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Lyman-Alpha Scattering in the Intergalactic Medium During the Epoch of Reionisation

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Declaration

I declare that this thesis is not substantially the same as any that I have submitted for a degree or diploma or other qualification at any other University. I further state that no part of my thesis has already been or is being concurrently submitted for any such degree, diploma or other qualification. This thesis is the outcome of my own work except where specifically indicated in the text.

Jonathan Higgins
Edinburgh
31st August, 2011

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Abstract

We examine resonant scattering of $\text{Ly}\alpha$ (Lyman-alpha) photons in the neutral hydrogen Intergalactic Medium (IGM) at high redshift. $\text{Ly}\alpha$ scattering plays a key role in the 21cm emission/absorption against the Cosmic Microwave Background via the ‘Wouthuysen-Field Effect’. Knowledge of the strength of $\text{Ly}\alpha$ scattering induced by the first sources will constitute a significant step in predicting and understanding the eventual observations of the impact of these objects on the signal from the IGM during the Epoch of Reionisation (EoR), using planned facilities such as the Square Kilometre Array. A quantitative analysis of the scattering rate requires formulation and solution of the radiative transfer equation for the system. We consider radiative transfer of $\text{Ly}\alpha$ scattering far from a source in the homogeneous expanding IGM for photons that free stream until scattering in the blue wing of the local line profile: we describe an approximation that ignores spatial diffusion of photons and assumes a locally homogeneous scattering medium, allowing the calculation of simple analytic solutions to examine the dependence of the local scattering rate on various physical effects such as local expansion/contraction, and extend our approach to determine time-dependent solutions. The more complex problem of $\text{Ly}\alpha$ photons scattering in both frequency and space within a spherically symmetric medium is subsequently solved for several test problems using both Monte Carlo methods and a method based on the ray and moment radiative transfer equations following an approach due to Mihalas et al. [1975, 1976]. We examine local $\text{Ly}\alpha$ scattering around a continuum source in the homogeneous expanding IGM using both methods, and compare our results with an analytic solution in the zero-temperature diffusion regime derived from an analogous solution for a monochromatic source found by Loeb and Rybicki [1999]. Our results are used to make estimates of the resulting size of the spherical region around the source that is rendered detectable via 21cm observations against the CMB background. We also examine cases with different density and velocity profiles and determine the effect on the scattering rate.

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CHAPTER 1

Introduction

In this chapter we give a detailed account of the background context and utility of the work presented in this thesis. In summary, our work is motivated by the Epoch of Reionisation (EoR), observation of which will rely on detection of the 21cm signal of the neutral hydrogen Intergalactic Medium (IGM) against the Cosmic Microwave Background (CMB). A key component necessary to render the neutral hydrogen detectable in 21cm emission/absorption against the CMB during the EoR is provided by scattering of Lyman-alpha or $\text{Ly}\alpha$ photons emitted by the first sources. We describe the dependence of the observed 21cm signal on the $\text{Ly}\alpha$ scattering rate experienced by the neutral hydrogen and the observational prospects for detecting the signal. We will also highlight the importance to predicting/interpreting the 21cm signal of in-depth radiative transfer calculations to compute the $\text{Ly}\alpha$ scattering rate arising from models of the EoR.

1.1 Background Cosmology

In order to describe the astrophysical context of our work in appropriate detail, we summarise several basic but important cosmological concepts. The universe is isotropic and, from isotropy and the cosmological principle that the properties of the universe are the same for all observers, homogeneous. Isotropy and homogeneity are observed on very large scales. The expansion of the universe is characterised by the scale factor $R(t)$, which dictates the dependence on cosmological time of any position vector $\mathbf{x}(t)$ as follows:

$$\mathbf{x}(t) = [R(t)/R_0]\mathbf{x}(t_0) \quad (1.1)$$

where t_0 is the cosmological time today and $R_0 = R(t_0)$ is the current value of the scale factor. The length $|\mathbf{x}(t)|$ is a ‘proper distance’, while the length $|\mathbf{x}(t_0)|$ is the corresponding ‘comoving distance’ measured today, independent of the expansion of the universe. The velocity of an object with position vector $\mathbf{x}(t)$ is written as:

$$\begin{aligned} \dot{\mathbf{x}}(t) &= [\dot{R}(t)/R_0]\mathbf{x}(t_0) \\ &= [\dot{R}(t)/R(t)]\mathbf{x}(t) = H(t)\mathbf{x}(t) \end{aligned} \quad (1.2)$$

where the ‘Hubble parameter’ $H(t) \equiv \dot{R}(t)/R(t)$ is the uniform velocity gradient of the expansion.

The Robertson-Walker spacetime metric for a homogeneous and isotropic Universe is written in terms of dimensionless, comoving coordinates (r, θ, ϕ) as (Peacock [1999]):

$$c^2 d\tau^2 = c^2 dt^2 - R^2(t) [dr^2 + S_k^2(r) d\psi^2] \quad (1.3)$$

where the contents of the square brackets multiplied by $R^2(t)$ is the squared line element for a space with constant curvature (required by homogeneity). The line element is factorised to highlight the effect of expansion and from isotropy is split into components describing comoving radial separation dr^2 and transverse angular separation $d\psi^2 = d\theta^2 + \sin^2\theta d\phi^2$. We see that the cosmological time t is explicitly the proper time measured by a ‘fundamental observer’ at rest with respect to the local matter distribution, with fixed (r, θ, ϕ) ; from homogeneity these observers can synchronise their

clocks with reference to any of the properties of the Universe such as the density. The function $S_k(r)$ is related to the curvature of the universe, denoted by k :

$$S_k(r) = \begin{cases} \sin r & ; \quad k = 1 \\ r & ; \quad k = 0 \\ \sinh r & ; \quad k = -1 \end{cases} \quad (1.4)$$

where $k = 1, 0, -1$ represents a spatially closed, flat and open universe respectively.

We consider the path of a photon emitted by some object at time t and received by an observer today at time t_0 . As photons have proper time $d\tau = 0$, the comoving distance travelled is determined from $dr = c dt/R(t)$:

$$r = \int_t^{t_0} \frac{c}{R(t)} dt = \int_{t+\delta t}^{t_0+\delta t_0} \frac{c}{R(t)} dt \quad (1.5)$$

where we have equated the comoving distance to that of a photon emitted and received at times $t+\delta t$ and $t_0+\delta t_0$ respectively. Thus for small $\delta t, \delta t_0$ we can say that $\delta t/R(t) = \delta t_0/R_0$ and thus if the δt 's represent a single period of the photon wave at emission and reception we can write:

$$1 + z \equiv \frac{\nu}{\nu_0} = \frac{R_0}{R(t)}. \quad (1.6)$$

As $R(t) < R_0$ we see that $\nu_0 < \nu$ and the photon has been redshifted. The number z is the 'cosmological redshift' of the universe at the time of emission; clearly $z = 0$ denotes the universe today, while the beginning of the universe is given by $R(t) \rightarrow 0$ and $z \rightarrow \infty$. An important change of variable between time and redshift is given by noting $\dot{z} = -(R_0/R^2)\dot{R} = -(1+z)H(z)$ and thus $dt = -dz/[(1+z)H(z)]$. The corresponding proper distance dl_p is given by $dl_p = R dr = c dt = -c dz/[(1+z)H(z)]$.

The dynamics of the expansion are governed by the Friedmann equation, essentially a statement of conservation of energy. A particle of mass m at proper radius $R(t)r$ has kinetic energy $K = m(\dot{R}r)^2$ and potential energy $V = -GMm/(Rr)$ for $M = (4/3)\pi(Rr)^3\rho$, with a fixed total energy $K + V$. The final form of the Friedmann equation can be written independently of the values of m and r (Peacock [1999]):

$$\dot{R}^2 = \frac{8\pi G\rho}{3}R^2 - kc^2 \quad (1.7)$$

$$\implies H^2 = \frac{8\pi G\rho}{3} - \frac{kc^2}{R^2} \quad (1.8)$$

where the value of the constant corresponding to the total energy is determined from a fully General Relativistic treatment and is related to the curvature of the universe. A $k = 0$ flat universe has a ‘critical density’ ρ_c defined as:

$$\rho_c \equiv \frac{3H^2}{8\pi G} \quad (1.9)$$

and we use this density to define a dimensionless density parameter Ω :

$$\Omega \equiv \rho/\rho_c = \frac{8\pi G\rho}{3H^2} \quad (1.10)$$

$$= 1 + \frac{kc^2}{H^2 R^2} \quad (1.11)$$

where the last equality follows by dividing Eq. (1.8) by H^2 . The relationship between the total mass density of the universe and its curvature is clear; $\Omega > 1$ corresponds to a closed universe with $k = 1$, $\Omega < 1$ corresponds to an open universe with $k = -1$, and $\Omega = 1$ with $k = 0$ is a flat universe.

The equation of motion for the scale factor $R(t)$ is obtained by differentiating the Friedmann equation with respect to t . It is thus necessary to know $\dot{\rho}$ which is found from conservation of energy in the form $dE = -P dV$ for a fluid with pressure P , or $d(\rho c^2 R^3) = -P d(R^3)$, giving:

$$\dot{\rho} = -3H \left[\rho + \frac{1}{c^2} P \right]. \quad (1.12)$$

The resulting equation of motion, known as the second Friedmann equation as both arise separately from General Relativity, is written:

$$\ddot{R} = -\frac{4\pi G}{3} R \left[\rho + \frac{3}{c^2} P \right] \quad (1.13)$$

where the quantity in the square brackets is the ‘active mass density’, a positive value for which results in a decelerating universe. It is of interest to consider the dependence of the density on the scale factor for various fluids.

- For a pressureless matter-dominated fluid, $P_m = 0$, giving $\dot{\rho}_m = -3(\dot{R}/R)\rho_m$ and thus $\rho_m \propto R^{-3}$. In terms of redshift and the current value of the matter density $\rho_{m,0}$ we write $\rho_m = \rho_{m,0}(1+z)^3$.

- A radiation-dominated fluid has the equation of state of radiation, $P_r = \rho_r c^2/3$ and thus $\dot{\rho}_r = -4(\dot{R}/R)\rho_r$ and $\rho_r \propto R^{-4}$; as the temperature T_r of black-body radiation satisfies $\rho_r \propto T_r^4$, we see that $T_r \propto R^{-1}$. Thus we write the density and black-body temperature of radiation in the universe as $\rho_r = \rho_{r,0}(1+z)^4$ and $T_r = T_{r,0}(1+z)$.
- The mass density of a homogeneous vacuum energy is denoted by the constant value $\rho_v \equiv \rho_{v,0}$. The corresponding pressure is negative, $P_v = -\rho_v c^2$, and a pure vacuum density has a negative active mass density resulting in $\ddot{R} > 0$ from Eq. (1.13), an accelerating universe.

The time dependence of the scale factor in any of the three special cases where the universe is matter-, radiation- or vacuum-dominated can be deduced by solving either of the Friedmann equations as ordinary differential equations. We omit details but we quote the results: $R(t) \propto t^{2/3}$ (matter-domination), $R(t) \propto t^{1/2}$ (radiation-domination) and $R(t) \propto e^{Ht}$ (vacuum-domination).

