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Spectral line formation with wave effects in optically thick plasmas

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Abstract. An extension of the radiative transfer theory is presented and applied to the formation of spectral lines in optically thick media. In the model, the radiation field is described with the quantum phase space formalism adapted to second quantization. Comparisons with the standard radiative transfer theory in ideal cases indicate that the latter may be inaccurate if the light’s coherence length is of the same order as or larger than the photon mean free path.

1. Introduction

Recent theoretical works have reported on an extension of the radiative transfer theory suitable for problems involving the wave nature of light. A derivation of the radiative transfer equation (RTE) from the first principles has been presented in [1]. The treatment involves the quantum phase space formalism adapted to second quantization and the result is an integro-differential equation for the one-photon Wigner function, a quantity interpretable as a phase space probability density with quantum features (e.g., it can be negative in domains violating the Heisenberg uncertainty relation). This “quantum” radiative transfer equation (hereafter referred to as QRTE) reduces to the usual RTE in the limit of small wavelength and coherence length. The applicability of this limit has been examined in ideal cases [2–4]. It has been shown that the spatial coherence of light leads to a distortion of the Wigner function if the coherence length is of the same order as or larger than the other spatial scales of interest. Hence, in such conditions, the use of the RTE for describing the formation of line shapes would be inappropriate and could lead to significant misestimates. In this work, we report on new calculations. Section 2 gives a brief overview of the standard RTE and the terminology used in the theory, the QRTE is presented in Sec. 3 and results are shown in Sec. 4.

2. Standard radiative transfer formalism

The fundamental quantity of interest in radiative transfer is the spectral energy flux $I(\omega,\vec{n},\vec{r},t)$ [J m$^{-2}$ s$^{-1}$ sr$^{-1}$ (rad/s)$^{-1}$], referred to as “specific intensity” (e.g. [5]). The RTE is a transport equation for this quantity, and it is obtained from balance considerations. In its usual form, this equation reads

$$\frac{1}{c} \frac{\partial}{\partial t} + \vec{n} \cdot \vec{V} + \chi I = \eta ,$$

where $\eta(\omega,\vec{n},\vec{r},t)$ and $\chi(\omega,\vec{n},\vec{r},t)$ are source and loss terms, respectively, and express the interaction between the radiation field and the constituents of the matter present in the medium under
consideration, for example atoms, molecules, or ions. For spectral line radiation with an atomic transition \( u \rightarrow d \), these terms are given by

\[
\eta(\omega, \vec{n}, \vec{r}, t) = \frac{\hbar \omega}{4\pi} N_u(\vec{r}, t) A_{ud} \phi(\omega, \vec{n}, \vec{r}, t),
\]

(2)

\[
\chi(\omega, \vec{n}, \vec{r}, t) = \frac{\hbar \omega}{4\pi} \left[ N_d(\vec{r}, t) B_{du} - N_u(\vec{r}, t) B_{ud} \right] \phi(\omega, \vec{n}, \vec{r}, t),
\]

(3)

where \( A_{ud}, B_{du}, B_{ud} \) are the Einstein coefficients for spontaneous emission, absorption, and stimulated emission, respectively; \( N_u, N_d \) are the densities of atoms in the upper and lower states; and \( \phi \) is the local spectral line shape normalized such that \( \int d\omega \int d\Omega \phi(\omega, \vec{n}, \vec{r}, t) = 4\pi \). It denotes the probability density function of emitting or absorbing a photon at the frequency \( \omega \). The fact that the stimulated emission is treated as a negative part in the absorption is only a matter of convention, which allows one to write the RTE in the compact form given in Eq. (1). The Einstein coefficients are related by \( g_d B_{ud} = g_d B_{du} = g_u A_{ud} \omega^2 c^2 / \hbar \omega_0^3 \), where \( g_u \) and \( g_d \) denote the statistical weights of the upper and lower level, respectively, and \( \omega_0 \) is the Bohr frequency of the transition under consideration.

The RTE looks like a Boltzmann equation. An examination of the loss term \( \chi \) shows that it has the dimensions of an inverse length, which suggests that it can be interpreted as an inverse monochromatic mean free path (when it is positive) for the radiation energy. Because the energy exchange processes occur through the creation and destruction of photons, it suggests that we can interpret \( \chi \) as an inverse mean free path for photons also. A similar argument for \( \eta \) leads to the conclusion that the radiative transfer equation is equivalent to a Boltzmann equation for a distribution function \( f(\vec{r}, \vec{p}, t) \) which describes photon transport in phase space, using the correspondence \( \vec{p} = \hbar \omega \vec{n} / c \) and the proportionality relation \( I = h c \vec{p} \cdot \vec{f} \).

