

Non-LTE Line Transfer with Diffusion of Excited Atoms

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The classical problem of radiative transfer in a spectral line, due to two-level atoms, in a homogeneous medium is reconsidered. It is pointed out that the source function used up to now in the literature neglects the diffusion of the excited atoms. In many cases this assumption is not justified. In the low-temperature limit $kT \ll h\nu$, the correct source function, allowing for diffusion of excited atoms, obeys an integro-differential equation.

1. Introduction

In this paper we wish to point out an inconsistency underlying all present-day investigations of radiative transfer in spectral lines in the absence of local thermodynamic equilibrium (LTE).

In non-LTE plasmas, the occupation numbers of atomic bound levels deviate from the Boltzmann value (and/or the degree of ionization from the Saha value). Non-LTE plasmas are, among others, low pressure gas discharges, the solar chromosphere, and many of the high-temperature plasmas encountered in fusion research. In such situations, the occupation numbers of the atomic levels must be calculated taking all relevant collisional and radiative processes into consideration. In particular, in optically thick plasmas, the equation of radiative transfer must be solved simultaneously with the rate equations for the atomic level populations, because the radiation field depends on the emission rates, and hence on the number of excited atoms, whereas the atomic occupation numbers, in turn, depend on the radiation field via the absorption rates. A self-consistent procedure must therefore be applied in order to calculate the intensities of emitted spectral lines (being an important energy loss of a plasma) and the corresponding line shapes (being useful for diagnostic purposes).

There is an extended literature on non-LTE line transfer (see Ref. 1—3a which all contain references to the original publications) which, however, has overlooked an effect that must be taken into account in order to obtain a self-consistent solution of the problem.

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Let us consider the simplest case: line formation in a homogeneous medium containing two-level atoms. This problem has been treated extensively in the literature^{1–3a}. The numerical calculations show, as expected, that in the optically thick case with no incident radiation from outside, the density of excited atoms increases when going from the boundary toward the interior, for this behavior simply reflects the fact that, near the boundary, the radiation field is weaker, and hence the absorption rate lower than in the interior. In other words, in all such systems there is a density gradient of excited atoms which gives rise to a corresponding diffusion current. However, the source function used in these calculations, which is due to Thomas⁴ and which goes back to Milne⁵, does not take particle diffusion into consideration. Clearly, this is an inconsistent procedure. The reason for this mistake is obvious: The system looks so “homogeneous” that one easily forgets that, in reality, it is not homogeneous due to the existence of boundaries.

In Section 2 of this paper we derive the equations which govern, in the low-temperature limit $kT \ll h\nu$ of the simple problem just discussed, the radiative transfer in the spectral line if diffusion of excited atoms is taken into account. Unlike the diffusionless case which leads to an algebraic expression in terms of the radiation intensity, one now obtains for the source function a differential equation with an inhomogeneous term depending on the radiation intensity. The dimensionless parameter, responsible for whether or not diffusion is important, is estimated for weakly ionized plasmas in Section 3. It turns out that, for not too low densities, many optical resonance lines require the explicit treatment of particle diffusion. Finally, in Section 4 we derive a



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closed integro-differential equation for the line source function in a plane parallel slab.

The aim of this paper is to draw attention to an inconsistency of non-LTE line transfer calculations. For this, the consideration of the simplest case is sufficient. It is evident that more complicated situations — inhomogeneous systems, multi-level atoms — must be treated along the same lines. In particular, when estimating the importance of convective transport in inhomogeneous systems, it must be kept in mind that, due to radiative transfer, the density gradients of excited atoms can be much steeper than those corresponding to the atomic species as a whole.

2. The Basic Equations

We consider a stationary and homogeneous system containing two-level atoms and electrons, i. e., the density of two-level atoms n_0 , the electron density n_e , and the (atom and electron) temperature T are constant, whereas the densities of atoms in the lower (1) and upper (2) level may be functions of the position \mathbf{r} ,

$$n_1(\mathbf{r}) + n_2(\mathbf{r}) = n_0. \quad (1)$$

We limit ourselves to the case of low temperature

$$e^{-h\nu_0/kT} \ll 1, \quad (g_2/g_1) e^{-h\nu_0/kT} \ll 1 \quad (2)$$

where $h\nu_0$ is the energy difference of the atomic levels, and g_1, g_2 their statistical weights. This means that even the Boltzmann value for n_2/n_1 is small compared to unity, and hence, a fortiori,

$$n_2 \ll n_1 \cong n_0. \quad (3)$$

Moreover, in this limit, induced emissions are negligible compared with spontaneous ones.