The total density for a universe consisting of contributions from all three fluids, weighted at redshift zero according to the values Ω_m , Ω_r and Ω_v where $\Omega_m + \Omega_r + \Omega_v = \Omega$, can be written:

$$\begin{aligned} \frac{8\pi G}{3}\rho &= \frac{8\pi G\rho_c(0)}{3} \times [\rho/\rho_c(0)] \\ &= H_0^2 [\Omega_m(1+z)^3 + \Omega_r(1+z)^4 + \Omega_v]. \end{aligned} \quad (1.14)$$

Thus from Equations (1.8) and (1.11) we find the full redshift dependence of the Hubble parameter:

$$H^2(z) = H_0^2 [\Omega_m(1+z)^3 + \Omega_v + \Omega_r(1+z)^4 + (1-\Omega)(1+z)^2]. \quad (1.15)$$

The Hubble constant H_0 is typically parameterised by the constant h according to:

$$H_0 = 100 h \text{ km s}^{-1} \text{ Mpc}^{-1}. \quad (1.16)$$

The value of H_0 is estimated by a ‘distance ladder’ of methods, such as observations of Cepheid variable stars and more distant Type-1a supernovae (SN1a), that attempt

to establish the distances d of objects sufficiently distant to minimise the relative effect of peculiar velocities, allowing use of the Hubble relation $V = H_0 d$ for the observed recession velocity V . The current size and age of the universe are of the order of the characteristic values given by the Hubble length $c/H_0 = 3000 h^{-1} \text{ Mpc}$ and the Hubble time $1/H_0 = 9.78 h^{-1} \text{ Gyr}$, respectively. The total density of the universe at the current epoch is given by $\rho(0) = \Omega \rho_c(0) = 1.88 \times 10^{-26} \Omega h^2 \text{ kg m}^{-3}$. Where the values of cosmological parameters or constraints are required explicitly by calculations we will assume the values given by Komatsu et al. [2011], including: $h = 0.70$, $\Omega_m = 0.27$, $\Omega_v = 0.73$.

In the remainder of this section we summarise the early evolution of the universe and describe the properties relevant to the study of the IGM and the Epoch of Reionisation. Seconds after the Big Bang, the expansion and cooling of the universe caused nucleons to decouple or ‘freezeout’ from the weak interactions keeping their abundances in thermal equilibrium, as the expansion timescale dropped below the interaction timescale. This ‘primordial nucleosynthesis’ is responsible for the deuterium and isotopes of helium, lithium and beryllium found today, outside of that generated by stars. A detailed understanding of the primordial nucleosynthesis reactions shows that the current abundances of deuterium and helium-3, the atomic forms of rare products of the reactions, are very sensitive to the total density of baryons in the universe Ω_b . These calculations and abundances, together with the total abundances of hydrogen and helium given respectively by mass fractions $X \simeq 0.75$ and $Y \simeq 0.25$, give the result $\Omega_b h^2 = 0.022$ or $\Omega_b = 0.045$.

From the scalings of the various density contributions in Eq. (1.14) it is clear that the early universe was radiation-dominated, and from the current energy density of photons comprising the CMB and the related neutrino energy density it is known that the current radiation density is $\Omega_r h^2 \simeq 4.2 \times 10^{-5}$. As the radiation density dropped faster with expansion than the matter density, the universe reached a state of matter-radiation equality at redshift $z \sim 3000$ and the density of the universe today is dominated by Ω_m and Ω_v . Observational evidence including SN1a and anisotropies in the CMB constrain these values to a flat universe with $\Omega_m + \Omega_v \simeq 1$. The vast majority of the matter in

the universe is non-baryonic, pressureless ‘dark matter’, generally believed to consist of massive frozen-out relic particles. The most popular models of the universe are those labelled with the descriptor ‘ Λ CDM’; the Λ denotes the large vacuum energy or ‘dark energy’ density, while the CDM denotes Cold Dark Matter, dark matter particles that are non-relativistic at the recombination epoch.

Cosmological recombination took place at $z \simeq 1100$, approximately 400,000 years after the Big Bang. Previously the universe was an ionised plasma, optically thick due to Compton scattering of photons by free electrons. At recombination this plasma cooled below $\sim 10^3$ K to allow formation of neutral atomic hydrogen and helium, locking up the vast majority of the free electrons and rendering the universe largely optically thin. The distribution of the redshift at which photons were last scattered is sharply peaked and they are considered to originate from a ‘last-scattering surface’ at the recombination redshift. These photons constitute the CMB, seen today as a black-body spectrum redshifted to temperature $T_{\text{CMB}} = 2.73$ K and isotropic to 1 part in 10^5 . The very weak anisotropies in the CMB contain significant information on the matter distribution of the universe at recombination. At general post-recombination redshifts we write the CMB temperature as $T_{\text{CMB}}(z) = 2.73(1+z)$ K.

After the radiation-dominated era, perturbations in the matter density of the universe developed through the influence of gravity on the pressureless dark matter. This ‘structure formation’ is well-understood theoretically for perturbations of low overdensity for which the dynamical equations can be reduced to the so-called linear regime, however when a perturbation of a particular scale significantly exceeds the mean density it will begin to develop non-linearly. Numerical N-body simulations of non-linear structure formation predict halos, filaments and sheets of dark matter with baryonic matter tracing these structures, formed in a hierarchical sequence of smaller objects accumulating to comprise larger structures. This picture is seen to be a broad match to that found from low-redshift observations on the largest scales, however much of the detail of the later stages of structure formation is not easily understood; the large density of baryons complicates the purely gravity-driven dark matter evolution by requiring treatment of electromagnetic ‘gastrophysical’ effects.

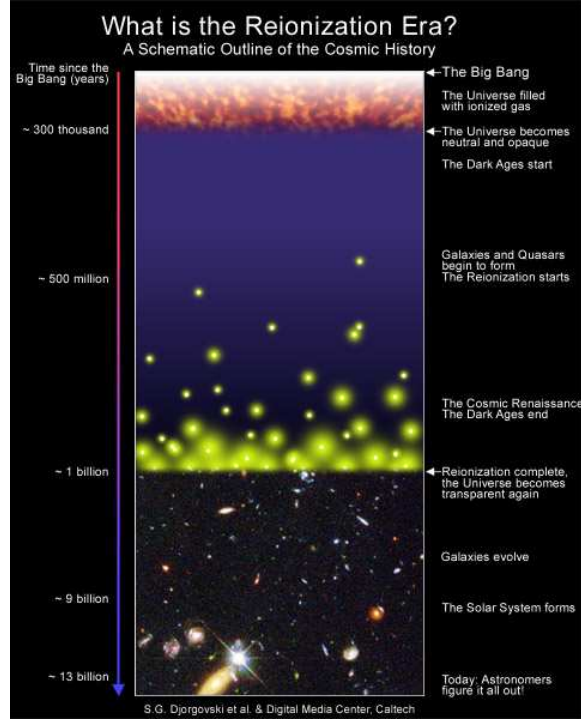


Figure 1.1: Timeline of the evolution of the universe illustrating the Epoch of Reionisation.

Following recombination, the universe entered an extended period distinguished observationally by the absence of sources of light and referred to as the cosmological Dark Ages. The eventual formation of the first light sources in the universe resulted in the emission of radiation by these sources capable of ionising hydrogen, causing the neutral hydrogen in the IGM to be reionised (see Figure 1.1). The period over which hydrogen reionisation took place is commonly described as the Epoch of Reionisation (EoR).¹ The first sources are believed to be the first galaxies formed in the universe, however high-redshift quasars, miniquasars and possibly the first generation of stars themselves, high-mass Population III stars, could also have contributed. Prospective determinations of the properties, effects and origins of the first sources have led to significant cosmological and astrophysical interest in the Epoch of Reionisation.

¹Reionisation of the helium content of the IGM occurred in two stages: He I was likely ionised to He II from the first sources during the EoR, while total helium ionisation is believed to have taken place later at $z \simeq 3.5$ following an increase in the population of energetic QSOs.

1.2 Motivation: Probing the Epoch of Reionisation

Direct observations of objects at the high redshifts corresponding to the Epoch of Reionisation are difficult due to low fluxes, cosmological dimming and absorption along the line of sight. A handful of galaxies, quasars and Gamma-Ray Bursts (GRBs) have been observed at these high redshifts, with the highest-confirmed-redshift belonging to a galaxy found by the Hubble Ultra Deep Field in the near-infrared at $z \simeq 8.5$ (Bouwens et al. [2010], McLure et al. [2010], Bunker et al. [2010]). These detections are rare and the maximum redshift of such objects is expected to advance only incrementally until the next generation of telescopes, including the James Webb Space Telescope (JWST) and the Very Large Telescope (VLT), begin operating. A significant source of information on the universe at these high redshifts is the IGM; studying the IGM during the Epoch of Reionisation allows direct determination of the progress of reionisation and indirect information on these first sources.

Much of our information about the IGM at high redshift comes from studies of the absorption spectra of quasars. A quasar emission spectrum shows a peak corresponding to Ly α emission at a rest frame wavelength $\lambda_\alpha = 1216 \text{ \AA}$. Consider observation of a quasar at redshift z_s ; if there is a distinct absorption system at intermediate redshift $z < z_s$, the system scatters photons out of the line of sight at the local Ly α wavelength, which is redshifted with respect to the emission in the quasar's rest frame due to the expansion of the universe. We detect an absorption line in the flux from the quasar at a wavelength $(1+z)\lambda_\alpha$, blueward of the Ly α emission peak seen at wavelength $(1+z_s)\lambda_\alpha$. Studying the detected flux as a function of wavelength shows a series of absorption lines blueward of the emission peak corresponding to intervening neutral hydrogen clouds along the line of sight, referred to as the 'Lyman-alpha Forest' (see Figure 1.2).

Absorption lines are seen as a suppression of the unabsorbed continuum flux by a factor $e^{-\tau_\nu}$, where the optical depth τ_ν is determined from the properties of the absorbing system:

$$\tau_\nu = \int \sigma_\nu n_{\text{HI}} dl \simeq \sigma_\nu N_{\text{HI}} \quad (1.17)$$

where $N_{\text{HI}} \equiv \int n_{\text{HI}} dl$ is the H I column density and σ_ν is the frequency- and

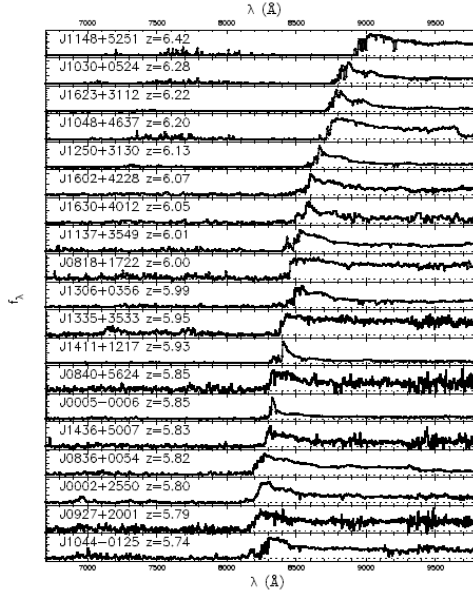


Figure 1.2: Plots of observed quasar absorption spectra for a series of different source redshifts, illustrating the Ly α forest and, for source redshifts $z \gtrsim 6.1$, the Gunn-Peterson trough (Fan et al. [2006]).

temperature-dependent Ly α absorption cross section. Note that more generally we should integrate n_1 , the number density of H I in the lower state capable of Ly α absorption, however in practice $n_1 \simeq n_{\text{HI}}$ for all temperatures of interest. High-resolution quasar spectra can allow determination of temperatures and column densities from absorption line properties. The clouds of neutral hydrogen responsible for the Lyman-alpha forest will have typical column densities satisfying $10^{12} \text{ cm}^{-2} < N_{\text{HI}} < 10^{17} \text{ cm}^{-2}$. The lower limit corresponds to clouds that are only just optically thick enough to be rendered detectable through their absorption signatures, while the upper limit represents a threshold beyond which the absorption signatures display additional properties. Column densities $N_{\text{HI}} > 10^{17} \text{ cm}^{-2}$ produce Lyman-Limit Systems (LLSs) which display a cutoff in the spectrum short of the Lyman-limit of 912 Å. For $N_{\text{HI}} > 10^{20} \text{ cm}^{-2}$ we detect Damped Lyman-alpha Absorbers (DLAs), for which the increasingly wide absorption lines display ‘damping wings’ corresponding to the shape of σ_ν far from line centre.

