation numbers (say \mathcal{N} of them) while \mathcal{A} is an $(\mathcal{N} \times \mathcal{N})$ matrix and \mathcal{B} is a vector in which only one element is nonzero [from equation (5-89) or (5-90)].

To make these considerations more definite, let us consider a case that is simple enough to be manageable and complicated enough to be of general applicability. Suppose we have an atmosphere composed entirely of hydrogen and helium (of abundance Y , by number, relative to hydrogen). We consider the helium to consist of a ladder of three ionization stages, He^0 , He^+ , and He^{++} , and we suppose that these ions have L_0 , L_+ , and 1 levels respectively. Further we write $M_{\text{He}} = L_0 + L_+ + 1$; i.e., M_{He} is the total number of helium states of all kinds. Similarly we consider L_{H} bound states

of hydrogen, yielding $M_{\text{H}} = L_{\text{H}} + 1$ states in all (including protons). Then, using X 's to denote nonzero elements, the rate matrix \mathcal{A} has the form

Row Number						
1	x x . . . x	x	0			0
2	x x
3
4
L_0	x x . . . x	x	0			0
$L_0 + 1$.	x x . . . x	x			0
.	.	x x
$L_0 + L_+$.	.	.			0
M_{He}	1 1 . . . 1	1 1 . . . 1	1	-y -y . . . -y	-y	
$M_{\text{He}} + 1$.	0	x x . . . x	x	x	
.	.	x x . . .	x	x	x	.
$M_{\text{He}} + L_{\text{H}}$
$M_{\text{He}} + M_{\text{H}}$	0 . . . 0	1 1 . . . 1	2	0 0 . . . 0	0	1
	1	L_0		M_{He}		$M_{\text{He}} + M_{\text{H}}$
					Column Number	

The first L_0 rows correspond to equation (5-87) for He^0 , the next L_+ rows give equation (5-87) for He^+ , the M_{He} th row gives the abundance equation (5-89), the next L_{H} rows give equation (5-87) for H, and the last row gives charge conservation. The vector \mathbf{n} consists of elements

$$\mathbf{n} = [n_1(\text{He}^0), \dots, n_{L_0}(\text{He}^0), n_1(\text{He}^+), \dots, n_{L_+}(\text{He}^+), n(\text{He}^{++}), n_1(\text{H}), \dots, n_{L_{\text{H}}}(\text{H}), n_p]^T \quad (5-92)$$

and

$$\mathcal{B} = (0, \dots, 0, n_e)^T \quad (5-92)$$

For given values of n_e , T , and the radiation field, equation (5-91) is a *linear system* in \mathbf{n} , and may be solved by standard numerical methods (526, Chapter 9).

5-5 The Non-LTE Equation of State

From the results of the preceding sections, we see that in LTE each occupation number at a specific point in the atmosphere is a function of only *two* thermodynamic variables; i.e., $n_i = n_i(N, T)$ where T is the *absolute* temperature at that point. In contrast, in the non-LTE case, the full rate equations imply that $n_i = n_i(N, T, J_v)$ where J_v denotes the frequency dependence of the radiation field over the entire spectrum and T is now a *kinetic* temperature describing only the particle velocity distribution function. We now have as many new (fundamental!) thermodynamic variables as are required to specify the *distribution* of radiation in frequency. [Note that if we could simplify the description of this distribution—e.g., if we could write $J_v \equiv WB_v(T)$ —then the situation would be vastly simplified; but in general we may need to consider perhaps hundreds of new variables.] As was the case for the LTE equation of state, the non-LTE statistical equilibrium equations are actually nonlinear in the electron density n_e , and we shall require a linearization procedure to solve for the occupation numbers; but now we shall have to extend the linearization to include changes in the radiation field as well. We shall see in §7-5 that this approach provides a method for coupling the transfer equations and statistical equilibrium equations together, and allows us to determine the global response of the gas to the radiation field simultaneously with the reciprocal response of the radiation field to material properties.

Before developing the linearization procedure required in the general case, it is worthwhile to consider a few examples that illustrate clearly the essential physical content of the statistical equilibrium equations.