The transfer equation for the specific intensity I_ν of frequency ν is

$$dI_\nu/ds = \kappa_\nu (S - I_\nu) \quad (4)$$

where $d/ds = \mathbf{n} \cdot \nabla$, \mathbf{n} being the unit vector specifying the considered direction. The line absorption coefficient κ_ν and the line source function S are given by^{1-3a}

$$\kappa_\nu = (h\nu_0/4\pi) B_{12} \varphi_\nu n_1 \cong (h\nu_0/4\pi) B_{12} \varphi_\nu n_0, \quad (5)$$

$$S = n_2 A_{21}/n_1 B_{12} \cong n_2 A_{21}/n_0 B_{12}. \quad (6)$$

Here φ_ν is the normalized absorption profile,

$$\int_{(\text{line})} \varphi_\nu d\nu = 1 \quad (7)$$

and A_{21}, B_{12} are the Einstein-Milne coefficients for spontaneous emission and absorption. We have made the approximation of complete redistribution, i. e., we have assumed equality of the emission and absorption profiles. This leads to the frequency-independence of the line source function (6)^{1-3a}.

On the other hand, the balance equation for the excited atoms is

$$\nabla \cdot \mathbf{I}_2 = \tilde{\nu}_2 \quad (8)$$

where \mathbf{I}_2 is the flux density and $\tilde{\nu}_2$ the net production rate of excited atoms. The atoms in the ground state need not be considered explicitly because $\tilde{\nu}_1 = -\tilde{\nu}_2$, and $\mathbf{I}_1 = -\mathbf{I}_2$ if the gas as a whole is at rest. One has

$$\mathbf{I}_2 = -D \nabla n_2 \quad (9)$$

where D is the diffusion constant, and

$$\begin{aligned} \tilde{\nu}_2 &= n_1 (B_{12} J + n_e C_{12}) - n_2 (A_{21} + n_e C_{21}) \\ &= n_0 (B_{12} J + n_e C_{12}) \\ &\quad - n_2 [A_{21} + B_{12} J + n_e (C_{21} + C_{12})] \\ &\cong n_0 (B_{12} J + n_e C_{12}) - n_2 (A_{21} + n_e C_{21}). \end{aligned} \quad (10)$$

Here

$$J = \iint I_\nu \varphi_\nu d\nu d\Omega/4\pi \quad (11)$$

where $d\Omega$ is the element of solid angle, and C_{12}, C_{21} are the rate coefficients for electronic excitation and de-excitation collisions, which are related to each other through

$$C_{12}/C_{21} = (g_2/g_1) e^{-h\nu_0/kT} \quad (12)$$

since the electron distribution function is Maxwellian. In view of Eq. (2) one has

$$C_{12}/C_{21} \ll 1. \quad (13)$$

Furthermore, using the well-known Einstein relation

$$A_{21}/B_{12} = (g_1/g_2) (2h\nu_0^3/c^2) \quad (14)$$

and observing that

$$B^W \equiv B_{\nu_0}^W(T) = (2h\nu_0^3/c^2) e^{-h\nu_0/kT} \quad (15)$$

is the Wien function, that is, the Planck function in the limiting case (2), one has

$$B_{12} J/A_{21} = (g_2/g_1) e^{-h\nu_0/kT} (J/B^W) \ll 1 \quad (16)$$

because of Eq. (2) and $J \leq B^W$. Relations (13) and (16) have been used in Equation (10).