Lyman-alpha forest features are typically identified with individual H I clouds, however we are more interested in the effect resulting from the large-scale neutral hydrogen distribution of the IGM prior to reionisation. We consider the optical depth in the limit of a uniform IGM with neutral hydrogen density $n_{\text{HI}}(z)$ along the line of sight to a quasar at redshift z_s :

$$\tau_\nu = \int_0^{z_s} \sigma_{(1+z)\nu} n_{\text{HI}}(z) \left| \frac{dl_p}{dz} \right| dz \quad (1.18)$$

where the frequency argument of the Ly α cross section is the rest-frame frequency at redshift z corresponding to the received frequency ν . Assuming a simplified Dirac delta-function form for the absorption cross section, $\sigma_\nu = \sigma \times \delta_D(\nu - \nu_\alpha)$ where $\sigma = 0.011 \text{ cm}^2 \text{ Hz}$ is the frequency-integrated Ly α cross section, gives (Peebles [1993]):

$$\begin{aligned} \tau_\nu &= \sigma c \int_0^{z_s} \frac{n_{\text{HI}}(z)}{(1+z)H(z)} \delta_D[(1+z)\nu - \nu_\alpha] dz \\ &= \sigma c \int_0^{z_s} \frac{n_{\text{HI}}(z)}{\nu(1+z)H(z)} \delta_D \left[z - \left(\frac{\nu_\alpha}{\nu} - 1 \right) \right] dz \\ &= \left. \frac{\sigma c n_{\text{HI}}(z)}{\nu_\alpha H(z)} \right|_{z=\nu_\alpha/\nu-1} ; \quad \frac{\nu_\alpha}{1+z_s} < \nu < \nu_\alpha. \end{aligned} \quad (1.19)$$

For non-negligible $n_{\text{HI}}(z)$ across the line of sight the optical depth is sufficiently large to completely suppress the source flux for observed wavelengths $\lambda_\alpha(1+z_s) > \lambda > \lambda_\alpha$. This effect is known as the Gunn-Peterson effect after Gunn and Peterson [1965], and the optical depth is known as the Gunn-Peterson optical depth, τ_{GP} . The cosmological hydrogen density of the universe scales with redshift according to $n_{\text{H}}(z) = n_{\text{H}}(0)(1+z)^3$, where the present-day value is given by $n_{\text{H}}(0) = (1-Y)\Omega_{\text{b}}\rho_{\text{c}}(0)/m_{\text{H}} \simeq 8.41(\Omega_{\text{b}}h^2) \text{ m}^{-3} \simeq 0.17 \text{ m}^{-3}$, and the Hubble parameter may be approximated using the form $H(z) \simeq H_0\Omega_{\text{m}}^{1/2}(1+z)^{3/2}$ applicable for large z ; thus we may write:

$$\tau_{\text{GP}} = \frac{\sigma c x_{\text{HI}} n_{\text{H}}(0)}{\nu_\alpha H_0 \Omega_{\text{m}}^{1/2}} (1+z)^{3/2} \simeq 3.5 \times 10^5 \left[\frac{\Omega_{\text{b}} h}{\Omega_{\text{m}}^{1/2}} \right] x_{\text{HI}} (1+z)^{3/2}. \quad (1.20)$$

At source redshifts z_s with a non-negligible neutral fraction x_{HI} , effectively zero emission from the quasar at wavelengths blueward of Ly α is detected. This effect has been observed for quasars with a minimum redshift $z_s \simeq 6.3$ (Becker et al. [2001]), suggesting that reionisation was completed by this redshift.

We can gain some insight into the redshift at which reionisation began from the anisotropies in the CMB. These anisotropies are primarily associated with the matter content of the universe at recombination, however a secondary effect is imposed by scattering of CMB photons by the increased abundance of free electrons generated by reionisation. Assuming reionisation occurred instantaneously at a redshift z_r , the Thomson scattering optical depth for CMB photons can be estimated as:

$$\tau_e = \int_0^{z_r} \sigma_t n_e(z) \left| \frac{dl_p}{dz} \right| dz \quad (1.21)$$

where $\sigma_t = 6.65 \times 10^{-25} \text{ cm}^2$ is the Thomson scattering cross section. The electron density can be approximated by the form $n_e(z) \simeq n_e(0)(1+z)^3$ corresponding to fully ionised helium: $n_e(0) = (1 - Y/2)\Omega_b\rho_c(0)/m_H \simeq 9.81(\Omega_b h^2) \text{ m}^{-3}$. The Hubble parameter can be approximated as $H(z) \simeq H_0[\Omega_m(1+z)^3 + \Omega_v]^{1/2}$ for a flat universe. The electron scattering optical depth is then estimated as follows:

$$\begin{aligned} \tau_e &\simeq \frac{\sigma_t c n_e(0)}{H_0} \int_0^{z_r} \frac{(1+z)^2}{[\Omega_m(1+z)^3 + \Omega_v]^{1/2}} dz \\ &= \frac{\sigma_t c n_e(0)}{H_0} \times \frac{1}{3\Omega_m} \int_1^{\Omega_m(1+z_r)^3 + \Omega_v} t^{-1/2} dt \\ &\simeq 0.04 \left[\frac{\Omega_b h}{\Omega_m} \right] \left\{ [\Omega_m(1+z_r)^3 + \Omega_v]^{1/2} - 1 \right\}. \end{aligned} \quad (1.22)$$

This optical depth dampens the fluctuations in the CMB for small angular scales and introduces anisotropies in the CMB polarisation at larger angular scales. 5-year WMAP (Wilkinson Microwave Anisotropy Probe) CMB polarisation data yield an optical depth $\tau_e = 0.087 \pm 0.017$; from a comparison with a detailed calculation of τ_e for instantaneous reionisation similar to Eq. (1.22), the model-dependent reionisation redshift is estimated as $z_r = 11.0 \pm 1.4$ (Dunkley et al. [2009]). Assuming a more complex reionisation history can significantly alter the estimated redshift at which reionisation began, however an instantaneous reionisation at $z \sim 6.3$ is ruled out and together with the QSO absorption data it is clear that reionisation was an extended process.

Future studies of the IGM during the Epoch of Reionisation will require observations of the 21 cm line of neutral hydrogen, resulting from the hyperfine states of the ground state. Hyperfine structure arises from different values of F , the sum of the nuclear spin

I and the total angular momentum $J = L + S$; the hydrogen $1s$ ground state has $L = 0$ and F is given by the sum of nuclear and electron spins (both $1/2$). The resulting energy levels E_u ($F = 1$) and E_l ($F = 0$) have a transition energy $E_u - E_l = h_P \nu_{ul}$ for $\nu_{ul} = 1.42 \times 10^9$ Hz or $\lambda_{ul} = c/\nu_{ul} = 21.1$ cm. The states have degeneracies given by $g_F = 2F + 1$, giving a triplet state ($F = 1$) with $g_u = 3$ and a singlet state ($F = 0$) with $g_l = 1$. The relative occupancies of the states are described by the spin temperature T_s :

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp \left[-\frac{h_P \nu_{ul}}{k_B T_s} \right] = 3 \exp \left[-\frac{T_*}{T_s} \right], \quad (1.23)$$

where n_u , n_l are the number densities of hydrogen in each of the hyperfine states and $T_* = h_P \nu_{ul}/k_B = 0.068$ K. We see that if the hydrogen is in thermal equilibrium then the Boltzmann relation applies for n_u/n_l and the spin temperature is equal to the thermal or kinetic temperature of the gas, T_K .

The 21 cm line arises from a forbidden transition with spontaneous emission coefficient $A_{ul} = 2.85 \times 10^{-15} \text{ s}^{-1}$. The characteristic temperature T_* is significantly lower than typical temperatures of neutral hydrogen in the IGM and for any realistic spin temperature we can write $n_u/n_l \simeq 3$ and $n_l \simeq (1/4)n_{\text{HI}}$, $n_u \simeq (3/4)n_{\text{HI}}$. This is in contrast to the case of Ly α for which $h_P \nu_{\alpha}/k_B \sim 10^5$ K and thus $n_u \simeq 0$. The optical depth is determined by a calculation analogous to Eq. (1.19) assuming a delta-function form for the 21 cm absorption cross section, $\sigma_{ul} \delta_D(\nu - \nu_{ul})$ where $\sigma_{ul} = 3A_{ul}\lambda_{ul}^2/(8\pi) \simeq 1.5 \times 10^{-13} \text{ cm}^2 \text{ Hz}$. The resulting line-of-sight optical depth at received wavelength $\lambda_{ul}(1+z)$, such that photons redshift into the 21 cm line at z , is given by:

$$\begin{aligned} \tau_\nu|_{\lambda=(1+z)\lambda_{ul}} &= \frac{3A_{ul}\lambda_{ul}^3 n_{\text{HI}}(z) T_*}{32\pi |dv_{\parallel}/dr_{\parallel}| T_s(z)} \\ &\simeq 0.14 \left[\frac{\Omega_b h}{\Omega_m^{1/2}} \right] (1+z)^{3/2} \times \frac{x_{\text{HI}}[1+\delta]H}{|dv_{\parallel}/dr_{\parallel}| T_s} \Big|_z. \end{aligned} \quad (1.24)$$

Note that the H I number density in Eq. (1.19) has been replaced by the level population of the singlet state $n_l \simeq n_{\text{HI}}/4$, and the result is multiplied by an additional factor correcting for stimulated emission given by $1 - e^{-T_*/T_s} \simeq T_*/T_s$ for $T_* \ll T_s$. We have also allowed for a general line of sight velocity gradient $|dv_{\parallel}/dr_{\parallel}|$ and a neutral hydrogen number density $n_{\text{H}} x_{\text{HI}}[1+\delta]$ with neutral fraction x_{HI} and overdensity δ .

By observing at different wavelengths, the signal corresponds to a different redshift of emission/absorption and thus ‘21 cm tomography’ is possible (Madau et al. [1997]).

The 21 cm signal of the neutral hydrogen in the IGM preceding and during the Epoch of Reionisation is typically considered in the case of emission or absorption against the CMB background. The brightness temperature in the Rayleigh-Jeans limit at wavelength $\lambda = 21(1+z)$ cm of some cloud of H I at redshift z is given by:

$$T_b = T_s(1 - e^{-\tau_\nu}) + T_{\text{CMB}}(z)e^{-\tau_\nu} \quad (1.25)$$

where T_s is the H I spin temperature of the cloud, $T_{\text{CMB}}(z)$ is the CMB temperature at redshift z and τ is the 21 cm optical depth presented by the cloud along the line of sight. The differential antenna temperature δT_b seen by a radio telescope in a comparison setup at $z = 0$ is (Madau et al. [1997]):

$$\begin{aligned} \delta T_b &= \frac{T_b - T_{\text{CMB}}(z)}{1+z} = \left[\frac{T_s - T_{\text{CMB}}(z)}{1+z} \right] (1 - e^{-\tau_\nu}) \\ &\simeq \frac{3A_{\text{ul}}\lambda_{\text{ul}}^3 n_{\text{HI}}(z) T_*}{32\pi(1+z)|dv_{\parallel}/dr_{\parallel}|} \left[\frac{T_s - T_{\text{CMB}}(z)}{T_s} \right] \end{aligned} \quad (1.26)$$

where we have written $1 - e^{-\tau_\nu} \simeq \tau_\nu$ following from $\tau_\nu \ll 1$. Thus the 21 cm signal of the neutral hydrogen in the IGM is critically dependent upon the difference between the spin temperature and the CMB temperature at the redshift of interest:

- If $T_s \gg T_{\text{CMB}}(z)$, the neutral gas is observed in emission and δT_b takes on a value independent of the spin temperature.
- If $T_s \ll T_{\text{CMB}}(z)$, $|\delta T_b| \propto T_{\text{CMB}}(z)/T_s$ and so the neutral gas is seen in absorption, with a stronger signal than that of emission, presumably making detection an easier task.
- If $T_s = T_{\text{CMB}}(z)$, $\delta T_b = 0$ and we do not detect the gas against the CMB.