LIMITING CASES

Consider first an atom consisting of a single bound level that can ionize to its continuum. We then have one rate equation which states that (ignoring stimulated emissions)

$$(n_1/n_1^*) = \left[4\pi \int_{v_0}^{\infty} (\alpha_v B_v/hv) dv + n_e q_{1\kappa} \right] / \left[4\pi \int_{v_0}^{\infty} (\alpha_v J_v/hv) dv + n_e q_{1\kappa} \right] \quad (5-94)$$

We note first that, as the electron density becomes very large, so that collisional rates exceed the radiative rates, then

$$\lim_{n_e \rightarrow \infty} (n_1/n_1^*) = \lim_{n_e \rightarrow \infty} (n_e q_{1\kappa} / n_e q_{1\kappa}) \equiv 1$$

i.e., LTE is recovered. Further, at very large optical depth, $J_v \rightarrow B_v$ and clearly $n_1/n_1^* \rightarrow 1$; i.e., if the radiation field is perfectly Planckian we recover

LTE, as expected. Two comments are necessary here, however. (a) To obtain LTE in a *multilevel* atom J_v must equal B_v in *all* transitions. If *any* transition is transparent, then LTE will *not* be obtained (unless densities are so high that collisions dominate), not only for the particular levels involved in the transition under consideration, but actually for *all* other levels as well because the radiation field in each transition influences the populations of *all* levels (see below). (b) We have left unanswered the question of how large is “*very large*” optical depth. As we have indicated earlier, $\tau_v \gtrsim 1$ is *not* sufficient to guarantee $J_v \rightarrow B_v$. Rather τ_v must exceed a *thermalization depth*, for which precise estimates will be given in Chapters 7 and 11. In the *low-density limit* (e.g., in a nebula), equation (5-94) reduces to

$$(n_1/n_1^*) = \int_{v_0}^{\infty} (\alpha_v B_v/hv) dv / \int_{v_0}^{\infty} (\alpha_v J_v/hv) dv \quad (5-95)$$

which states that, if the recombination rate exceeds the photoionization rate, the level is overpopulated; and it is underpopulated if the reverse is true. Equation (5-95) is, of course, equivalent to equation (5-46) which is often applied in nebular analyses. In the *coronal* case, we have $T_e (\sim 10^6 \text{ K}) \gg T_R (\sim 6000 \text{ K})$, which implies that collisional ionizations exceed radiative [see equation (5-44) and related discussion] while radiative plus dielectronic recombinations, both of which proceed at a rate specified by T_e , exceed collisional recombinations. Then

$$n_1 n_e q_{1\kappa} = n_e n_e (\alpha_{RR} + \alpha_{DR})$$

so that $(n_e/n_1) = q_{1\kappa} / (\alpha_{RR} + \alpha_{DR}) = f(T)$ (5-96)

That is, the coronal ionization balance depends only on temperature and is independent of the electron density, a fact that vastly simplifies analysis of the corona. Both the coronal and nebular situations represent extreme departures from LTE.

Let us now consider some multilevel problems. Suppose we have a volume of pure hydrogen gas illuminated by a very dilute radiation field (i.e., a nebula). We anticipate that virtually all of the hydrogen will be in its ground state, and we assume that all the resonance lines are completely opaque (and hence in detailed balance). Further, we assume that, after an atom is photoionized from the ground state, recombinations occur to *all* states, but the populations of the upper states are so small and the incident radiation field so diluted that (a) we can ignore photoionization out of these states, and (b) electrons in any excited state cascade downward at rates determined by the Einstein coefficients A_{ji} without reabsorption upward (i.e., the subordinate lines are *transparent*). We further assume densities are so low that we

may neglect collisions. Then we have an ionization equation

$$n_1 R_{1\kappa} = n_e^2 \sum_{i=1}^I \alpha_{RR}(i, T) \quad (5-97a)$$

and a number conservation equation

$$\sum_{i=1}^I n_i + n_e = n_H \quad (5-97b)$$

where n_H is the (given) hydrogen density, I is the total number of bound states considered, and $n_e = n_p$ (for pure hydrogen). $R_{1\kappa}$ is assumed given in terms of $J_v = WB_v(T_R)$, as in equation (5-40). For any subordinate state we can calculate the population in terms of the branching ratios $a_{ji} \equiv A_{ji}/\sum_{l < j} A_{jl}$, and the cascade probabilities p_{ji} which are defined recursively as $p_{i+1,i} \equiv a_{i+1,i}$, and $p_{ji} \equiv a_{ji} + \sum_{k=i+1}^{j-1} p_{jk} a_{ki}$ for $(j = i+2, \dots, I)$. Then for level i we find

$$\begin{aligned} n_i \sum_{l < i} A_{il} &= n_e^2 \alpha_{RR}(i, T) + \sum_{j > i}^I A_{ji} n_j \\ &= n_e^2 \left[\alpha_{RR}(i, T) + \sum_{j > i}^I p_{ji} \alpha_{RR}(j, T) \right] \end{aligned} \quad (5-98)$$

Exercise 5-8: (a) Verify the expressions for p_{ji} given above and derive equation (5-98). (HINT: Start with level 1 and work downward.) (b) Show that equations (5-97) and (5-98) yield a quadratic equation in n_e that allows the determination of $n_e(n_H, T)$, and hence all the n_i 's. (c) Show that $p_{j1} = 1$ ($j > 1$); interpret this result physically.

