Review

J. Astrophys. Astr., Vol. 36, No. 4, December 2015, pp. 605–611

Radiative Transfer Reconsidered as a Quantum Kinetic Theory Problem

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Received 12 June 2015; accepted 27 July 2015
DOI: 10.1007/s12036-015-9349-6

Abstract. We revisit the radiative transfer theory from first principles approach, inspired from quantum kinetic theory. The radiation field is described within the second quantization formalism. A master equation for the radiation density operator is derived and transformed into a balance relation in the phase space, which involves nonlocal terms owing to radiation coherence. In a perturbative framework, we focus on the lowest order term in $\hbar$-expansion and show that the radiation coherence results in an alteration of the photon group velocity. An application to the formation of hydrogen lines in stellar atmospheres is performed as an illustration.

Key words. Radiative transfer—quantum kinetic theory—anomalous dispersion.

1. Introduction

The radiative transfer equation is commonly presented as a balance relation for the electromagnetic radiation energy (Chandrasekhar 1960; Pomraning 1973; Mihalas 1978; Oxenius 1986; Milonni & Eberly 1988; Wang & Wu 2007); it has a structure similar to the Boltzmann equation involved in classical kinetic theory, making it suitable for the elaboration of transport codes (e.g. based on the Monte-Carlo technique (Reiter *et al.* 2002)) or the elaboration of a fluid model. In this framework, the radiation field is viewed as a set of particles (photons) evolving along straight lines and interacting locally with massive particles (e.g. atoms) through emission, absorption and scattering processes. While convenient for numerical applications, the radiative transfer equation can be inaccurate if the radiation has a narrow spectral band Δk, sufficiently so that the coherence length $1/\Delta k$ (Born & Wolf 1964) becomes comparable to relevant gradient lengths. In this work, we revisit this issue from the first principles. We derive the radiative transfer equation from QED master equations and consider an extension suitable for a description of radiation coherence. The treatment follows previous works (Rosato 2011, 2013, 2015).

2. Specific intensity and phase space distribution

The specific intensity $I(\omega, \mathbf{n}, \mathbf{r}, t)$ is defined in such a way that the amount of energy transported by a radiation pencil crossing a surface element $\mathrm{d}\sigma$ located at $\mathbf{r}$, between times t and $t+\mathrm{d}t$, is given by

$$\delta E = I(\omega, \mathbf{n}, \mathbf{r}, t) \cos\theta \mathrm{d}\omega \mathrm{d}\Omega \mathrm{d}\sigma \mathrm{d}t, \tag{1}$$

where θ is the angle between the propagation direction $\mathbf{n}$ and the normal to the surface, $\mathrm{d}\Omega$ denotes the angular aperture, and $[\omega, \omega+\mathrm{d}\omega]$ is the frequency range of the radiation pencil. Several conventions can be found in the literature. For example, an alternative definition involves the frequency ν instead of the angular frequency ω. In the following, we adopt the angular frequency convention and take equation (1) as a definition of the specific intensity in order to make the notation consistent with previous works (Rosato 2011, 2013, 2015). In a kinetic theory context, the specific intensity can be written in terms of the one-photon phase space distribution $f(\mathbf{r}, \mathbf{p}, t)$ ($\mathbf{p} = \hbar\omega\mathbf{n}/c$ stands for the momentum): $I(\omega, \mathbf{n}, \mathbf{r}, t) = \hbar c p^3 f(\mathbf{r}, \mathbf{p}, t)$. In a strict sense, this function is not a true probability density function but rather a quasiprobability (Wigner) distribution, which can take negative values on phase space volumes of typical extent $\hbar^3$. An observable signal (e.g., on a spectrometer) with positive values can be obtained from a phase space average using an appropriate detector function (Rosato 2013). The Wigner function is defined in terms of the QED photon creation and annihilation operators as

$$f(\mathbf{r}, \mathbf{p}, t) = \left(\frac{2}{\hbar L}\right)^3 \sum_{jj'} \delta_{\varepsilon_j \varepsilon_{j'}} \delta\left(\mathbf{k}_j + \mathbf{k}_{j'} - \frac{2\mathbf{p}}{\hbar}\right) \langle a_j^+ a_{j'} \rangle(t) \mathrm{e}^{-i\mathbf{k}_{jj'}\cdot\mathbf{r}}. \tag{2}$$

Here, j refers to a discretized mode $(\mathbf{k}_j, \varepsilon_j)$ (ε_j is a polarization vector), $\mathbf{k}_{jj'} \equiv \mathbf{k}_j - \mathbf{k}_{j'}$, and the brackets $\langle \cdots \rangle (t)$ denote average at time t using the radiation density operator.