A detailed understanding of the physical mechanisms that determine the spin temperature is necessary to enable predictions of the observed 21 cm signal.

Radiation at the resonant frequency of the transition can cause absorption and stimulated emission, altering the hyperfine level populations and affecting the spin temperature. In the context of H I in the high-redshift universe, such radiation is provided

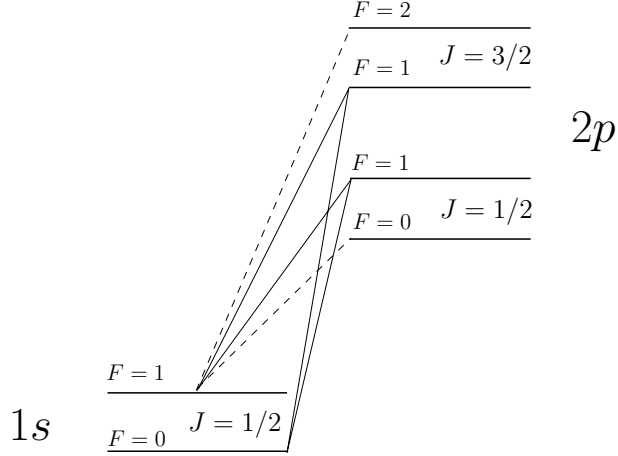


Figure 1.3: Energy level diagram of the $1s$ ground state and $2p$ excited state of hydrogen. The solid and dashed lines show allowed $\text{Ly}\alpha$ transitions, with the solid lines identifying those transitions responsible for the Wouthuysen-Field Effect.

by the continuum spectrum of the CMB at 21 cm. In the absence of other interactions, hydrogen bathed in CMB photons will have its spin temperature approach the frequency-independent (due to the black-body nature of the CMB) brightness temperature $T_{\text{CMB}} = 2.73(1+z)\text{K}$, on a timescale much less than the age of the universe. There are two important mechanisms in the high-redshift IGM that can compete with this process:

- (i) Collisions with other hydrogen atoms or electrons resulting in ‘spin exchange’, a reversal of the spin of the $1s$ electron, and eventual thermalisation with the kinetic temperature of the gas i.e. $T_s \rightarrow T_K$ (Purcell and Field [1956]). In the post-recombination universe such collisions are predominantly between hydrogen atoms.
- (ii) Scattering of $\text{Ly}\alpha$ photons which affect the H I spin temperature by the ‘Wouthuysen-Field Effect’ (WFE). A $\text{Ly}\alpha$ photon is absorbed by an H I atom, exciting the atom from the $1s$ state to the $2p$ state; the subsequent spontaneous emission of a $\text{Ly}\alpha$ photon can leave the atom in either of the $1s$ hyperfine states, see Figure 1.3. In the limit of many scatters the spin temperature will approach the $\text{Ly}\alpha$ colour temperature T_α of the radiation field, which itself will quickly thermalise with the kinetic temperature of the gas i.e. $T_s \rightarrow T_\alpha \rightarrow T_K$ (Wouthuysen [1952], Field [1958]).

1.2.1 Computation of 21cm Spin Temperature

In this section we outline the calculation of the spin temperature resulting from the influence of the CMB, collisions and Ly α scattering. The direct excitation and de-excitation rates for the hydrogen 1s hyperfine states due to scattering of 21 cm radiation are given respectively by:

$$P_{\text{lu}}^{\text{r}} = \bar{J}_{\text{ul}} B_{\text{lu}} = \frac{2k_{\text{B}}T_{\text{r}}}{\lambda_{\text{ul}}^2} \times \frac{g_{\text{u}}}{g_{\text{l}}} \left(\frac{c^2}{2h\nu_{\text{ul}}^3} \right) A_{\text{ul}} = 3 \left(\frac{T_{\text{r}}}{T_{*}} \right) A_{\text{ul}}, \quad (1.27)$$

$$P_{\text{ul}}^{\text{r}} = A_{\text{ul}} + \bar{J}_{\text{ul}} B_{\text{ul}} = \left(1 + \frac{T_{\text{r}}}{T_{*}} \right) A_{\text{ul}}, \quad (1.28)$$

where $\bar{J}_{\text{ul}}$ is the intensity of radiation at 21 cm averaged over angle and frequency, $T_{\text{r}} = T_{\text{CMB}}$ is the corresponding 21 cm radiation brightness temperature in the Rayleigh-Jeans limit and B_{lu} , B_{ul} are the Einstein B-coefficients for absorption and stimulated emission. In the absence of spin-exchange collisions or Ly α scattering, the hyperfine level populations will reach a steady state with $T_{\text{s}} = T_{\text{CMB}} = 2.73(1+z)$ K in the timescale $1/P^{\text{r}} \sim T_{*}/(A_{\text{ul}}T_{\text{r}}) \simeq 3 \times 10^5(1+z)^{-1}$ yr, effectively negligible by cosmological standards.

We now consider the corresponding rates arising from spin-exchange collisions between hydrogen atoms. The rates are written as $P_{\text{ul}}^{\text{c}} = n_{\text{H}}\kappa_{\text{ul}}(T_{\text{K}})$ and $P_{\text{lu}}^{\text{c}} = n_{\text{H}}\kappa_{\text{lu}}(T_{\text{K}})$ where the κ 's are rate coefficients dependent on the kinetic temperature of the gas T_{K} , and determined by quantum mechanical scattering calculations (see e.g. Furlanetto et al. [2006]). The ratio of the rate coefficients is given by the reciprocity relation $\kappa_{\text{lu}}/\kappa_{\text{ul}} = 3e^{-T_{*}/T_{\text{K}}}$ and thus:

$$\frac{P_{\text{lu}}^{\text{c}}}{P_{\text{ul}}^{\text{c}}} = 3 \exp \left[-\frac{T_{*}}{T_{\text{K}}} \right] \simeq 3 \left[1 - \frac{T_{*}}{T_{\text{K}}} \right], \quad (1.29)$$

where the small value of T_{*} relative to any realistic value of T_{K} permits us to expand the exponential.

Finally we consider the transition rates between the hyperfine states arising indirectly from the Ly α scattering Wouthuysen-Field Effect. The details of this process were described quantitatively by Field [1958]; by considering the hyperfine structure in both the 1s and 2p levels of hydrogen, Field showed that the effectiveness of the WFE in depopulating the triplet state is given by $P_{\text{ul}}^{\alpha} = (4/27)P_{\alpha}$ where P_{α} is the rate of

Ly α scattering of a hydrogen atom. Following Eq. (1.29) relating the transition rates between the H I hyperfine levels for the case of interaction with hydrogen atoms described by a kinetic temperature T_K , we suppose that the WFE rates P_{lu}^α , P_{ul}^α can be similarly related by:

$$\frac{P_{lu}^\alpha}{P_{ul}^\alpha} = 3 \left[1 - \frac{T_*}{T_\alpha} \right], \quad (1.30)$$

for a Ly α colour temperature T_α . It will be convenient to postpone the details of how P_α and T_α are explicitly determined from the radiation field until the next chapter. Wouthuysen argued that the colour temperature would, with an effectively infinite number of scatterings, tend to the kinetic temperature of the gas as the Ly α radiation field thermalised with the scattering medium (Wouthuysen [1952]).

We now seek to use these rates to specify the spin temperature. Following Field, we assume statistical equilibrium of the hyperfine levels so that $n_u P_{ul} = n_l P_{lu}$, thus:

$$\frac{P_{lu}^r + P_{lu}^c + P_{lu}^\alpha}{P_{ul}^r + P_{ul}^c + P_{ul}^\alpha} \equiv \frac{P_{lu}}{P_{ul}} = \frac{n_u}{n_l} \equiv 3 \exp \left[-\frac{T_*}{T_s} \right] \simeq 3 \left[1 - \frac{T_*}{T_s} \right]. \quad (1.31)$$

By using Equations (1.27) and (1.28) for the direct radiative (de-)excitation rates together with the ratios given in Equations (1.29) and (1.30), we obtain for T_s :

$$T_s = \frac{T_{\text{CMB}} + \gamma_c T_K + \gamma_\alpha T_\alpha}{1 + \gamma_c + \gamma_\alpha} \quad (1.32)$$

where the ‘pumping efficiencies’ for collisions and Ly α scattering are given respectively by γ_c and γ_α :

$$\gamma_c = \frac{T_*}{T_K} \frac{P_{ul}^c}{A_{ul}}, \quad (1.33)$$

$$\gamma_\alpha = \frac{T_*}{T_\alpha} \frac{P_{ul}^\alpha}{A_{ul}} = \frac{T_*}{T_\alpha} \frac{4P_\alpha}{27A_{ul}}. \quad (1.34)$$

Thus the efficiencies determine the spin temperature through a weighted average of the CMB temperature, the kinetic temperature of the hydrogen gas, and the colour temperature of the Ly α radiation. During the Epoch of Reionisation, the spin temperature is critically dependent upon the Ly α scattering rate P_α . Madau et al. [1997] define a threshold ‘thermalisation rate’ P_{th} from $\gamma_\alpha T_\alpha = T_{\text{CMB}}$:

$$P_{\text{th}} = \frac{27A_{ul}T_{\text{CMB}}}{4T_*} = 7.7 \times 10^{-13} (1+z) \text{ s}^{-1}. \quad (1.35)$$

For $P_\alpha \gg P_{\text{th}}$ we have $T_s \simeq T_\alpha \simeq T_K$: the $\text{Ly}\alpha$ scattering interaction acts as an intermediary to couple the spin temperature to the kinetic temperature of the gas.

1.2.2 Observations of the EoR 21cm Signal

The 21 cm signal at the Epoch of Reionisation is redshifted by the expansion of the universe and detected today at a frequency $\nu_{\text{ul}}/(1+z) \simeq 1.42 \text{ GHz}/(1+z) \simeq 129 \text{ MHz}$ for $z = 10$, corresponding to metre wavelengths. Detailed reviews of the observational prospects for detecting various signatures of the EoR are available, including Carilli [2008], Furlanetto et al. [2006] and Pritchard and Loeb [2011]. The most basic observations of the neutral hydrogen signal measure the sky-averaged global 21 cm signal against the CMB background; the resulting brightness temperature associated with the neutral hydrogen can be estimated, following Eq. (1.26) in the absence of any peculiar velocity or overdensity, as:

$$\begin{aligned} \delta T_{\text{b}} &= \frac{3A_{\text{ul}}\lambda_{\text{ul}}^3 n_{\text{HI}}(z) T_*}{32\pi(1+z)H(z)} \left[1 - \frac{T_{\text{CMB}}}{T_s} \right] \\ &\simeq 25x_{\text{HI}} \left[\frac{1+z}{10} \right]^{1/2} \left[1 - \frac{T_{\text{CMB}}}{T_s} \right] \text{ mK}. \end{aligned} \quad (1.36)$$

To understand the expected global H I 21cm signature during the EoR, we discuss the dependence on redshift of the spin temperature and the ionisation fraction:

- At very high redshifts $z \gtrsim 200$, the density of free electrons is sufficient to maintain thermal equilibrium between the CMB radiation and the matter by Compton scattering and thus $T_s = T_K = T_{\text{CMB}}$ and no 21 cm detection is possible.
- Below $z \sim 200$ the gas and radiation components thermally decouple and the adiabatic expansion of the universe gives the scaling $T_K \propto (1+z)^2$, while $T_{\text{CMB}} \propto (1+z)$. At these redshifts, the high density of baryons in the universe ensures that particle collisions couple the spin temperature to the gas temperature. Thus, as the gas cools faster than the radiation, the spin temperature will couple to $T_K < T_{\text{CMB}}$ and we would detect an H I absorption signature, although the signal would be observed at very low frequencies due to redshifting.