If D is constant, Eq. (8) now takes the form

$$-D \nabla^2 n_2 = n_0 (B_{12} J + n_e C_{12}) - n_2 (A_{21} + n_e C_{21}). \quad (17)$$

Inserting here the source function (6), one obtains after a little algebra the following equation for S

$$S - \frac{D/A_{21}}{1 + \varepsilon} \nabla^2 S = \frac{J + \varepsilon B^W}{1 + \varepsilon} \quad (18)$$

where

$$\varepsilon = n_e C_{21}/A_{21} \quad (19)$$

is the dimensionless parameter which determines whether excited atoms are de-excited primarily by inelastic collisions ($\varepsilon \gg 1$) or by spontaneous emissions ($\varepsilon \ll 1$).

If diffusion is negligible ($D \cong 0$), one recovers, of course, the Thomas-Milne source function^{4, 5}

$$S = (J + \varepsilon B^W)/(1 + \varepsilon). \quad (20)$$

Equations (4) and (18), together with suitable boundary conditions for I_ν and S , govern the line formation of the considered system.

3. Numerical Estimates

Let us estimate the importance of the diffusion term in Equation (18). For the sake of simplicity, we consider only weakly ionized plasmas, such as in gas discharges or stellar atmospheres, where the diffusion is mainly due to collisions with neutral particles. In this case the diffusion constant is, for particles of mass m , approximately given by⁶

$$D \cong kT/m\gamma \quad (21)$$

where

$$\gamma \cong n_s Q (kT/m)^{1/2} \quad (22)$$

is the collision frequency with particles of density n_s , Q being the corresponding cross section.

The characteristic length of our problem is κ_0^{-1} where $\kappa_0 \equiv \kappa_{\nu_0}$ is the absorption coefficient in the line center. In view of Eq. (18), it is thus the dimensionless parameter

$$\delta = \kappa_0^2 D/A_{21} \quad (23)$$

which determines whether diffusion is important ($\delta \gg 1$) or not ($\delta \ll 1$). Note that, in our example, appreciable density gradients of excited atoms may occur only in optically thick systems with $\varepsilon \ll 1$.

Since, for all densities of practical interest, the line core is determined by Doppler broadening, we may put, up to factors of the order of unity,

$$\varphi_{\nu_0} \cong (\Delta\nu_D)^{-1} \quad (24)$$

with the Doppler width

$$\Delta\nu_D = (\nu_0/c) (2kT/m)^{1/2}. \quad (25)$$

Introducing the absorption oscillator strength f_{12} through

$$A_{21} = (g_1/g_2) (8\pi^2 e^2 \nu_0^2/m_e c^3) f_{12} \quad (26)$$

where e is the elementary charge and m_e the electron mass, one has

$$\kappa_0 \cong (\pi e^2/m_e c) (f_{12}/\Delta\nu_D) n_0. \quad (27)$$

From all these relations one finally derives

$$\delta \cong \frac{g_2}{16g_1} f_{12} \frac{e^2}{m_e c} \left(\frac{m}{kT} \right)^{1/2} \frac{\lambda_0^4}{Q} \frac{n_0^2}{n_s} \quad (28)$$

where $\lambda_0 = c/\nu_0$ is the wavelength of the line. Because of Eq. (2) one must have $kT < h\nu_0 = hc/\lambda_0$.

Table 1 quotes order of magnitudes of the quantity δ for two different wavelengths and some densities. We have considered the cases $n_0 = n_s$ and $n_0 = 10^{-2} n_s$, the former corresponding to a system containing only two-level atoms, and the latter to a case where the two-level atoms are "impurities". Table 1 has been calculated using the following values: $g_2 f_{12}/g_1 \sim 1$, $T \lesssim 10^4$ °K, $Q \sim 10^{-16}$ cm², $m \gtrsim 10^{-24}$ g.

Inspection of Table 1 shows that many strong, optical and uv resonance lines of laboratory discharges and stellar atmospheres require the consideration of the diffusion of excited atoms.

4. Integro-differential Equation for S

From the two coupled Eqs. (4) and (18) one can eliminate the intensity I_ν , thus forming a closed equation for S alone. We briefly recall this procedure for the case of a plane parallel slab with no incident radiation from outside (cf. Figure 1).

