ON THE TRANSFER OF RESONANT-LINE RADIATION IN MESH SIMULATIONS

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ABSTRACT

The last decade has seen applications of adaptive mesh refinement (AMR) methods for a wide range of problems from space physics to cosmology. With the advent of these methods, in which space is discretized into a mesh of many individual cubic elements, the contemporary analog of the extensively studied line radiative transfer (RT) in a semi-infinite slab is that of RT in a cube. In this study we provide an approximate solution of the RT equation, as well as analytic expressions for the probability distribution functions (PDFs) of the properties of photons emerging from a cube, and compare them with the corresponding slab problem. These PDFs can be used to perform fast resonant-line RT in optically thick AMR cells where, otherwise, it could take unrealistically long times to transfer even a handful of photons.

Subject headings: line: formation — line: profiles — radiative transfer — scattering

1. INTRODUCTION

The classic problem of resonant radiative transfer (RT) in a semi-infinite slab has been extensively studied in literature (e.g., Harrington 1973; Neufeld 1990). On the other hand, the last decade has seen applications of adaptive mesh refinement (AMR) methods to problems as diverse as solar physics, supernovae and nucleosynthesis, interstellar medium physics, star formation, astrophysical jets, cosmology, etc. (for a summary, see, e.g., Norman 2004). In mesh-based methods the continuous domain of interest is discretized into a grid of many individual cubic elements. With the advent of AMR codes, the contemporary analog, at least in terms of usefulness and applicability range, of the extensively studied problem of resonant-line RT in a slab is the relatively unexplored problem of RT in a cube.

Understanding resonant RT in optically thick cubes is useful in particular because to perform RT in AMR simulations, one must solve numerous cube RT problems, since each time a photon enters an AMR cell one has a new cube RT problem. Furthermore, as is the case, e.g., for LyC line RT in cosmological simulations of galaxy formation, the high resolution achieved with AMR codes (along with the cooling of the gas) leads to very high scattering optical depths (see Tasitsiomi 2006). To obtain results within realistic times, we need a very fast RT algorithm, faster than the standard direct Monte Carlo approach, in which one follows the detailed scattering of photons in each one of the cells. A way to obtain this very fast algorithm is to study a priori the RT in cubes of various physical conditions. Using the results of such a study, we can avoid following the detailed photon scattering in each cell. Instead, we can immediately take the photon out of the cell, treating thus the problem on a per cell rather than on a per scattering basis, thus accelerating the RT scheme considerably. In this paper we discuss results on the resonant RT in a cube, and in comparison with resonant RT in a slab of similar physical conditions.

2. DESCRIPTION OF THE PROBLEM AND DEFINITIONS

In what follows we assume slab and cube configurations for the scattering medium. The slab is semi-infinite; namely, it is finite in one spatial dimension and infinite in the other two. The scattering medium is uniform in its properties and has a central source of center-of-line photons that scatter resonantly before escaping. Harrington (1973) has solved the slab RT equation in the limit of high optical depths and obtained a one-parameter solution (see also Neufeld 1990). The parameter is \( \alpha \tau_0 \), where \( \alpha = \Delta \nu_L / 2 \Delta \nu_D \), \( \Delta \nu_L \) and \( \Delta \nu_D \) are the line natural and thermal Doppler widths, respectively, and \( \tau_0 \) is the center-of-line optical depth from the center of the scattering medium to one of its edges. More specifically, \( \tau_0 \) is defined so that the optical depth at frequency shift \( \chi_f = (\nu - \nu_0) \Delta \nu_D \) is \( \tau_0 = \tau_f(\chi_f) \), with \( \phi(\chi_f) \) the normalized line profile. The discussion that follows applies to optically thick media (\( \alpha \tau_0 > 1 \)).