- At lower redshifts $z \lesssim 30$, the hydrogen density is low enough to render the effect of collisions on the spin temperature negligible, and T_s will subsequently tend to thermalise with the CMB. The 21 cm signal is suppressed.
- When sources of light in the universe begin to appear and emit UV radiation at $z \lesssim 15$, scattering of Ly α photons will couple T_s to the gas temperature T_K . Thus such sources will produce a 21cm absorption signature in the surrounding neutral gas.
- The large-scale heating of the IGM by X-rays from e.g. black hole accretion disks will eventually raise T_K above T_{CMB} (Madau et al. [1997], Chen and Miralda-Escudé [2004]). The absorption signal will become an emission signal.
- The progress of reionisation will reduce the volume of neutral hydrogen and begin to suppress the emission signal, which will eventually vanish entirely for $z \lesssim 6$.

The brightness temperature arising from the first sources, including various sources of heating, have been studied in many simulations by e.g. Gnedin and Shaver [2004] and Pritchard and Loeb [2010], while calculations of the absorption signature arising from collisions during the Dark Ages have been performed by Scott and Rees [1990]. An example model of the redshift-dependence of the EoR signal, from the collisional coupling during the Dark Ages to the end of reionisation and including heating effects, is displayed in Figure 1.4.

At metre wavelengths corresponding to the signal from Ly α coupling, major observational challenges are presented by foreground radiation arising from galactic synchrotron emission, radio-loud point sources, the Earth’s ionosphere and terrestrial Radio Frequency Interference (RFI). The foreground comprises a brightness temperature of several hundred Kelvin, many orders of magnitude greater than that of the neutral hydrogen during the EoR; in order to detect the reionisation signal we must somehow excise the foreground signal. Strategies to solve this problem are being developed based on the expected smoothness in frequency space of the foreground sources compared to the EoR signal. Observational prospects for detecting the all-sky signal do not require high angular resolution and can be performed by just a single dipole, as is the case with

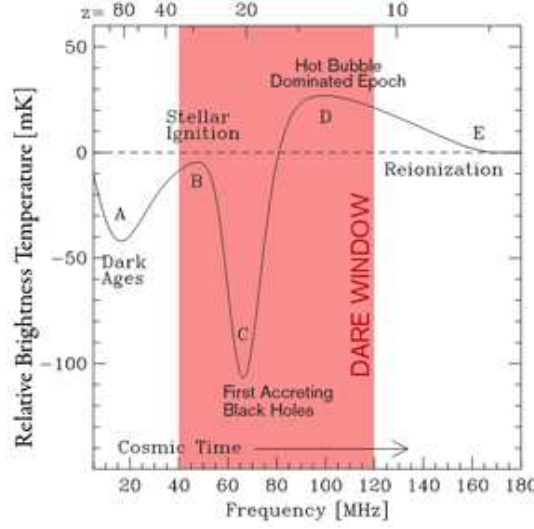


Figure 1.4: Model of expected 21 cm brightness temperature as a function of frequency and the corresponding H I redshift, from Burns et al. [2012]. The range of frequencies that will be studied by the Dark Ages Radio Explorer are highlighted and the epochs or events associated with the turning points marked A to E in the curve are labelled.

the Experiment to Detect the Global EoR Step² (EDGES) which has already yielded constraints on models of reionisation. More information on the EoR will be recovered from future projects such as the Dark Ages Radio Explorer³ (DARE). The DARE satellite will seek to study the global 21 cm signature from orbit about the moon, eliminating the ionosphere and providing a shield from RFI by taking measurements from the far side. DARE will launch in ~ 2016 and make observations of the global 21 cm signal for ~ 3 years in order to measure the frequencies and slopes of the turning points marked B, C and D in Figure 1.4, constraining properties of the first stars, the first X-ray sources and the early stages of reionisation. It should be noted that the signal from the collisionally coupled Dark Ages is observed at very low frequencies at which the foregrounds are much greater than at metre wavelengths; consequently all current and planned observational efforts are focused on the era of first light or later.

²<http://www.haystack.mit.edu/ast/arrays/Edges/>

³<http://lunar.colorado.edu/dare/>

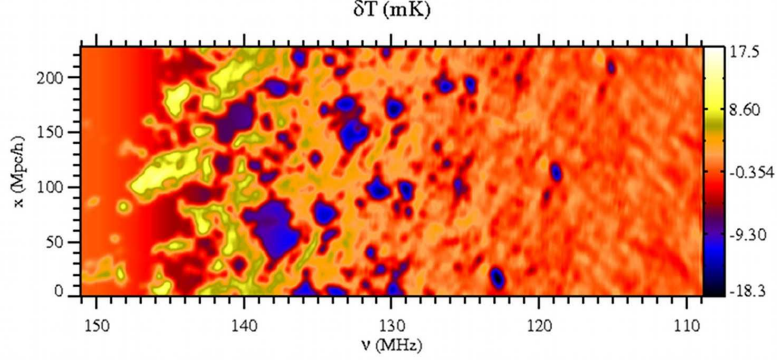


Figure 1.5: Variation of 21 cm brightness temperature with frequency and along a single spatial dimension arising from a simulation of reionisation and heating effects of the first sources. The frequency axis corresponds to $z \simeq 8.5 \rightarrow 11$. Image credit: Garrelt Mellema, Ilian Iliev.

A more detailed description of the EoR will be obtained from studying the power spectrum of fluctuations in the 21 cm signal, arising from fluctuations in H I overdensity, peculiar velocity, ionisation and radiation fields responsible for the spin temperature by Ly α coupling and X-ray heating [see Eq. (1.26)]. An example simulation of the variation in the detected signal, along an axis on the sky and with frequency, is displayed in Figure 1.5; the power spectrum is a three-dimensional quantity that characterises the fluctuations in the plane of the sky and along the line of sight (responsible for frequency fluctuations). Studies of the 21 cm power spectrum require high angular resolution and therefore large-baseline interferometric arrays are necessary, in contrast to the modest requirements for resolving the global signal. The observed power spectrum is strongly contaminated by radio sources and much investigation is being undertaken to enable extraction of this and other foreground contributions. Arrays such as the Giant Meterwave Radio Telescope⁴ (GMRT) have placed upper limits on the magnitude of the power from the EoR at a limited selection of redshifts (Paciga et al. [2011]), however a range of projects developed with the EoR 21 cm fluctuations as primary science goals will improve on these detections. Interferometric arrays studying the EoR fluctuations

⁴<http://www.gmrt.ncra.tifr.res.in/>

need to have wide fields of view, providing many independent samples for computing the power spectrum, as well as excellent frequency sensitivity as will be required to allow accurate removal of foreground contamination. A relatively low-cost tool for the study of the EoR signal is the Precision Array for Probing the Epoch of Reionisation⁵ (PAPER), a dipole array interferometer with collecting area $\sim 10^3 \text{ m}^2$. Studies are also feasible with the greater sensitivity provided by the general-purpose LOw Frequency ARray⁶ (LOFAR, $\sim 10^5 \text{ m}^2$) and the wider field-of-view Murchison Widefield Array⁷ (MWA, $\sim 10^4 \text{ m}^2$). These projects are all currently making observations and results should be forthcoming in the near future, although the focus at present is firmly centred on tackling the foreground removal problem and concrete results on the EoR signal will be slower to arrive. In addition to studies of the power spectrum, PAPER, LOFAR and the MWA are also expected to detect signatures of Cosmic Stromgren Spheres, large H II regions carved out by QSOs or groups of galaxies during the latter stages of reionisation. These are seen as roughly spherical dark patches against the surrounding H I 21 cm emission.

The study of the power spectrum of 21 cm fluctuations falls short of full 21 cm tomography, direct imaging of the EoR. Such observations will require extremely high angular resolution, as well as even more accurate methods of foreground removal. The baselines necessary could be provided by the Square Kilometre Array⁹ (SKA), which will provide an effective collecting area of 10^6 m^2 . Construction will begin in ~ 2016 before completion sometime in the next decade. A simulated radio map is displayed in Figure 1.6 as a speculative example of the kind of imaging possible with the SKA; there is the potential to image neutral hydrogen on scales down to a comoving Megaparsec.

A possible avenue of cosmological H I detection using the 21 cm line with an entirely different physical origin is absorption against sources of radio emission, the so-called ‘21 cm forest’ caused by neutral hydrogen concentrations along the line of sight. The

⁵<http://eor.berkeley.edu/>

⁶<http://www.lofar.org>

⁷<http://www.mwatelescope.org/>

⁹<http://www.skatelescope.org/>

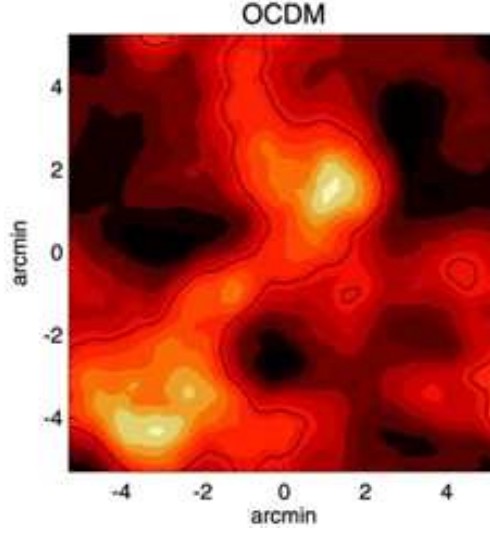


Figure 1.6: Simulated radio image of a 21 cm emission signature of cosmological density fluctuations (the ‘cosmic web’) at $z = 8.5$, for a box of side $20h^{-1}$ Mpc (comoving), assuming an open, CDM-dominated universe with $\Omega_m = 0.4$, $\Omega_v = 0$ and $h = 0.65$. The colour intensity represents a flux of $1 \rightarrow 6 \mu\text{Jy}$ per beam on a linear scale, while the contours denote emission exceeding $4 \mu\text{Jy}$ per beam. Taken from Tozzi et al. [2000].

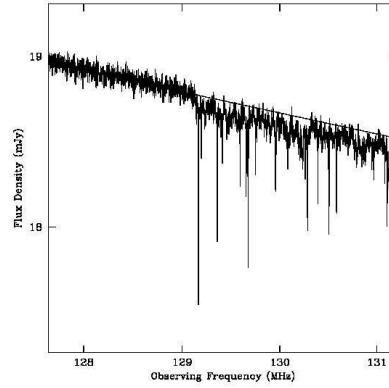


Figure 1.7: Simulated spectrum of continuum source at $z = 10$ based on SKA-derived observational parameters. Absorption lines analogous to the $\text{Ly}\alpha$ forest, and a mean decrement in the flux arising from a value of the 21 cm Gunn-Peterson optical depth $\tau_{\text{GP}}^{21} \ll 1$, are seen for frequencies greater than $\nu_{\text{ul}}/(1+z) \simeq 129$ MHz. Taken from Carilli et al. [2002].

21 cm optical depth is typically much less than unity, and thus these observations are in principle more sensitive to gas density compared with the Ly α absorption studies. An example of these observations based on simulations is given in Figure 1.7; this approach has the advantage of not limiting the spatial resolution that can be probed, allowing detection of e.g. filaments of H I structure or minihaloes (Meiksin [2011]), although the number of sufficiently bright sources at these high redshifts is currently unknown and presumably limited.

1.3 Ly α Scattering

Prediction and interpretation of the redshifted neutral hydrogen 21 cm signal corresponding to the Epoch of Reionisation will require detailed simulations of the fluctuations in the H I spin temperature caused by Ly α scattering. This Ly α scattering is dominated by UV emission from the first sources; a photon emitted at a frequency between Ly α and the higher-energy Lyman-beta resonance will be scattered when its redshifted frequency seen by a Hydrogen atom comoving with the expansion of the universe approaches the Ly α frequency. As the distributions, emissivities, lifetimes and other properties of the first sources are not known, however, simplified models are typically used to represent the Ly α scattering and the WFE during the EoR.