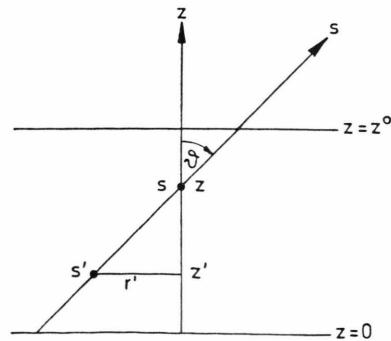


Fig. 1. Definition of geometrical variables in a plane parallel slab.

n_0 ($=n_s$)	λ_0 10000 Å	λ_0 1000 Å	n_0 ($=10^{-2} n_s$)	λ_0 10000 Å	λ_0 1000 Å
10^8 cm^{-3}	10^{-1}	10^{-5}	10^8 cm^{-3}	10^{-3}	10^{-7}
10^{12} cm^{-3}	10^3	10^{-1}	10^{12} cm^{-3}	10	10^{-3}
10^{16} cm^{-3}	10^7	10^3	10^{16} cm^{-3}	10^5	10

Table 1. Values of the dimensionless quantity δ [Equation (28)].

The transfer equation (4) has the formal solution

$$I_\nu(s) = \int_0^s \kappa_\nu S(s') e^{-\kappa_\nu(s-s')} ds', \quad (29)$$

from which one gets the mean intensity \bar{I}_ν ,

$$\bar{I}_\nu(z) \equiv \int I_\nu(s) \frac{d\Omega}{4\pi} \quad (30)$$

$$= \frac{\kappa_\nu}{4\pi} \int_{(\text{vol})} S(z') e^{-\kappa_\nu(s-s')} \frac{dV'}{(s-s')^2}$$

since the volume element is $dV' = (s-s')^2 ds' d\Omega$, $d\Omega = 2\pi \sin \vartheta d\vartheta$ being the element of solid angle, so that

$$ds' d\Omega = dV' / (s-s')^2. \quad (31)$$

In Eq. (30) we have indicated explicitly that \bar{I}_ν and S depend only on the z -coordinate. But (cf. Fig. 1)

$$s-s' = +[(z-z')^2 + r'^2]^{1/2}, \quad (32)$$

$$dV' = 2\pi r' dr' dz', \quad (33)$$

so that

$$\bar{I}_\nu(z) = \frac{\kappa_\nu}{2} \int_0^{z^0} dz' S(z') \int_0^\infty \frac{\exp\{-\kappa_\nu[(z-z')^2 + r'^2]^{1/2}\}}{(z-z')^2 + r'^2} r' dr' \quad (34)$$

$$= \frac{1}{2} \kappa_\nu \int_0^{z^0} S(z') E_1(\kappa_\nu |z-z'|) dz'$$

where z^0 is the thickness of the slab, and

$$E_1(u) = \int_u^\infty (e^{-t}/t) dt \quad (35)$$

the exponential integral.

Inserting Eq. (34) in Eq. (18) leads to the following integro-differential equation for S

$$S(z) - \frac{D/A_{21}}{1+\varepsilon} \frac{d^2 S}{dz^2} = \frac{\varepsilon}{1+\varepsilon} B^W + \int_0^{z^0} K(z, z') S(z') dz' \quad (36)$$

with the kernel

$$K(z, z') = \frac{1}{2(1+\varepsilon)} \int \kappa_\nu \varphi_\nu E_1(\kappa_\nu |z-z'|) d\nu, \quad (37)$$

which has to be supplemented by two boundary conditions. For instance, if there is no exchange of matter with the surroundings, the particle fluxes must vanish at the boundaries, and hence

$$S'(0) = S'(z^0) = 0 \quad (38)$$

where $S'(z) = dS/dz$.

In conclusion, we have seen that there are situations where the diffusion of excited atoms plays a role in determining the spectroscopic state of a gas. The mathematical description then becomes more complicated than in the diffusionless case. From a physical point of view, the main effect of the diffusion is, of course, the flattening of the density profiles of excited atoms, compared to cases without diffusion, affecting hereby the intensities and line shapes of emitted spectral lines. Numerical calculations are required in order to study these effects quantitatively.

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