3. RESULTS

3.1. Emerging Frequency Distribution

3.1.1. Approximate Analytic Solution for Resonant RT in a Cube

Following Harrington (1973), one can show that the RT equation we need to solve is

\[
\nabla^2 \bar{J}(\tau; \sigma) + \frac{\partial^2 \bar{J}}{\partial \sigma^2} = -3\phi^2(\chi_f) \frac{J(\tau)}{4\pi},
\]

where \( J \) is the zeroth moment of the intensity \( I \), \( \sigma \) is defined through \( \partial \chi_f / \partial \sigma = (3/2)^{1/2} \phi(\chi_f) \), \( \tau \) is defined through \( d \sigma = \phi(\chi_f) d\chi_f \), \( J(\tau) \) is the emissivity, and \( \tau \) is measured from the center of the cube. This equation is identical to the equation used previously for a semi-infinite slab (Unno 1955; Harrington 1973; Neufeld 1990) or a spherically symmetric distribution (e.g., Dijkstra et al. 2006). The only difference is that those previous cases were for one spatial dimension, hence \( \nabla^2 \) consisted of only one term, whereas in the case of a cube, it has contributions from all three dimensions, i.e., \( \nabla^2 = \partial^2 / \partial x^2 + \partial^2 / \partial y^2 + \partial^2 / \partial z^2 \), with \( x, y, \) and \( z \) as the components of \( \tau \) along the \( x \)-, \( y \)-, and \( z \)-axes, respectively.

Equation (1) is a linear, inhomogeneous, partial differential equation. To solve it we use the eigenfunction expansion method.

\[\text{Thus, for } d\tau = -\kappa_0 ds \text{ with } s \text{ measured along the photon propagation direction and } \kappa_0 \text{ such that } \kappa_0 \phi(\chi_f) \text{ is the "absorption coefficient," } \tau_x, \tau_y, \text{ and } \tau_z \text{ are such that } d\tau_x = -\kappa_0 dx, d\tau_y = -\kappa_0 dy, \text{ and } d\tau_z = -\kappa_0 dz \text{, respectively. In simple terms, } \tau_x, \tau_y, \text{ and } \tau_z \text{ are (modulo a factor } \kappa_0 \text{ that depends on the density of the scattering medium) equivalent to spatial coordinates within the cube.} \]
Namely, motivated by the method of separation of variables (applicable in the case of the corresponding homogeneous equation), we assume that the solution can be written as

$$J(\tau; \sigma) = \sum_{\alpha, \beta, \gamma = 1}^{\infty} X_\alpha(\tau_x) Y_\beta(\tau_y) Z_\gamma(\tau_z) G_{\alpha, \beta, \gamma}(\sigma).$$  \hspace{1cm} (2)$$

When applying this expansion method in inhomogeneous problems, the idea is that $X_\alpha$, $Y_\beta$, and $Z_\gamma$ will be known (eigen)functions, and $G_{\alpha, \beta, \gamma}$ will be the unknown coefficients of the sum (here frequency dependent) that are to be determined through the solution process. In reality, we have to specify all four functions, since we do not have any “known” eigenfunctions. We take the “known” (eigen)functions of position to be the solutions to the “associated” homogeneous ordinary differential equations. The term “associated” here implies that the best choice for the basis position (eigen)functions should be the solution sets from Sturm-Liouville problems that closely resemble the problem being addressed. This will give a set of functions that are orthogonal over the domain defined by the problem. Thus, to find the position (eigen)functions, we focus first on the solution of the corresponding homogeneous equation. We assume that the solution is separable, namely, that $J(\tau, \sigma) = R(\tau)G(\sigma)$. Substituting in equation (1) and after some rearrangement, we get

$$\frac{\nabla^2 R(\tau)}{R(\tau)} = -\frac{1}{G(\sigma)} \frac{\partial^2 G(\sigma)}{\partial \sigma^2} = -\lambda^2,$$  \hspace{1cm} (3)

where we have performed a first separation with separation constant $-\lambda^2$. As already implied by equation (2), we furthermore assume that $R(\tau) = X(\tau_x)Y(\tau_y)Z(\tau_z)$ in Cartesian coordinates. After performing additional separations, we end up with equations of the form