Preliminary investigations of the 21 cm signal during the EoR postulated a homogeneous Ly α background spectrum resulting from the summed emission from many sources (Madau et al. [1997]). The range in redshift, if any, over which such a background might provide a good description of the Ly α radiation field during the EoR is poorly understood. Several studies have focused on the signal induced by a single source, presumably applicable at least for the very first UV sources. A trivial solution for this problem is obtained by assuming photons travel uninterrupted before scattering at the local Ly α frequency, resulting in a $1/r^2$ radius dependence for P_α . However, these basic treatments ignore much of the physics behind resonance-line scattering that affects the spectrum and the scattering rate as determined by detailed radiative transfer calculations or Monte Carlo simulations.

Radiative transfer is necessary for accurate quantitative treatments of $\text{Ly}\alpha$ scattering. Many authors have sought a homogeneous background spectrum that has a frequency-dependence derived from the radiative transfer equation for an infinite homogeneous medium (e.g. Chen and Miralda-Escudé [2004], Furlanetto and Pritchard [2006]). The properties of such solutions have been well-developed, however they are limited in how they can represent the real universe during the EoR. Attempts to examine the effect of radiative transfer for a single source have used Monte Carlo methods to determine the variation of the $\text{Ly}\alpha$ scattering rate as a function of radius for various spherically symmetric configurations (e.g. Chuzhoy and Zheng [2007], Semelin et al. [2007]). Inevitably, the definitive quantitative analyses on this topic will only come from complex codes developed to treat the radiative transfer for general configurations of sources and neutral hydrogen density, with properties derived from cosmological simulations. Many groups are developing and applying codes of this type offering various levels of functionality (e.g. Pierleoni et al. [2007], Semelin et al. [2007]).

We present a detailed summary of the physics and mathematical description of resonance-line scattering necessary to solve the radiative transfer problem in order to compute the line photon spectrum and line photon scattering rate per atom, as well as existing test problems and solutions, in Chapter 2. Subsequent chapters present our own work: we look at the $\text{Ly}\alpha$ scattering radiative transfer in homogeneous and spherically symmetric systems. We place emphasis on problems relevant to the $\text{Ly}\alpha$ scattering during the early stages of the Epoch of Reionisation. In chapter 3 we obtain simple steady-state analytic solutions in a locally homogeneous approximation that allow qualitative insight into the effects of the density and velocity structure of the IGM on the $\text{Ly}\alpha$ scattering rate. We also solve the corresponding time-dependent problem numerically in a number of cases. In chapters 4 and 5 we describe implementations and tests for Monte Carlo and grid-based strategies, respectively, for solving the transfer problem in spherical symmetry. In chapter 6 we apply both methods to the problem of a continuum source in a uniform IGM undergoing expansion with the Hubble law. We examine the applicability of these methods to a more general spherically symmetric problem with example profiles for the density and velocity.

CHAPTER 2

Ly α Radiative Transfer

In our introduction we discussed the astrophysical context to our work, the Epoch of Reionisation, and outlined the basic physics of the neutral hydrogen 21 cm signal and its dependence on the Ly α scattering rate via the Wouthuysen-Field Effect. As the radiative transfer of Ly α resonance-line scattering plays a vital part in our work, this chapter aims to provide a detailed account of the relevant background theory before providing a summary of various existing results found in the literature. The contents of this chapter are ordered as follows:

- In section 2.1 we describe the effect of an atomic resonance line on the frequency and direction of a scattered photon and define the scattering redistribution function.
- In sections 2.2 and 2.3 we summarise the physical processes such as natural and thermal broadening that affect the form of the type II frequency redistribution function and the associated absorption profile. We summarise useful approximate forms for these functions in the line core and line wing frequency regimes.
- In section 2.4 we examine the equation of radiative transfer for the resonance-line scattering process in various geometries using the redistribution function to specify

the emission and absorption coefficients, and some widely-used approximations to these equations are described.

- In section 2.5 we outline an alternative approach to solving the radiative transfer problem using Monte Carlo methodology.
- Section 2.6 briefly outlines the calculation of the Ly α scattering rate P_α and other physically relevant quantities from the Ly α radiation spectrum.
- In sections 2.7 and 2.8 we summarise existing solutions and results for radiative transfer in a homogeneous medium and a spatially one-dimensional medium respectively.

Note that this chapter is a somewhat exhaustive description of the language used and example results found in the literature on Ly α scattering but it can easily be skipped over by the reader initially and referred back to later if needed.

2.1 Scattering Description

The Ly α scattering process responsible for the Wouthuysen-Field effect is a common example in astrophysics of the general process of resonance line scattering. Resonance line scattering can be described in the context of the simple 2-level model of the atom as follows (see Figure 2.1):

- A photon of frequency ν' travelling in direction $\mathbf{n}'$ is absorbed by an atom of resonance frequency ν_0 , moving with a thermal velocity $\mathbf{v}$; the photon causes radiative excitation of the atom i.e. promotes an electron from the lower state (l) to the upper state (u).
- The atom decays back to the initial state ($u \rightarrow l$), emitting a photon of frequency ν in direction $\mathbf{n}$; generally we will have $\mathbf{n} \neq \mathbf{n}'$ and thus $\nu \neq \nu'$ (due to Doppler shifting at the very least, see later).

The photon's interaction with the resonance line of the atom causes a deflection and a change in frequency.

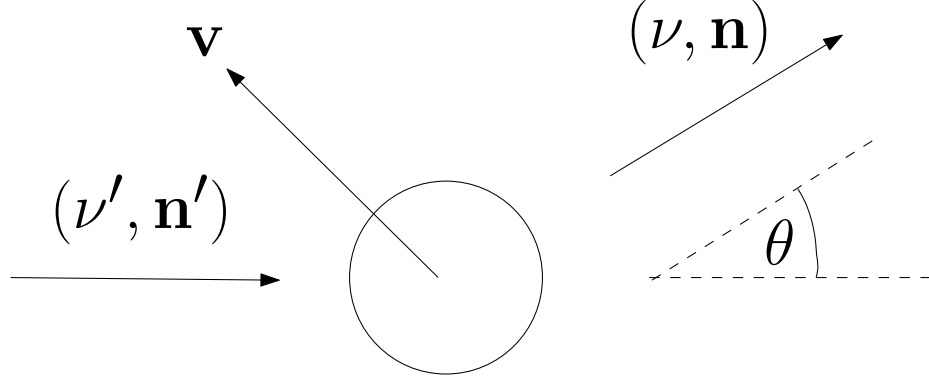


Figure 2.1: Sketch of absorbed photon $(\nu', \mathbf{n}')$, re-emitted photon $(\nu, \mathbf{n})$ and scattering atom (thermal velocity $\mathbf{v}$).

To describe quantitatively the effects of resonance line scattering we use the ‘redistribution function’ $R(\nu', \mathbf{n}'; \nu, \mathbf{n})$, defined (in accordance with the conventions of Mihalas [1978] Ch.13) such that the probability of scattering of a photon from frequency $\nu' \rightarrow \nu' + d\nu'$ and direction within solid angle $d\omega'$ about $\mathbf{n}'$ to frequency $\nu \rightarrow \nu + d\nu$ and direction within solid angle $d\omega$ about $\mathbf{n}$ is given by:

$$R(\nu', \mathbf{n}'; \nu, \mathbf{n}) d\nu' d\nu \frac{d\omega'}{4\pi} \frac{d\omega}{4\pi}. \quad (2.1)$$

This function is normalised such that integration over all 4 variables (incoming direction and frequency, outgoing direction and frequency) gives unity. An important quantity related to the redistribution function is the ‘line absorption profile’ $\varphi(\nu)$;

$$\varphi(\nu') = \frac{1}{4\pi} \oint d\omega \int_0^\infty d\nu R(\nu', \mathbf{n}'; \nu, \mathbf{n}). \quad (2.2)$$

This acts as a probability distribution function for the frequency at which the photon is absorbed; from the interpretation of the redistribution function, we can say that $\varphi(\nu') d\nu'$ is the probability of scattering from $\nu' \rightarrow \nu' + d\nu'$ to any other frequency (equivalently interpreted as the probability of absorption). Note that the line profile is normalised according to $\int_0^\infty \varphi(\nu) d\nu = 1$. In the following sections we will describe the physics relevant to the astrophysical Ly α resonance line scattering process and the corresponding forms for the line profile and the redistribution function.

2.2 Absorption Profile

For a resonance line centred on some frequency ν_0 , a first approximation to the absorption profile is provided by a Dirac delta-function at the resonant frequency, $\varphi(\nu) = \delta_D(\nu - \nu_0)$; no photons are absorbed other than those with exactly the right frequency to excite the relevant atomic transition. In attempts to quantify Ly α scattering in an astrophysical context it will prove necessary to consider a broadened line profile, with a non-zero probability for absorption in some narrow region about ν_0 .

First we examine the origin of ‘natural broadening’, associated with the finite energy width of the excited state. Consider an isolated 2-level atom in its rest frame, with an excited state of finite lifetime τ_u and corresponding decay rate $\Gamma \equiv A_{ul} = \tau_u^{-1}$; the uncertainty principle tells us that the excited state has a finite energy width $\Delta E \approx \hbar\Gamma$, while the ground state is assumed to have an infinite lifetime and therefore zero line width. A quantum mechanical justification for the shape of the naturally-broadened profile is given by Mihalas, following the theory developed by Weisskopf and Wigner; the wavefunction of the excited state has time dependence $\sim \exp(-[i\omega_0 + \Gamma/2]t)$, where $\omega_0 = 2\pi\nu_0$ and the $\Gamma/2$ component is required by noting that the corresponding probability of finding the atom in the excited state decays as $\exp(-\Gamma t)$. The probability distribution for the energy of the excited state is given by the squared modulus of the Fourier transform of the wavefunction:

$$P(\omega) \propto \left| \int_0^\infty \exp([i(\omega - \omega_0) - \Gamma/2]t) dt \right|^2 = [(\omega - \omega_0)^2 + (\Gamma/2)^2]^{-1}$$

and thus the normalised absorption profile as a function of frequency is:

$$\varphi(\nu) = \frac{\Gamma}{4\pi^2} \left[\frac{1}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2} \right] \quad (2.3)$$

i.e. the line shape adopts a Lorentz profile, analogous to the energy spectrum of a damped classical oscillator with damping constant Γ .