3. Photon master equation

In the following we consider a system of identical two-level atoms (dipoles) immersed in a plasma, emitting and absorbing photons. The radiation density operator implied in the average $\langle \cdots \rangle$ in equation (2) is defined by partial trace of the total density operator ρ over the atoms' Hilbert space A: $\rho_R = \mathrm{Tr}_A(\rho)$. A closed master equation for this quantity (hence a closed equation for the Wigner function) can be obtained by tracing the Liouville–von Neumann equation

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} + i\hat{L}\right)\rho = 0 \xrightarrow{\mathrm{Tr}_A} \left(\frac{\mathrm{d}}{\mathrm{d}t} + i\hat{L}_R\right)\rho_R = -i\mathrm{Tr}_A(\hat{V}\rho), \tag{3}$$

and using an appropriate model for the right-hand side (r.h.s.). Here ^ denotes Liouville superoperators defined in terms of commutators: $\hat{L}X = [H, X]/\hbar$, $\hat{L}_R X = [H_R, X]/\hbar$, $\hat{V}X = [V, X]/\hbar$ for any operator X, where $H = H_A + H_R + V$ is the Hamiltonian of the total system (same notations as in Rosato (2013) are used). The interaction term V can be written as the sum $\Sigma_a V_a$, where a refers to an individual atom, hence the r.h.s. of equation (3) becomes

$$-i\mathrm{Tr}_A(\hat{V}\rho) = -i\mathcal{N}\mathrm{Tr}_1(\hat{V}_1\rho_{R,1}), \tag{4}$$

where $\mathcal{N}$ is the number of atoms, $\hat{V}_1$ refers to the interaction with an individual atom numbered '1', and $\rho_{R,1} = \mathrm{Tr}_{2\ldots\mathcal{N}}\rho$ is the restriction of the density operator to the subspace associated with the radiation and atom 1. An explicit expression for this quantity can be obtained using BBGKY hierarchy techniques. For simplicity we describe the interaction term $\hat{V}_1$ perturbatively at the first non-vanishing order (weak coupling approximation) and we apply the Markov approximation. In this framework, the following relation holds (Rosato 2015):

$$\rho_{R,1} \approx \rho_1\rho_R - i\int_0^\infty \mathrm{d}\tau\, \tilde{\hat{V}}_1(-\tau)[\rho_1\rho_R], \tag{5}$$

and equation (3) becomes a closed relation for ρ_R:

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} + i\hat{L}_R\right)\rho_R = -\mathcal{N}\mathrm{Tr}_1\int_0^\infty \mathrm{d}\tau\, \hat{V}_1\tilde{\hat{V}}_1(-\tau)[\rho_1\rho_R]. \tag{6}$$

Here, ρ_1 denotes the restriction of the density operator to the subspace associated with atom 1 and the tilde symbol stands for the interaction picture with respect to H_A+H_R. The r.h.s. can be split into a Hamiltonian term and a dissipator, in a fashion similar to that done in the derivation of the Lindblad equation (Breuer & Petruccione 2002). For radiative transfer, it is more convenient to deal with a master equation for the quantity $\langle a_j^+ a_{j'}\rangle \equiv N_{jj'}$ rather than for the density operator; such an equation can be obtained from equation (6), multiplying by $a_j^+ a_{j'}$, tracing and neglecting terms proportional to $\langle a_j^+ a_{j'}^+\rangle$ and $\langle a_j a_{j'}\rangle$ (rotating wave approximation) (Rosato 2013):

$$\left(\frac{\mathrm{d}}{\mathrm{d}t} - i\omega_{jj'}\right)N_{jj'} = \gamma_{2jj'} - \sum_{j''}(\Gamma_{jj''}N_{j''j'} + \Gamma^*_{j'j''}N_{j''j}). \tag{7}$$