From equation (5-98) we may estimate ratios of occupation numbers, and hence ratios of line intensities along a series. For example we can compute the relative intensities of the Balmer lines (the *Balmer decrement*) as

$$I(H_k)/I(H_J) = (n_k A_{k2} h\nu_{k2})/(n_J A_{J2} h\nu_{J2})$$

and compare the theoretical results with observation. The approach outlined in equations (5-97) and (5-98) (with extensive elaboration and refinement!) forms the basis for the analysis of nebulae [see (15, Chaps. 23–25; 10, Chap. 4; 415, pp. 40–110; and 350, Chaps. 1–3)].

Finally, consider an atom that consists of three states (1, 2, 3) in order of increasing energy in a rarefied medium (neglect collisions) and a dilute radiation field. A famous result regarding such a system is *Rosseland's theorem of cycles*, which states that the number of radiative transitions in the direction $1 \rightarrow 3 \rightarrow 2 \rightarrow 1$ exceeds the number in the inverse direction $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$. A consequence of this result is that energetic photons are systematically

degraded from high energies (say far ultraviolet) to low (visible and infrared); for example, in a nebula, Lyman continuum photons are degraded—e.g., into Balmer continuum photons plus $L\alpha$ photons (state 1 = 1s, state 2 = 2p, state 3 = continuum). We may calculate the ratio $R_{1 \rightarrow 3 \rightarrow 2 \rightarrow 1}/R_{1 \rightarrow 2 \rightarrow 3 \rightarrow 1}$ quite easily. The number of excitations $1 \rightarrow 3$ is $n_1 B_{13} WB(v_{13})$. Of the excited atoms in state 3, a fraction $A_{32}/(A_{32} + A_{31})$ decays to state 2, and of the atoms in state 2 a fraction $A_{21}/[A_{21} + B_{23} WB(v_{23})]$ decays to state 1 (here we have ignored stimulated emission). Thus

$$n_1 R_{1 \rightarrow 3 \rightarrow 2 \rightarrow 1} = \frac{n_1 B_{13} WB(v_{13}) A_{32} A_{21}}{(A_{32} + A_{31})(A_{21} + B_{23} WB(v_{23}))} \quad (5-99)$$

By similar reasoning

$$n_1 R_{1 \rightarrow 2 \rightarrow 3 \rightarrow 1} = \frac{n_1 B_{12} WB(v_{12}) B_{23} WB(v_{23}) A_{31}}{[A_{21} + B_{23} WB(v_{23})](A_{32} + A_{31})} \quad (5-100)$$

so that

$$\begin{aligned} R_{1 \rightarrow 2 \rightarrow 3 \rightarrow 1}/R_{1 \rightarrow 3 \rightarrow 2 \rightarrow 1} \\ = W[B_{12} B(v_{12})/A_{21}][B_{23} B(v_{23})/A_{32}][A_{31}/B_{13} B(v_{13})] \end{aligned} \quad (5-101)$$

But using the relations among the Einstein coefficients and writing B_v in the Wien approximation ($h\nu/kT \gg 1$) one finds $[B_{ij} B(v_{ij})/A_{ji}] = (n_j/n_i)^*$, so equation (5-101) reduces to $R_{1 \rightarrow 2 \rightarrow 3 \rightarrow 1}/R_{1 \rightarrow 3 \rightarrow 2 \rightarrow 1} = W < 1$, which proves the theorem. The result clearly follows from the fact that in the cycle $1 \rightarrow 3 \rightarrow 2 \rightarrow 1$ the dilution factor enters only once, while in the reverse process it enters twice. In stellar atmospheres, Rosseland's theorem is relevant because at certain depths one may have resonance lines that are opaque (i.e., $W = 1$) exciting atoms to upper states, from which the subordinate lines are transparent; in such cases we anticipate a systematic photon degradation.

LINEARIZATION

As mentioned before, the general system $\mathcal{An} = \mathcal{B}$ can be solved as a linear system for n if n_e , T , and J_v are all specified. But, in practice, we do not know exact values for these variables in the course of a model-atmosphere computation (recall the discussion for the LTE equation of state) but have only current estimates in an overall iterative process. We expect all of these variables to change by amounts δn_e , δT , δJ_v , etc. to satisfy better the constraints of energy and pressure balance, and must evaluate the response of n to these changes, in the form

$$\delta n = (\partial n / \partial n_e) \delta n_e + (\partial n / \partial T) \delta T + \sum_{k=1}^K (\partial n / \partial J_k) \delta J_k \quad (5-102)$$