3. The quantum radiative transfer equation

The particle picture of radiation transport leads to ambiguities inherent to the definition of a photon in quantum mechanics. Symmetry considerations show that a position operator is not well defined for this particle, because it has zero mass and spin 1 [6]. Furthermore, if ever such an operator did exist, the Heisenberg uncertainty relation would prevent from knowing the position and momentum of a photon simultaneously, in contrast with that assumed in the standard radiative transfer theory. A remedy to this problem is provided by the quantum phase space formalism developed by Wigner [7]. This formalism involves “quasi-probability” distributions \( W(\vec{r}, \vec{p}, t) \), which are generalizations of the s-particle phase space distribution functions used in classical kinetic theory. They account for nonclassical features such as the uncertainty principle and quantum entanglement. “Quasi-probability” means that these functions may become negative. This occurs for physical states that have no classical equivalent. A coarse graining procedure is done to avoid such a peculiarity, with a spatial scale much larger than the particle’s thermal de Broglie wavelength \( \hbar / \Delta \rho \) (where \( \Delta \rho \) is the typical momentum dispersion). For photons, the thermal wavelength denotes the coherence length \( \lambda_c \sim c / \Delta \omega_{\lambda / 2} \) where \( \Delta \omega_{\lambda / 2} \) is the half width at half maximum (e.g. [8]). In the following, we use an adaptation of the Wigner formalism to second quantization and focus on the one-photon distribution \( W(\vec{r}, \vec{p}, t) = W(\vec{r}, \vec{p}, t) \). The development is detailed in [1] and follows early works reported in [9–11]. The Wigner function is defined as the average of the phase space photon number operator \( N(\vec{r}, \vec{p}) \):

\[
W(\vec{r}, \vec{p}, t) = \text{Tr}\{\rho(t)N(\vec{r}, \vec{p})\},
\]

\[
N(\vec{r}, \vec{p}) = \sum_z \frac{1}{(2\pi \hbar)^3} \int d^3k a_z^\dagger \left( \frac{\vec{p}}{\hbar} - \frac{\vec{k}}{2} \right) a_z \left( \frac{\vec{p} + \vec{k}}{\hbar} \right) e^{i\vec{k} \cdot \vec{r}}.
\]
Here, $\rho(t)$ is the density operator of the total (radiation + matter) system, $a_\epsilon^\dagger(\vec{k})$ and $a_\epsilon(\vec{k})$ are respectively the creation and annihilation operators corresponding to a photon of wavevector $\vec{k}$ and polarization $\vec{\epsilon}$, and $\text{Tr}\{\ldots\}$ denotes a trace over the whole system’s Hilbert space. The creation and annihilation operators obey the commutation rules $[a_\epsilon(\vec{k}),a_\epsilon^\dagger(\vec{k}')] = \delta_{\epsilon,\epsilon'}\delta(\vec{k} - \vec{k}')$ and $[a_\epsilon(\vec{k}),a_\epsilon(\vec{k}')] = 0 = [a_\epsilon^\dagger(\vec{k}),a_\epsilon^\dagger(\vec{k}')]$. The sum over the polarizations performed in Eq. (5) is due to an assumption of unpolarized radiation used here. Examination of Eqs. (4) and (5) shows that $W(\vec{r}, \vec{p}, t)$ is normalized to the total number of photons. A closed transport equation for the one-photon Wigner function is obtained by applying the differential operator $\left[\partial_t + c(\vec{p}/p)\cdot \vec{V}\right]$ to each side of Eq. (4) and by using appropriate assumptions [1]. The Lagrangian derivative involves two terms of different physical origins. (i) $DN/Dt$ denotes the time variation of the phase space number operator along a trajectory. It is identically zero in the short wavelength limit, which corresponds to propagation along defined straight rays. We will assume this condition satisfied in the following. (ii) $D\rho/Dt$ denotes evolution of the Wigner distribution due to the interactions between the radiation field and the plasma, i.e., the emission and absorption of photons. This term can be described using a quantum master equation [12–14]. This treatment yields the following transport equation

$$\left(\frac{\partial}{\partial t} + c \frac{\vec{p}}{p} \cdot \vec{V}\right) W(\vec{r}, \vec{p}, t) = S(\vec{r}, \vec{p}, t) - \int d^3 r' d^3 p' K(\vec{r}, \vec{p}, t; \vec{r}', \vec{p}') W(\vec{r}', \vec{p}', t),$$