In typical astrophysical situations we have to deal with a further contribution to the line broadening arising when we consider the absorption profile of an ensemble of atoms with a thermal velocity distribution, ‘Doppler broadening’. Consider an atom seen to have thermal velocity component $v_{\parallel}$ along the line of sight from the observer;

if the observer then sends a photon of frequency ν towards the atom, the atom (in its rest frame) will see the photon at frequency $\nu(1 - v_{\parallel}/c) \simeq \nu - \nu_0(v_{\parallel}/c)$. The resulting absorption profile then becomes a convolution of the rest-frame profile (which we denote φ^{RF}) and the Maxwellian distribution of the thermal velocity component along the line of sight; for atoms of mass m at temperature T :

$$\varphi(\nu) = \int_{-\infty}^{\infty} \varphi^{\text{RF}} [\nu - (\nu_0/c)v_{\parallel}] p(v_{\parallel}) dv_{\parallel}, \quad (2.4)$$

where the velocity component has the distribution

$$p(v_{\parallel}) = \left(\frac{m}{2\pi k_{\text{B}} T} \right)^{1/2} e^{-mv_{\parallel}^2/2k_{\text{B}} T}. \quad (2.5)$$

In the case of an excited state with infinitely-long lifetime the convolution yields the Doppler profile, a Gaussian centred on ν_0 :

$$\begin{aligned} \varphi(\nu) &= \int_{-\infty}^{\infty} \delta_{\text{D}} [\nu - \nu_0 - (\nu_0/c)v_{\parallel}] p(v_{\parallel}) dv_{\parallel}, \\ &= \frac{c}{\nu_0} \left(\frac{m}{2\pi k_{\text{B}} T} \right)^{1/2} \exp \left[-\frac{mc^2(\nu - \nu_0)^2}{2\nu_0^2 k_{\text{B}} T} \right]. \end{aligned} \quad (2.6)$$

At this stage a particularly useful change of variables becomes apparent. If we define the typical thermal velocity or Doppler ‘b parameter’ $b \equiv (2k_{\text{B}}T/m)^{1/2}$, we see that we can write the Doppler width as $\Delta\nu_{\text{D}} = \nu_0(b/c)$, defined such that the exponential in Eq. (2.6) becomes $\exp [-(\nu - \nu_0)^2/(\Delta\nu_{\text{D}})^2]$. We now introduce the variable $x \equiv (\nu - \nu_0)/\Delta\nu_{\text{D}}$, the frequency offset from line centre in Doppler widths. We can then write the line absorption profile as a function of x , $\phi(x) = (\Delta\nu_{\text{D}})\varphi(\nu)$, in the case of both the Doppler and Lorentz profiles respectively as:

$$\phi_{\text{D}}(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}, \quad (2.7)$$

$$\phi_{\text{L}}(a, x) = \frac{a}{\pi} \left[\frac{1}{a^2 + x^2} \right]. \quad (2.8)$$

In Eq. (2.8) we have introduced the ‘Voigt parameter’ $a \equiv \Gamma/(4\pi\Delta\nu_{\text{D}})$ which gives an indication of the width of the Lorentz profile relative to the Doppler profile. For Ly α scattering we can take $\nu_0 = \nu_{\alpha} = 2.47 \times 10^{15}$ Hz and $\Gamma = \Gamma_{\alpha} = 6.26 \times 10^8$ Hz, while $m = m_{\text{H}} = 1.66 \times 10^{-27}$ kg and we obtain $a \simeq 0.0472(T/\text{K})^{-1/2}$.

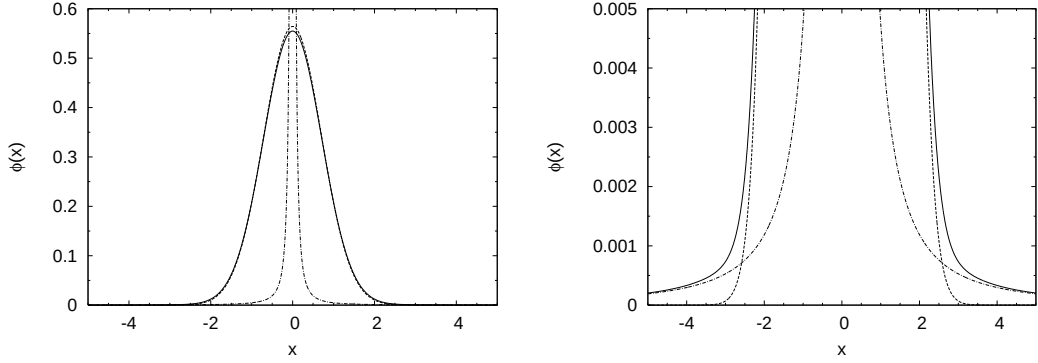


Figure 2.2: Left panel: normalised line profiles for $T = 10$ K: Voigt profile (Eq. (2.9), solid line), Doppler profile (Eq. (2.7), dotted line) and Lorentz profile (Eq. (2.8), dotted-dashed line). Right panel: Zoomed-in view to highlight behaviour in the wings.

While it is useful to study both natural broadening and Doppler broadening in isolation, we need to look at the more applicable case of a naturally-broadened line profile that undergoes further Doppler broadening. If we take the Lorentz profile of Eq. (2.3) to be the rest-frame profile $\varphi^{\text{RF}}(\nu)$ in Eq. (2.4), adopt the integration variable $y = v_{\parallel}/b$, and adopt x as the frequency variable, we obtain (see e.g. Rybicki and Lightman [1979]):

$$\phi_V(a, x) = \pi^{-1/2} H(a, x), \quad (2.9)$$

$$H(a, x) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{a^2 + (x - y)^2} dy. \quad (2.10)$$

This form for the absorption line profile is called the Voigt profile and is plotted in Figure 2.2, along with the Lorentz and Doppler profiles.

Clearly the Voigt profile resembles the Doppler profile near line centre ($x = 0$) and at large x begins to resemble the Lorentz profile. As such we adopt the following approximation for the Voigt profile that divides the functional form into a ‘Doppler core’ about line centre and ‘Lorentz wings’ outside this region (see Mihalas for a mathematical justification arising from an expansion of the integrand of $H(a, x)$):

$$\phi_V(a, x) = \begin{cases} \frac{1}{\sqrt{\pi}} e^{-x^2} & ; \quad |x| \leq x_m \\ \frac{a}{\pi x^2} & ; \quad |x| > x_m \end{cases} \quad (2.11)$$

where we have assumed $x \gg a$ in the wings and the boundary is set to the outermost crossover of the two functional forms. For $T = 10\text{ K}$ and $a = 0.015$, this is given by $x_m = 2.58$. While Eq. (2.9) suggests numerical integration is required to evaluate the Voigt profile, the form given by Eq. (2.11) is useful in approximate analytic calculations.

2.3 Redistribution Function

In this section we expand on the physics of resonance line scattering and introduce the appropriate form for the previously defined redistribution function, before examining some of its more important properties. Many of the arguments and results summarised in this section are expounded comprehensively in Hummer [1962]. As mentioned previously, line scattering involves photon absorption followed by photon emission. We start by considering absorption and re-emission of a photon in the rest frame of the scattering atom. We can write the redistribution function for scattering in the rest frame as follows:

$$R^{\text{RF}}(\xi', \mathbf{n}'; \xi, \mathbf{n}) = \varphi^{\text{RF}}(\xi') \times p^{\text{RF}}(\xi | \xi') \times g(\mathbf{n}', \mathbf{n}) \quad (2.12)$$

where we have used ξ to represent rest frame photon frequencies; the function $p^{\text{RF}}(\xi | \xi')$ acts as a conditional probability distribution function for the emission frequency ξ given absorption at frequency ξ' , while the phase function $g(\mathbf{n}', \mathbf{n})$ describes the directional redistribution. We can deduce the forms that these functions will take by interpreting a broadened excited state in terms of ‘substates’: the excited state (e.g. state ‘u’ of the 2-level atom) is comprised of a continuum of substates, the probability density distribution of which in frequency space determines a range of frequencies at which a photon can be absorbed and is given by the line absorption profile. Now consider the form of the factorised redistribution function in the rest frame (we assume our atom to be excited from the ground state):

- The upper level has finite width thus the absorption profile (and therefore the substate distribution about the resonant frequency) adopts a Lorentz profile $\varphi(\xi') = (\Gamma/4\pi^2)[(\xi' - \nu_0)^2 + (\Gamma/4\pi)^2]^{-1}$. The Lorentz profile is used as natural broadening is the only source of line broadening in the atomic rest frame.

- The atom absorbs at frequency ξ' ; thus the atom is excited to the substate of energy $h_P \xi'$. Upon return from this substate to the ground state a photon of frequency ξ is emitted, but as the ground state has fixed energy we know $\xi = \xi'$ (this argument assumes there is no mechanism to allow the atom to alter the excited substate prior to re-emission, such as collisions between atoms). Thus $p(\xi | \xi') = \delta_D(\xi - \xi')$.
- The phase function $g(\mathbf{n}', \mathbf{n})$ should really be written $g(\mathbf{n}' \cdot \mathbf{n})$, as it is invariably a function of the angle between the 2 directions only; the form of the functional dependence is determined by the quantum numbers involved in the transition. It is usual to assume isotropy i.e. $g(\mathbf{n}' \cdot \mathbf{n}) = 1$, although dipole scattering for which $g(\mathbf{n}' \cdot \mathbf{n}) = \frac{3}{4}[1 + (\mathbf{n}' \cdot \mathbf{n})^2]$ may also be appropriate.

The single-atom redistribution function in the laboratory frame is then obtained by applying the following Doppler shifts to Eq. (2.12):

$$\nu' = \xi' + \nu_0 \left[\frac{\mathbf{v} \cdot \mathbf{n}'}{c} \right], \quad \nu = \xi + \nu_0 \left[\frac{\mathbf{v} \cdot \mathbf{n}}{c} \right] \quad (2.13)$$

where $\mathbf{v}$ is the velocity of the atom in the lab frame due to thermal motions. Note that while the frequencies are transformed between the 2 frames, aberration of the photon direction vectors is neglected. To obtain a redistribution function that will be applicable to a population of atoms it is then necessary to average over the Maxwellian thermal velocity distribution for $\mathbf{v}$. The result, written in terms of Doppler widths from line centre x where $R(x', \mathbf{n}'; x, \mathbf{n}) = (\Delta\nu_D)^2 R(\nu', \mathbf{n}'; \nu, \mathbf{n})$, is:

$$\begin{aligned} R_{\Pi}(x', \mathbf{n}'; x, \mathbf{n}) &= \frac{g(\mathbf{n}', \mathbf{n})}{\pi \sin \theta} \exp \left[- \left(\frac{x' - x}{2} \right)^2 \csc^2 (\theta/2) \right] \\ &\times H \left(a \sec (\theta/2), \frac{1}{2}(x' + x) \sec (\theta/2) \right) \end{aligned} \quad (2.14)$$

where θ is the angle between the photon directions and H is the Voigt function defined in Eq. (2.9). From this form we obtain the angle-averaged redistribution function $R(x', x) = (1/4\pi) \oint d\omega R(x', \mathbf{n}'; x, \mathbf{n})$:

$$R_{\Pi}(x', x) = \frac{1}{\pi^{3/2}} \int_{(\bar{x}-\underline{x})/2}^{\infty} \left[\tan^{-1} \left(\frac{\underline{x} + u}{a} \right) - \tan^{-1} \left(\frac{\bar{x} - u}{a} \right) \right] e^{-u^2} du \quad (2.15)$$

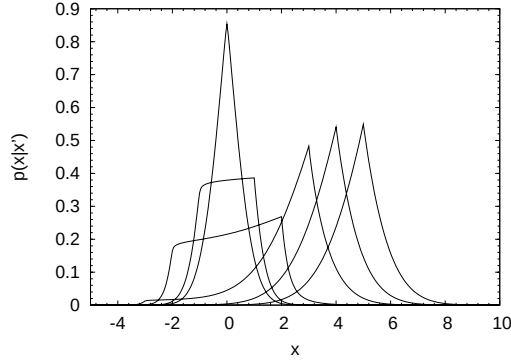


Figure 2.3: $p(x|x') = R_{\text{II}}(x', x)/\phi_V(a, x')$ for $x' = 0, 1, 2, 3, 4, 5$ in order of peak value from left to right with $a = 0.015$ ($T = 10$ K).

where $\bar{x} = \max(x, x')$ and $\underline{x} = \min(x, x')$. The subscript ‘II’ is used here as this redistribution function applies to ‘type II redistribution’: the atom in the rest frame is excited from the ground state to some naturally broadened upper state, and the medium is assumed to have a sufficiently low density that there is no broadening from collisions between atoms. These are the same conditions that determine a Voigt function line profile and the integration of R_{II} over all emitted frequencies recovers the Voigt profile, $\phi_V(x) = \int_{-\infty}^{\infty} R_{\text{II}}(x, x') dx'$. Type II applies in astrophysical scattering problems including Ly α scattering in low-density H I media. It is worth noting that type I redistribution is the limit of type II when the upper state has zero energy width, while types III and IV correspond to redistribution with collisional broadening of the upper state (important in high density media), and natural broadening of both the upper and lower state (important if the transition occurs between 2 excited states) respectively. Detailed examinations of the various redistribution functions are provided by Hummer [1962] and Mihalas [1978] Ch.13.