$$1 \frac{\partial^2 X}{\partial \tau_x^2} = -l^2,$$  \hspace{1cm} (4)

and similarly, for $Y(\tau_y)$ and $Z(\tau_z)$ with separation constants $-m^2$ and $-n^2$, respectively, and with $l^2 = m^2 + l^2 + m^2$. The general solution for each one of these equations consists of both sine and cosine terms. Since we only consider central point sources, i.e., $f(\tau) = \delta(\tau_x)\delta(\tau_y)\delta(\tau_z)$, each one of the functions $X$, $Y$, and $Z$ must be separable even. Thus, we set $X(\tau_x) = A \cos(\lambda \tau_x)$, $Y(\tau_y) = B \cos(m \tau_y)$, and $Z(\tau_z) = C \cos(n \tau_z)$.

We calculate the constants $A$, $B$, and $C$ using boundary conditions that are generated assuming the Eddington approximation (see, e.g., Eddington 1926, p. 322), where near isotropy is assumed. Given the optical depths we are concerned with, the near isotropy assumption should be fairly accurate. In fact, we adapt the isotropy assumption should be fairly accurate. In fact, we adapt the assumptions that are generated assuming the Eddington approximation (see Harrington 1973). Plugging all these in equation (7) and since we are interested in the overall spectrum of radiation emerging from one side of the cube, say, along the $z$-axis, after integrating over $\tau_x$, $\tau_y$, and setting $\tau_z = \tau_0$, we get

$$J(\tau_0, \sigma) = \sum_{\alpha, \beta, \gamma = 1}^{\infty} \sin(l_\alpha \tau_0) \sin(m_\beta \tau_0) \cos(n_\gamma \tau_0)$$
\begin{equation}
\times \frac{\sqrt{6} e^{-l_\alpha m_\beta n_\gamma}}{2 \pi \sqrt{(l_\alpha \tau_0)^2 + (m_\beta \tau_0)^2 + (n_\gamma \tau_0)^2}}, \hspace{1cm} (11)
\end{equation}

At this last step, we also substituted $j_{\alpha, \beta, \gamma}^2$ with $l^2_\alpha + m^2_\beta + n^2_\gamma$. For a comparison of the spectrum emerging from one side of a cube
to that emerging from one of the two “sides” of a slab, we must multiply our cube solution by a factor of 3 so that both solutions have the same normalization. This is so because for the same central source we expect 1/6 of the photons to emerge from a certain cube side and 1/2 of the photons to emerge from a certain slab “side.”

Each individual series term for both the cube and the slab solution (given in Harrington 1973) depends only on \( C_{11}/C_{28} \). This becomes obvious when one takes into account the definition of \( C_{27} \) and the approximation for \( C_{30} \) \((xf)\). The slab solution is an alternate series and can be written in closed form. The cube solution cannot be written in closed form, but using equations (5) and (6), we see that sin \((l, \tau_0) \) \(\sim (-1)^{n-1} \) and cos \((n, \tau_0) = 2n/3(\phi(xf)(-1)^{n-1}. Thus, the sin \((l, \tau_0) \sin (m, \tau_0) \cos (n, \tau_0) \) term in equation (11) can be written as \(-(-1)^{n+\beta+\gamma} \), indicating that the cube series may also be alternating. Writing this three-sum series as one sum, i.e., \( \sum_{i=1}^{\infty} c_i \), we find that indeed the cube series is alternating as well. Some of the first finite sums of the alternating series for a \( \tau_0 = 2 \times 10^4 \) cube and slab are shown in the top two panels and the bottom left panel of Figure 1, respectively. In the case of the cube the infinite number of terms result (solid histograms) is obtained by the Monte Carlo method described in detail in Tasitsiomi (2006), whereas for the slab we use the closed-form slab analytical solution of Harrington (1973).