(6)

where $S$ denotes a source corresponding to spontaneous emission and the integral term describes the contribution of the absorption corrected by stimulated emission. Explicitly, $S$ and $K$ are given by

$$S(\vec{r}, \vec{p}, t) = \frac{1}{(\pi\hbar)^3} \text{Re} \int d^3 r' d^3 p' \eta_\epsilon(\vec{r}', \vec{p}', t) e^{-2i(\vec{p}\cdot \vec{r} + \vec{r}\cdot \vec{p}')/\hbar},$$

(7)

$$K(\vec{r}, \vec{p}, t; \vec{r}', \vec{p}') = \frac{c}{(\pi\hbar)^3} \text{Re} \int d^3 r'' d^3 p'' \chi_\epsilon(\vec{r}'', \vec{p}'', t) e^{2i(\vec{p}\cdot \vec{r} + \vec{r}\cdot \vec{p}')/(\hbar)},$$

(8)

where $\eta_\epsilon$ and $\chi_\epsilon$ are complex generalizations of the emission and absorption coefficients used in the radiative transfer theory. They have a structure similar to Eqs. (2) and (3). The complex line shape function is given by the following relation [2] ($\vec{n}, \vec{r}, t$ are not written explicitly)

$$\phi_\epsilon(\omega) = \frac{1}{\pi} \int_0^\infty d\tau C(\tau) e^{-i\omega\tau},$$

(9)

with $C(\tau)$ being the atomic dipole autocorrelation function. The line shape function introduced in Sec. 2 corresponds to the real part of Eq. (9). If the Doppler effect is important, this expression is convolved with the atoms’ velocity distribution function.

The transport equation (6) is more general than the standard RTE. The presence of an integral in the right-hand side denotes delocalization of the absorption and the stimulated emission processes on a phase space volume of typical extent $\hbar^3$. This result is in agreement with the Heisenberg uncertainty principle. A consequence is that the processes are delocalized spatially over a region of typical volume $\lambda_v^3$. There is also a delocalization of the emission and absorption processes with respect to the emitters’ and absorbers’ location, which stems from the integrals present in the source and the kernel terms [Eqs. (7) and (8)]. Equation (6) reduces to the radiative transfer equation when $\lambda_v \rightarrow 0$. In the general case, we will refer to it as a “quantum” radiative transfer equation (QRTE). The QRTE can be interpreted as a transport equation governing the evolution of quasi-particles (also: wave packets) of spatial volume $\lambda_v^3$ and with the momentum dispersion $\Delta p^3$. Figure 1 shows an illustration of the spontaneous emission and the evolution of such a quasi-particle. An ideal case is considered: we assume an isolated, motionless, and perfectly localized atom, emitting in a given direction (one-dimensional geometry). There are no absorbers, so that $K \equiv 0$ in the QRTE. In the source term, the atomic density (which appears in the complex emissivity $\eta_\epsilon$) is set equal to $\delta(z)\exp(-A_{\text{mf}}z)$, with $z$
being the direction under consideration. The exponential denotes depopulation due to the spontaneous emission. In a similar fashion, there is also an exponential in the dipole autocorrelation function present in the complex line shape Eq. (9) in such a way to account for natural line broadening (here: the damping factor is \(A_{\omega d}/2\)). As can be seen in the figure, the Wigner function presents a bump structure of size \(\lambda_c \times \Delta p\) after a few coherence times (here the coherence time is estimated as \(\tau_c = 1/A_{\omega d}\)), which indicates the presence and the propagation of the quasi-particle. Although obtained here within a pure quantum approach, the delocalization effect induced by the spatial coherence is also expected from classical electromagnetism. A sketch of the derivation of a transport equation accounting for spatial coherence, with a classical picture, is presented in the Appendix. The result shown in Fig. 1 completes a preliminary study reported in [2]. Note, in the latter reference, an absolute value is missing on the y axis label of Fig. 2. This omission does not affect the conclusion of this work because the spread of the Wigner function over the coherence length, illustrated through the figure, does not depend on the sign of the momentum.