Here the notation $\omega_{jj'} \equiv \omega_j - \omega_{j'}$ with $\omega_j = |\mathbf{k}_j|c$ has been used. The first term of the right-hand side is a source corresponding to spontaneous emission and the second term accounts for absorption and stimulated emission and can be interpreted as a loss if the medium is not amplifying. The rates can be written explicitly as (the time t is not written explicitly)

$$\Gamma_{jj'} = \frac{c\delta_{\varepsilon_j\varepsilon_{j'}}}{2L^3}\int \mathrm{d}^3r e^{i\mathbf{k}_{jj'}\cdot\mathbf{r}}\chi_c(\mathbf{r}, \hbar\mathbf{k}_{j'}), \tag{8}$$

$$\gamma_{2jj'} = \frac{c\delta_{\varepsilon_j\varepsilon_{j'}}}{2L^3}\int \mathrm{d}^3r e^{i\mathbf{k}_{jj'}\cdot\mathbf{r}}[\chi_{c,em}(\mathbf{r}, \hbar\mathbf{k}_{j'}) + \chi^*_{c,em}(\mathbf{r}, \hbar\mathbf{k}_j)], \tag{9}$$

with

$$\chi_c(\mathbf{r}, \mathbf{p}) = \frac{\hbar\omega_0}{4\pi}\left[B_{12}N_1(\mathbf{r}) - B_{21}N_2(\mathbf{r})\right]\phi_c(\omega, \mathbf{n}, \mathbf{r}), \tag{10}$$

$$\chi_{c,em}(\mathbf{r},\mathbf{p}) = \frac{\hbar\omega_0}{4\pi} B_{21} N_2(\mathbf{r}) \phi_c(\omega,\mathbf{n},\mathbf{r}), \tag{11}$$

$$\phi_c(\omega,\mathbf{n},\mathbf{r}) = \frac{1}{\pi}\int_0^\infty \mathrm{d}\tau C(\tau;\mathbf{n},\mathbf{r})\mathrm{e}^{-i\omega\tau}. \tag{12}$$

χ_c and ϕ_c are complex generalizations of the extinction coefficient and the normalized line shape function. C denotes the atomic dipole autocorrelation function in reduced units. In the case where Doppler broadening is important, the line shape involves a convolution with the atomic velocity distribution function.

4. Radiative transfer equation

The master equation (7) can be transformed into a balance relation in the phase space. The calculation involves tedious manipulations with sums and integrals and will not be detailed here. For simplicity, we focus on a case where the line shape function is not space dependent. In this framework, the Wigner function obeys the following transport equation (Rosato 2014):

$$\frac{\partial f}{\partial t} + \{f, H_c\}_A = S - \{f, L\}_S. \tag{13}$$

Here, $\{,\}_A$ and $\{,\}_S$ denote the antisymmetric and symmetric brackets associated with the Moyal star product: their action on two functions f, g yields

$$\{f,g\}_A = \frac{1}{i\hbar}(f * g - g^* f), \tag{14}$$

$$\{f,g\}_S = \frac{1}{2}(f * g + g^* f). \tag{15}$$

The star product is defined by an integral ($\mathrm{d}1 \equiv \mathrm{d}^3 r_1 \mathrm{d}^3 p_1$, $\mathrm{d}2 \equiv \mathrm{d}^3 r_2 \mathrm{d}^3 p_2$),

$$(f * g)(\mathbf{r},\mathbf{p}) = \frac{1}{(\pi\hbar)^6}\int \mathrm{d}1 \int \mathrm{d}2 f(\mathbf{r}+\mathbf{r}_1,\mathbf{p}+\mathbf{p}_1) g(\mathbf{r}+\mathbf{r}_2,\mathbf{p}+\mathbf{p}_2)\mathrm{e}^{2i(\mathbf{r}_1\cdot\mathbf{p}_2-\mathbf{r}_2\cdot\mathbf{p}_1)/\hbar}. \tag{16}$$