The cube series solution will be of some practical value only if a few first terms contribute significantly to the sum. The exponential decay in \( |\phi| \) indicates that the terms should die off for “high” \( \alpha, \beta, \) and \( \gamma \) values, with the exact values where this happens dependent on the frequency (or \( \sigma \)) at which one calculates the spectrum. The logarithm of the absolute ratio of the series terms, \( c_i \), in units of the first term, \( c_1 \), for three different values of the

![Figure 1](image-url)
frequency shift is shown in the bottom right panel of Figure 1. As before, \( \alpha \tau_0 = 2 \times 10^4 \), but we find that these “convergence curves” remain identical for all cube \( \alpha \tau_0 \) at the extremely optically thick regime. The dash-dotted line is the convergence curve for a slab for frequency shift equal to the shift where the emergent spectrum is known to have a maximum \( \sim 0.9(\alpha \tau_0)^{1/3} \) \[103\]. Harrington 1973]. Away from this maximum the slab convergence curves look identical to those of the cube \( \text{(dotted and dashed lines)} \). Clearly, the rate of convergence depends on the frequency at which the spectrum is calculated. Given that the series is alternating, with the absolute value of the terms decreasing monotonically \( \text{(for most } \sigma \text{ values)} \), the absolute error we make by truncating the series at the \( i \)th term is less or equal to the \( i + 1 \) term. From the plot this means that if we keep only the first term, the actual infinite series limit \( S \) will be \( \sim (1 \pm 10^{-4}) S_i \) for \( \sigma_f = 39 \) and \( \sim (1 \pm 0.3) S_i \) for \( x = x_{\text{max}}, \) with \( S_i \) the \( i \)th partial sum. We can achieve a 3% accuracy at the peak if we go to \( i = 4 \) \( \text{(i.e., } |S - S_4|/|S| \leq 0.03 \) \), whereas for better accuracy we must exceed \( i = 30 \). Convergence becomes extremely slow at values close to the resonance, \( e.g., \ x = 2 \). Furthermore, we find that the terms up to \( i = 30 \) for \( x = 2 \) do not decrease monotonically in the case of the cube; they do decrease for the slab but extremely slowly.

The usefulness of the slab series solution derived here depends on the application in mind. For example, when studying Ly\( \alpha \) emitters at very high redshifts, it is expected that the blue frequencies will be absorbed anyway because of hydrogen intervening between the emitter and the observer and the red wavelengths near the resonance will also be absorbed by the red damping wing. In this case, the poor convergence at frequencies near resonance \( \text{(and, more generally, over the } |x| \leq x_{\text{max}} \text{ range)} \) may not be a problem. Clearly, one must decide on the usefulness of the series solution based on the specifics of the application.

3.1.2. Approximate Cube Spectrum in Closed Form

Based on the similarities between the cube and the slab spectra, one might think that the spectrum emerging from one side of a cube may be well described by the slab closed-form solution, but for a different, smaller \( \alpha \tau_0 \) than the actual \( \alpha \tau_0 \) of the cube. Because, for example, when observing the spectrum emerging from a cube along the \( z \)-direction, we lose all photons that in the case of a slab would wander and scatter many times along the infinite dimensions until they finally escape from the \( z \)-plane. In the case of the cube, these photons do not contribute to the spectrum we observe from the \( z \)-direction, because they have already exited the cube along directions other than \( z \). This argument has been already used in Tasitsiomi \( \text{(2006)} \), where the slab solution was used to describe the spectrum for a cube by plugging in the slab solution an \( \alpha \tau_0 \) equal to \( 2/3 \) the actual cube \( \alpha \tau_0 \). This value was motivated by comparing the mean number of scatterings, \( N_{\text{sc}} \), for photon escape in cubes and slabs. Since \( N_{\text{sc}} \) scales linearly with \( \tau_0 \) for extremely optically thick media \( \text{(Adams 1972)} \), by comparing \( N_{\text{sc}} \) for cubes and slabs, one can guess a correct effective \( \tau_0 \) and thus \( \alpha \tau_0 \). For the purposes of this previous study, this effective thickness gave good agreement with simulated spectra for a wide range of physical conditions.