Here $J_k (k = 1, \dots, K)$ is the mean intensity at discrete frequencies that sample the spectrum. These frequencies are chosen such that all integrals over frequency are replaced by *quadrature sums*—i.e.,

$$\int F(v) dv = \sum_{k=1}^K w_k F(v_k) \quad (5-103)$$

We obtain equation (5-102) by linearization of the original equations (5-91) [and also can find parallel linearized equations that give, in essence, $\delta J_k (\delta T, \delta n_e, \delta n)$ from the transfer equations; cf. §7-5]. Equations of the form (5-102) are required in two contexts: (a) model atmosphere calculations where all variables may change in an iteration cycle, and (b) multilevel statistical equilibrium calculations for a *given* model (n_e , T , and total particle density *fixed*). The procedure for case (b) will be deferred until Chapter 12, and we shall consider only case (a) here. [In case (b) one may use a special technique motivated by consideration of the computational methods of solving transfer equations, to be developed in Chapter 6.]

If x denotes any variable, then by linearization of equation (5-91) we have

$$\frac{\partial n}{\partial x} = \mathcal{A}^{-1} \left[\frac{\partial \mathcal{B}}{\partial x} - \left(\frac{\partial \mathcal{A}}{\partial x} \cdot n \right) \right] \quad (5-104)$$

where we have assumed that n is the solution of the *current system* $\mathcal{A}n = \mathcal{B}$ (we might introduce a subscript zero, or some similar device, but it would become unwieldy). An extremely important feature of this approach is that every derivative in equations (5-102) and (5-104) can be written down *analytically* (though the inverse \mathcal{A}^{-1} must be computed numerically); this produces a system of high accuracy and reliability. To illustrate the procedure, we shall write down some representative derivatives for the model atoms discussed at the end of §5-4; more comprehensive collections of formulae are given in (42) and (437). In what follows, we use the auxiliary vector $a \equiv (\partial \mathcal{A} / \partial x) \cdot n$. Suppose we choose some frequency v_k , and wish to calculate $(\partial n / \partial J_k)$. Except for the “special” rows of \mathcal{A} that express abundance and charge conservation, we will generally have

$$(\partial \mathcal{A} / \partial J_k)_{ij} = -4\pi w_k \alpha_{ji}(v_k) / h v_k, \quad (j < i) \quad (5-105a)$$

$$(\partial \mathcal{A} / \partial J_k)_{ii} = (4\pi w_k / h v_k) \left[\sum_{j>i} \alpha_{ij}(v_k) + \sum_{j< i} \alpha_{ji}(v_k) (n_j / n_i)^* e^{-h v_k / kT} \right] \quad (5-105b)$$

and $(\partial \mathcal{A} / \partial J_k)_{ij} = -[4\pi w_k \alpha_{ij}(v_k) / h v_k] (n_i / n_j)^* e^{-h v_k / kT}, \quad (j > i) \quad (5-105c)$

from which we find

$$\begin{aligned} a_i &= [(\partial \mathcal{A} / \partial J_k) \cdot n]_i \\ &= (4\pi w_k / h v_k) \left\{ \sum_{j>i} \alpha_{ij}(v_k) [n_i - n_j (n_i / n_j)^* e^{-h v_k / kT}] \right. \\ &\quad \left. - \sum_{j< i} \alpha_{ji}(v_k) [n_j - n_i (n_j / n_i)^* e^{-h v_k / kT}] \right\} \end{aligned} \quad (5-106)$$

We then can construct

$$(\partial n / \partial J_k)_l = -\sum_m \mathcal{A}_{lm}^{-1} a_m \quad (5-107)$$

It is particularly instructive to consider the case where *only one* ($i \rightarrow j$) transition can absorb at v_k , and all the other $\alpha_{lm}(v_k)$'s are zero.

Exercise 5-9: Show that, for the case just described, equation (5-108) is valid.

$$(\partial n / \partial J_k)_l = (\mathcal{A}_{lj}^{-1} - \mathcal{A}_{li}^{-1}) [4\pi w_k \alpha_{ij}(v_k) / h v_k] [n_i - n_j (n_i / n_j)^* e^{-h v_k / kT}] \quad (5-108)$$

This result, besides being simple, shows clearly that, because \mathcal{A}^{-1} must in general be a *full* matrix, a change in the radiation field at *any* frequency v_k causes a change in the occupation numbers of *every* level l , even if l cannot absorb or emit photons of that frequency. Of course the elements \mathcal{A}_{li}^{-1} and \mathcal{A}_{lj}^{-1} may be small, and the coupling weak, but the basic physical point remains true. Similar results for $(\partial / \partial n_e)$ and $(\partial / \partial T)$ are given in the references cited.