4. Application to the formation of spectral lines
The delocalizing integrals in Eqs. (6) – (8) are a feature of the light’s spatial coherence. The latter is not retained in the standard RTE. This suggests that the usual RTE may be inaccurate in cases where the coherence length is significant with respect to the other spatial scales of interest. We have examined this point by applying the QRTE to the formation of spectral lines in one-dimensional geometry. A slab of size \(L\) containing a homogeneous hydrogen gas, between two perfectly absorbing walls at \(z = \pm L/2\), is considered. We assume \(p_x = 0 = p_y, p_z > 0\) (radiation propagating towards the \(z > 0\) direction) and assume \(W(-L/2) = 0\) (no incoming radiation). The Wigner function in stationary regime can be written for \(z \in [-L/2, L/2]\) as a Fourier series

\[
W(z) = \sum_{n=-\infty}^{\infty} W_n e^{2\pi i n z / L},
\]

and the value at the boundary \(z = L/2\) is given by

\[
W(L/2) = 2 \sum_{n=-\infty}^{\infty} W_n (-1)^n,
\]

where we have used that the periodization of \(W\) has a discontinuity at \(z = L/2\) (Dirichlet’s theorem). Each Fourier coefficient can be approximated as [4]

\[
W_n = \frac{S_0 \delta_{n0} L - (-1)^n W(L/2)}{2i \pi n + L^2 K_0 n},
\]
In Eq. (12), $S_0 = \eta/\hbar c p^3$ and $\delta_{\alpha\beta}$ stands for the Kronecker symbol. Equations (11), (12), and (13) form a closed set, which provides the Fourier coefficients. The solution of the QRTE is obtained from solving this set for a sufficiently large number of coefficients and inserting them into Eq. (10). Figure 2 shows an application of the solution to the Lyman $\alpha$ line, assuming $L = 1$ mm, $N_1 = 10^{15}$ cm$^{-3}$, and $T = 1$ eV (with $N_1$, $T$ being the density of atoms in the fundamental state and their temperature, respectively). At these conditions, the product $\lambda_c \times \chi_0$ between the coherence length [estimated as $c/\Delta\omega_D$ with $\Delta\omega_D = (\omega_0/c)\sqrt{(2T/m_p)}$ being the Doppler width] and the extinction coefficient at the line center ($\omega = \omega_0$) is of the order of unity, hence, we are in conditions such that the RTE may be inaccurate. As can be seen in the figure, a noticeable increase of the Wigner function is present at the line center. This stems from the delocalization of the photon emission and absorption processes, and it indicates that the gas seems less opaque when the delocalization is important. It should be noted that this curve does not directly represent an observable spectrum since, by construction, the Wigner function can take negative values. A proper characterization of an observable spectrum should involve a phase space integral denoting a suitable detector response. In general, the effect of spatial coherence depends of the line under consideration. This point is illustrated in Fig. 3, where a plot of the Lyman $\beta$ Wigner function obtained
in the same plasma conditions is shown. Here the results of the QRTE and those of the RTE are close to each other because the parameter $\lambda_c \times \chi_0$ is smaller than unity in this case. A consequence of the line dependence is that line ratios can be affected by the spatial coherence. In a diagnostic context, this means that spectra may be misinterpreted if coherence effects are not well accounted for.

5. Conclusion
The radiative transfer equation widely used in opacity problems can be derived from first principles, using the Wigner quantum phase space formalism adapted to second quantization. Such a derivation has the advantage of providing physical insight in the mechanisms involved in radiation-matter interactions. We have considered an extension of the radiative transfer equation suitable for problems involving the wave nature of light. This equation accounts for spatial coherence and reduces to the usual radiative transfer equation in the limit $\lambda_c \rightarrow 0$. An application of this equation to an ideal case has indicated significant deviations from the result of the usual radiative transfer theory. In a diagnostic context, this suggests the possibility of spectra misinterpretation if coherence effects are not well accounted for. This result is preliminary. A more rigorous treatment of the quantum radiative transfer equation, using realistic geometry, is required. Further work should also consist in comparison to experiments.

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Appendix
A radiation transport equation accounting for spatial coherence can be obtained from classical electromagnetism. The classical counterpart of the Wigner function is given by

$$W(\vec{r}, \hat{p}, t) = \frac{1}{(2\pi\hbar)^3} \int d^3k \tilde{\alpha} \left( \frac{\hat{p}}{\hbar} - \frac{\vec{k}}{2}, t \right) \cdot \left( \frac{\hat{p}}{\hbar} + \frac{\vec{k}}{2}, t \right) e^{i \vec{k} \cdot \vec{r}},$$