Applying a more detailed treatment, we fit cube spectra with the slab solution for the fraction \( f \) of \( \alpha \tau_0 \) that must be used in this solution to get the best fit. We find that \( f \) varies in the 0.66–0.77 range for \( \alpha \tau_0 \) values in the \( 2 \times 10^3–10^8 \) range. We find no trend of \( f \) with \( \alpha \tau_0 \). Within errors, one can use a constant fraction in the above \( f \)-range regardless of \( \alpha \tau_0 \), since we find that we cannot distinguish between the fits obtained when \( 2/3 \) or the exact \( f \)-value are used. An example of a fit of the cube spectrum using the slab solution and \( f = 2/3 \) is shown in the top right panel of Figure 1 \( \text{(the best-fit } f \text{-value for this example is 0.72)} \). Furthermore, in terms of the spectrum shape \( \text{(e.g., maximum location and intensity)} \), the above range of \( f \)-values lead to spectra indistinguishable by currently existing instruments.
3.2. Distribution of Exiting Direction and Point

Referring to $\mu$, the cosine of the angle with which the photon is exiting, measured with respect to the normal to the exiting surface, we show its cumulative probability distribution function (CPDF) in the top panel of Figure 2. We find that this CPDF is the same for a slab or a cube and clearly deviates from isotropy (dashed line). We verify the findings of other studies that in optically thick media, photons tend to exit in directions perpendicular to the exiting surface (see, e.g., Phillips & Meszaros 1986; Ahn et al. 2002).

In cases of very optically thick media, the emerging radiation directionality approaches the Thomson-scattered radiation emergent from a Thomson-thick electron medium. Phillips & Meszaros (1986) found that for a Thomson-thick medium, $I(\mu)/I(0) = (1 + 2\mu)/3$.

Since the number of photons emerging at $\mu$ is $\propto I(\mu)\,d\mu$, we get

$$P(\leq \mu) = \frac{\int_0^\mu (1 + 2\mu)\,d\mu}{\int_0^1 (1 + 2\mu)\,d\mu} = \frac{\mu^2}{\pi} (3 + 4\mu). \quad (12)$$

This dependence is shown in Figure 2 with the solid line. It is an excellent description of the directionality of the spectrum, and hence, equation (12) can be used to determine the photon-exiting direction. It has been suggested by some authors (Ahn et al. 2002) that the fact that in optically thick media RT occurs mostly via wing photons, with the latter being described by a dipole phase function (Stenflo 1980) and the fact that Thomson scattering is also described by a dipole-scattering phase function explain why the resulting $\mu$ CPDFs are similar. However, we find the same CPDF if we use either an isotropic or a dipole phase distribution.

For such optical thicknesses the details of the exact phase function do not matter, at least not with respect to the exiting angle CPDF. Regardless of scattering phase function, in such media photons tend to escape along the normal to the exiting surface where the opacity is smaller. The results shown are for $\alpha \tau_0 = 2 \times 10^3$, but similar distributions are obtained for thicker media.

In the case of the slab, the azimuthal angle $\phi$ is distributed uniformly in $[0, 2\pi]$. In the case of the cube, there are small deviations from uniformity. This is expected, since the previous distribution for $\mu$ is found to be valid for all sides of the cube. In the simplest case, in which we observe along the $z$-axis (in which case the spherical coordinate $\phi$ angle is the actual azimuthal angle we refer to), all direction cosines ($\cos \theta, \sin \theta \cos \phi, \text{and } \sin \theta \sin \phi$) follow the distribution given in equation (12); thus, $\phi$ cannot be exactly uniformly distributed. However, the deviations from uniformity are small.

The distribution of exiting points for both a cube and a slab are shown in the bottom panel of Figure 2. For this figure we assume that we observe photons emerging along the $z$-direction, and we record the $x$- and $y$-coordinates of their exit points (in units of the size of the cube). In the case of RT in a cube, the distribution is pretty close to uniform. In the case of the slab, despite it being semi-infinite, for any practical purposes one can assume that all photons exit at most within $|x| (|y|) \leq 5$ (not shown in figure).

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