It can be expanded as a power series of $\hbar$. At the first order, the symmetric bracket reduces to multiplication and the antisymmetric bracket is equivalent to the Poisson bracket involved in Hamiltonian mechanics. H_c is a scalar Hamiltonian function:

$$H_c = pc + \frac{c\hbar}{2}\mathrm{Im}\chi_W. \tag{17}$$

It involves the free photon's energy $E = pc$ and a dispersion term. The χ_W coefficient is defined by

$$\chi_W = \frac{\hbar\omega_0}{4\pi}(B_{12}N_1 - B_{21}N_2)^* \phi_c^*. \tag{18}$$

S, L are source and loss terms denoting spontaneous emission, stimulated emission and absorption:

$$S = c\,\mathrm{Re}\chi_{W,e} \times \frac{2}{(2\pi\hbar)^3}, \tag{19}$$

$$L = c\,\mathrm{Re}\chi_W \tag{20}$$

with

$$\chi_{W,e} = \frac{\hbar\omega_0}{4\pi} B_{21} N_2 * \phi_c^*. \tag{21}$$

Note, the Einstein A_{21} coefficient is obtained if one multiplies with the factor $2/(2\pi\hbar)^3$ (equation (19)) and the factor $\hbar c p^3$ (cf. section 2). The delocalization implied in the star product (equation (16)) is a feature of the wave nature of light. It can be important if the coherence length (identical to the radiation's thermal de Broglie length) is significant with respect to relevant gradient lengths. Equation (13) reduces to the common radiative transfer equation given in textbooks (Chandrasekhar 1960; Pomraning 1973; Mihalas 1978; Oxenius 1986; Milonni & Eberly 1988; Wang & Wu 2007) at the large spectral band limit (incoherent radiation). Note, scattering is implied and described within the complete redistribution approximation. This stems from the closure relation (5). A generalization that accounts for incomplete redistribution can be obtained using a non-Markovian closure relation (Rosato 2015; Bommier 1997).

5. Application

Equation (13) presents a challenging computational issue due to the six-dimensional integrals implied in the Moyal products. It has been solved in specific cases in Rosato (2011, 2012, 2013, 2014), using simplifications (e.g. slab geometry with localized boundary conditions), in order to illustrate the possible inaccuracy of the standard radiative transfer theory at regimes with significant coherence length. We present hereafter an application to hydrogen line radiation in conditions relevant to stellar atmospheres. For the sake of simplicity, in numerical calculations we consider a homogeneous medium with slab geometry and we keep terms of first order in $\hbar$ in the Moyal product. The atomic populations are also assumed at local thermodynamic equilibrium. The radiative transfer equation (13) in stationary regime reads

$$v_g \frac{\partial f}{\partial x} = -L_0 (f - f_0) \tag{22}$$

and has the following solution:

$$f(x, p) = f_0 (1 - \exp(-L_0 x / v_g)) + f(x = 0) \exp(-L_0 x / v_g). \tag{23}$$

x denotes the coordinate along the slab depth. f_0 corresponds to the equilibrium (black body) distribution evaluated at the Bohr frequency of the transition ω_0:

$$f_0 = \frac{2}{(2\pi\hbar)^3} \times \frac{1}{\mathrm{e}^{\hbar\omega_0/T} - 1}. \tag{24}$$

L_0 is defined by

$$L_0 = \frac{\hbar\omega_0 c}{4\pi} B_{12} N_1 (1 - \mathrm{e}^{-\hbar\omega_0/T}) \phi, \tag{25}$$

where $\phi = \text{Re}\,\phi_c$ denotes the real line shape function. v_g is the group velocity,

$$v_g = c\left[1 - \frac{\hbar\omega_0 c}{8\pi} B_{12} N_1 (1 - e^{-\hbar\omega_0/T}) \text{Im}\,\phi_c'(\omega)\right]. \tag{26}$$

It can be significantly larger than c near a resonance line (anomalous dispersion). Figure 1 illustrates this point. The radiation's group velocity is plotted against the frequency detuning $\Delta\omega = \omega - \omega_0$ of hydrogen Lyman α, assuming $N_1 = 5 \times 10^{13}$