(A1)

where $\tilde{\alpha}(\vec{k}, t)$ is the normal variable of the electromagnetic field in the Fourier mode $\vec{k}$. This quantity is defined in terms of the Fourier transform of the electric and magnetic fields $\hat{E}, \hat{B}$ [12]

$$\tilde{\alpha}(\vec{k}, t) = -\frac{i}{2} \sqrt{2\varepsilon_0 (2\pi) \hbar \omega} \left[ \hat{E}(\vec{k}, t) - c \frac{\vec{k}}{k} \times \hat{B}(\vec{k}, t) \right],$$

(A2)

and it obeys the following evolution equation, obtained from the Maxwell equations:

$$\frac{\partial \tilde{\alpha}}{\partial t} = -i \omega \tilde{\alpha} + \frac{i}{2\varepsilon_0} \sqrt{\frac{2\varepsilon_0 (2\pi) \hbar \omega}{\hbar \omega}} \hat{j}.$$  

(A3)

Here, $\omega = kc$ and $\hat{j}$ is the transverse part (i.e., perpendicular to $\vec{k}$) of the Fourier transform of the current density associated with the atomic dipoles. A classical-harmonic-oscillator description of the dipoles (Thomson model) is suitable here. The response of a dipole $\vec{d}$ to the electric field is given by

$$\vec{d}(t) = \frac{e^2}{m_e \omega_0} \int_0^\varepsilon d\omega' e^{-\gamma\omega'} \sin(\omega_0\tau) \hat{E}(\vec{R}, t - \tau),$$

(A4)

where $\omega_0$ is the atomic frequency, $\gamma$ is proportional to the inverse lifetime of the oscillator, and $\vec{R}$ is the atom’s position vector. Equation (A4) is obtained from the solution of the classical equation of motion assuming $\gamma \ll \omega_0$ (e.g. [15] for details on the classical atomic model). The exponential
corresponds to the dipole autocorrelation function involved in the line shape function. If we assume non-interacting dipoles, the $\gamma$ factor is identical to $\frac{A_{du}}{2}$. This factor can also be written explicitly in terms of the parameters of the classical oscillator as $\gamma = r_e \alpha_0 \sqrt[3]{3c}$ where $r_e$ is the classical electron radius. The current density in real space $\vec{j}$ is obtained after deriving Eq. (A4) with respect to time and multiplying the result by the density of dipoles $N$:

$$\vec{j}(\vec{r}, t) = \frac{e^2 N(\vec{r}, t)}{m_e} \int_0^\infty d\tau \ e^{-i\omega \tau} \cos(\omega_0 \tau) \vec{E}(\vec{r}, t - \tau).$$  \hspace{1cm} (A5)

We now consider the following approximation for the electric field

$$\vec{E}(\vec{R}, t - \tau) \approx \frac{1}{(2\pi)^{3/2}} \int d^3 k \vec{E}(\vec{k}, t) e^{i(\vec{k} \cdot \vec{r} + \omega \tau)}$$

$$\approx \frac{1}{(2\pi)^{3/2}} \int d^3 k \ i \ \sqrt{\frac{\hbar \omega}{2\varepsilon_0 (2\pi)^3}} \vec{\alpha}(\vec{k}, t) e^{i(\vec{k} \cdot \vec{r} + \omega \tau)},$$  \hspace{1cm} (A6)

which stems from the fact that the radiation field in spectral line is nearly monochromatic. The time integral in Eq. (A5) combined with Eq. (A6) yields the complex line shape function involved in the QRTE and the current density can be written explicitly in terms of the complex extinction coefficient, using the identity $N_d B_{du} - N_d B_{aw} = N \times \alpha_a \times 2 \gamma \times 4\pi c^2/h\alpha_0^3$ with $\alpha_a = 3$:

$$\vec{j}(\vec{r}, t) = \frac{e_0 c}{(2\pi)^{3/2}} \int d^3 k \ i \ \sqrt{\frac{\hbar \omega}{2\varepsilon_0 (2\pi)^3}} \vec{\alpha}(\vec{k}, t) e^{i(\vec{k} \cdot \vec{r} + \omega \tau)} \chi^*_c(\vec{r}, \hbar \vec{k}, t).$$  \hspace{1cm} (A7)

A transport equation for the classical Wigner function is obtained by applying the Lagrangian derivative $\{\dot{\rho}, + c(\vec{p}/p) \cdot \vec{V}\} = D/Dt$ to each side of Eq. (A1), using Eq. (A3), the Fourier transform of Eq. (A7), and the approximation $\omega \approx \omega_0$ in the square root factors (short wavelength approximation). A calculation leads to the QRTE Eq. (6) with $S \equiv 0$, i.e. with no spontaneous emission, consistently with the classical assumption considered in this appendix.

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