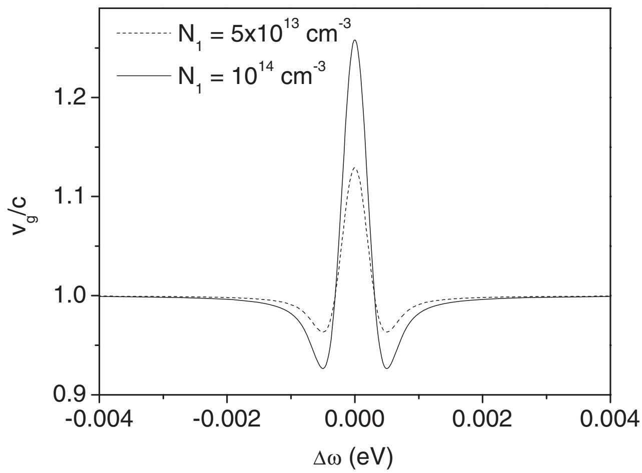

Figure 1. Plot of the ratio between the radiation's group velocity and the speed of light, at the vicinity of the hydrogen Lyman α transition. Two atomic densities are assumed. Only Doppler line broadening is retained, with a temperature of 0.5 eV. The ratio is larger than unity near the line center, which indicates anomalous dispersion.

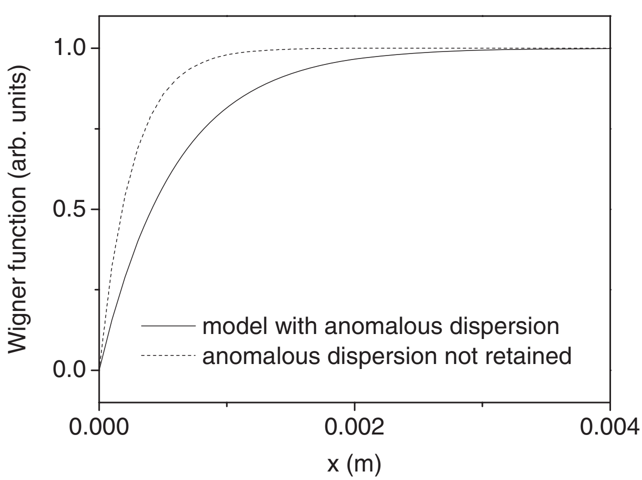

Figure 2. The characteristic length scale involved in the relaxation to thermal equilibrium is sensitive to the coherence properties of radiation. When dispersion effects are retained, the group velocity becomes larger than c near the line center, which results in an effective reduction of opacity.

cm^{-3} and 10^{14} cm^{-3}, and a temperature of 0.5 eV. Only Doppler line broadening has been retained. The deviation to c increases with density. Figure 2 shows the photon distribution at the central frequency ($p = \hbar\omega_0/c$) calculated from the solution (23) and normalized to the equilibrium distribution f_0. No incoming radiation has been assumed [$f(x = 0) \equiv 0$]. The atomic density has been set equal to 5×10^{14} cm^{-3}. Also shown in the figure is the result of a calculation assuming $v_g = c$, i.e. neglecting anomalous dispersion. As can be seen, the relaxation to thermal radiation occurs on a larger scale if the anomalous dispersion is retained.

6. Conclusion

In this work, we have reconsidered the radiative transfer theory from first principles approach inspired from quantum kinetic theory. The radiation field is quantized and described with a Wigner function. The evolution is governed by a master equation for the density operator. By using an appropriate closure relation, we have derived a generalization of the radiative transfer equation that accounts for spatial coherence. If the coherence length is significant with respect to relevant gradient lengths, the photon emission and absorption processes are delocalized. The transport equation can be written in a compact form involving Moyal brackets. At the first order in $\hbar$, it yields a transport equation of Boltzmann type, where the group velocity of radiation wave packets appears explicitly. An application to stellar atmospheres has indicated the possibility for an alteration of the relaxation to thermal radiation. These results are still qualitative and require a further examination with confrontations to experiments. A possible extension of the work could involve the analysis of atomic lines observed in discharge lamps. On the theoretical side, an extension to radiation transport in transient regimes is presently under consideration.

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