It is worthwhile to look at the conditional probability that a photon absorbed at x' will be re-emitted at x , obtained from the redistribution function by appropriate normalisation: $p(x|x') = R(x', x)/\phi(x')$. This function is plotted in Figure 2.3 for a series of values of x' . Following Mihalas, we can explain the displayed frequency distributions qualitatively. Consider the extreme case of a delta-function line profile in the atom’s rest frame (actually type I redistribution): the atom can only absorb

at $\xi' = \xi_0$ i.e. $x' = (\mathbf{v} \cdot \mathbf{n}')/b$. For a given value of x' , that the photon was absorbed implies the atom has velocity $\mathbf{v}$ such that $v/b > |x'|$. The emitted photon will have $x = (\mathbf{v} \cdot \mathbf{n})/b$; due to the isotropic nature of the scattering, we can see that the emitted photon frequencies are equally distributed on $[-x', x']$, while the probability distribution for frequencies outwith this range will drop off exponentially as the required value for v increases. In Figure 2.3, we see that curves corresponding to absorption near the line centre ($x' = 0, 1, 2$) closely resemble the result predicted; this can be understood if we argue that the atoms' thermal velocities allow them to absorb primarily at line centre in the rest frame. At larger x' few atoms have a sufficient thermal velocity to allow them to absorb at line centre, and consequently those atoms with low thermal velocity absorb in the wings of the Lorentz profile (again in the rest frame). The subsequent output frequencies are tightly distributed about x' due to the weakened Doppler broadening, resulting in scattering events that are nearly coherent ($x \simeq x'$).

2.3.1 Approximations and Limiting Behaviour

Similarly to the piecewise approximation to the Voigt profile, it is useful to be able to use a simpler form for the R_{II} redistribution function applicable in a given frequency regime. Making use of an expansion of $H(a, x)$ in Eq. (2.14) and looking at the resulting angle-average gives a series expansion for R_{II} (see Adams et al. [1971]). The zeroth order term in a (the appropriate form to use when $a \rightarrow 0$) has the form:

$$R_{\text{I}}(x|x') = \frac{1}{\sqrt{\pi}} \int_{|x|}^{\infty} e^{-u^2} du \quad (2.16)$$

where $\overline{|x|} = \max(|x|, |x'|)$. This particular form is labelled R_{I} as it is exactly the redistribution function appropriate in type I redistribution (the absence of natural damping, consistent with the limit $a = 0$). Integration over outgoing frequencies yields the Doppler line profile, $\phi_{\text{D}}(x)$. The probability density curves $p(x|x') = R_{\text{I}}(x', x)/\phi_{\text{D}}(x)$ resulting from Eq. (2.16) are shown in Figure 2.4. Photons are re-emitted with a frequency distribution symmetric about the line centre and constant on $[-x', x']$. The probability distribution curves have the same form as those for the type II redistribution function for absorption near line centre and Eq. (2.16) is clearly a good approxi-

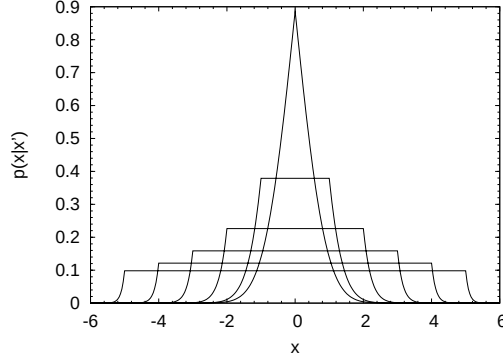


Figure 2.4: $p(x|x') = R_I(x', x)/\phi_D(x')$ for $x' = 0, 1, 2, 3, 4, 5$ in order of decreasing height.

mation for frequency redistribution within the core of the line, where the wings have no influence.

The first order term in a in the expansion of $H(a, x)$ gives a more complicated contribution to the redistribution function. The resulting term in the limit of small $|x - x'|$ can be written as:

$$R(x', x) = \frac{a}{\pi} \left(\frac{x + x'}{2} \right)^{-2} \text{ierfc} \left(\frac{\bar{x} - \underline{x}}{2} \right) \quad (2.17)$$

where

$$\text{ierfc}(y) \equiv \int_y^\infty \text{erfc}(t) dt = \frac{1}{\sqrt{\pi}} e^{-y^2} - y \text{erfc}(y). \quad (2.18)$$

With the condition that $|x - x'|$ is small and $|x|, |x'| \gg 1$, i.e. redistribution in the wings of the line, it is found that the form above is an excellent approximation to the full R_{II} function (Unno [1952]). We can simplify this further if we make the approximation $x/x' \approx 1$; in this case upon dividing through by the wing form of $\phi(x)$, given by $a/(\pi x^2)$, the probability distribution for the emitted frequency becomes $p(x|x') \simeq \text{ierfc}(\Delta)$, $\Delta \equiv (\bar{x} - \underline{x})/2$ i.e. the emitted frequency distribution is a function only of the difference from the absorbed frequency. Figure 2.5 shows the accuracy resulting from the two approximate forms of the redistribution function discussed here.

Finally for this section we look at two idealised forms of the redistribution function appropriate in particular limits, coherent redistribution and complete redistribution:

(i) Coherent redistribution: The photon is absorbed at lab frame frequency shift x'

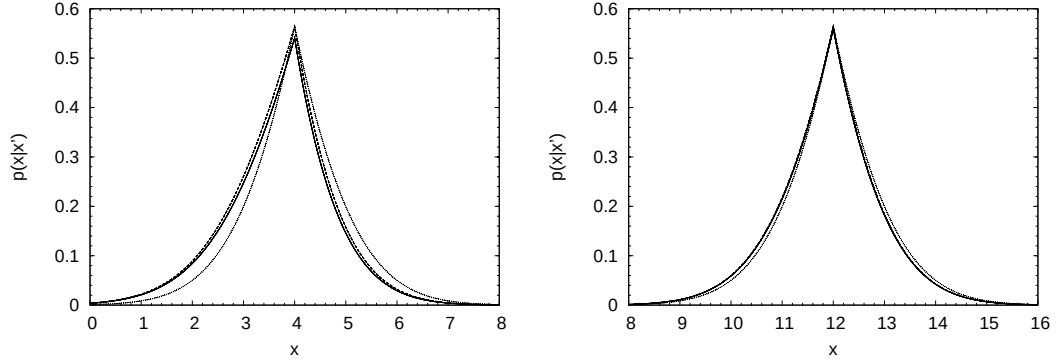


Figure 2.5: Frequency redistribution curves $p(x|x')$ in the wings for (left) $x' = 4$ and (right) $x' = 12$, with $T = 10$ K. Forms plotted come from full R_{II} redistribution function (solid line), the approximate form given in Eq. (2.17) (dashed line) and $p(x|x') = \text{ierfc}(\Delta)$ (dotted line).

(distributed as the absorption line profile) and re-emitted at $x = x'$; we represent this via the angle-averaged redistribution function

$$R(x', x) = \phi(x') \delta_{\text{D}}(x' - x) = \phi(x) \delta_{\text{D}}(x' - x). \quad (2.19)$$

(ii) Complete redistribution: The photon is absorbed at x' and re-emitted at frequency shift x , where x' and x are distributed about line centre according to the line profile $\phi(x)$:

$$R(x', x) = \phi(x') \phi(x). \quad (2.20)$$

Consideration of the R_{II} redistribution probability curves in Figure 2.3 leads us to a useful application of these limiting cases. Photons absorbed in the wings scatter in a roughly coherent manner, while photons absorbed nearer the line centre undergo an almost random frequency reshuffling. A very basic approximation to the full redistribution function is given by taking a weighted sum of both forms, Equations (2.19) and (2.20), such that they dominate in the line wings and core respectively (see Jefferies and White [1960]).

2.3.2 Effect of Atomic Recoil

Adopting the frame in which the scattering atom is initially at rest, if the atom absorbs a photon and subsequently re-emits in any direction other than that of the original

photon, it must adopt some recoil velocity $\mathbf{v}_{\text{rec}}$ to ensure momentum conservation. The energy transferred to the atom comes from the incident photon, and so the re-emitted photon will have a lower frequency from conservation of energy. In this section we outline the effect of the recoil of the atom on the redistribution function, considered in detail by Field [1959b].

Consider absorption of a photon $(x', \mathbf{n}')$ followed by emission of a photon $(x, \mathbf{n})$. Conservation of 4-momentum tells us that, to first order in v_{rec}/c and $h_P\nu_0/(mc^2)$, the frequency shift (comparing the incoming and outgoing photons) is given by:

$$x - x' = -\epsilon(1 - \mathbf{n} \cdot \mathbf{n}'), \quad (2.21)$$

where we have introduced the ‘recoil parameter’ ϵ :

$$\epsilon = \frac{c}{b} \left(\frac{h_P\nu_0}{mc^2} \right) = \frac{h\nu_0}{\sqrt{2k_B T} mc^2}. \quad (2.22)$$

Assuming Ly α scattering enables us to write Eq. (2.22) as $\epsilon = 0.025(T/\text{K})^{-1/2}$. Referring to Eq. (2.21), (analogous to Compton scattering) the frequency shift is zero for parallel photon directions and a maximum for anti-parallel photon directions, with the scale of the shift given by the ratio of the photon momentum to the atom’s thermal momentum. The frequency of the photon will decrease as it loses energy to provide the kinetic energy of the atom. The effect of recoil increases with decreasing temperature as the atoms are more easily influenced by the photon momentum. We note that the approximations implicit in this simple treatment correspond to an accuracy first-order in $(b/c)\epsilon = h_P\nu_0/(mc^2)$; for Ly α scattering this is of order 10^{-8} and thus Eq. (2.21) is a suitable approximation.

The effect of recoil upon the scattered photon frequency alters the form of the frequency redistribution function. Referring to Eq. (2.12), it is necessary to proceed using $p(\xi | \xi') = \delta_D[\xi' - \xi - \Delta\nu_D\epsilon(1 - \mu)]$, where μ is the cosine of the angle between the incoming and outgoing photons. We label the resulting form analogous to R_{II} as $R_{\text{II},\epsilon}$ (Basko [1978]):

$$\begin{aligned} R_{\text{II},\epsilon}(x', x) &= \frac{a}{2\pi} \exp[-\epsilon(x - x') - \epsilon^2] \\ &\times \int_{-\infty}^{\infty} \frac{e^{2\epsilon p} \text{erfc}(|p| + \frac{1}{2}|x - x'|)}{a^2 + [p - \frac{1}{2}(x + x') - \epsilon]^2} dp. \end{aligned} \quad (2.23)$$

This form is seen to reduce to the redistribution function without recoil by setting $\epsilon = 0$, although the form written in Eq. (2.15) is only recovered after writing the complementary error function as an explicit integral and interchanging the order of integration with the integral over p . The resulting probability distribution profiles for the output frequency look very similar to those found in the case without recoil (see Figure 2.3), but at low temperatures they display a bias towards redder frequencies.

2.4 Equation of Radiative Transfer

The previous sections have looked at the physics involved in the resonance-line scattering process and the quantitative descriptions of the process provided by the redistribution function. Now we establish the utility of the redistribution function in the radiative transfer equation, which specifies the evolution of the radiation field upon interaction with the transfer medium. The generalised form of the radiative transfer equation is given by:

$$\left[\frac{1}{c} \frac{\partial}{\partial t} + \mathbf{n} \cdot \nabla \right] I_\nu(\mathbf{r}, \mathbf{n}, t) = -\chi_\nu(\mathbf{r}, \mathbf{n}, t) I_\nu(\mathbf{r}, \mathbf{n}, t) + \eta_\nu(\mathbf{r}, \mathbf{n}, t) \quad (2.24)$$

where the specific intensity $I_\nu(\mathbf{r}, \mathbf{n}, t)$ determines $dE = I_\nu(\mathbf{r}, \mathbf{n}, t) dA d\omega d\nu dt$, the energy transferred in time dt by radiation in frequency range $\nu \rightarrow \nu + d\nu$, contained in solid angle $d\omega$ about $\mathbf{n}$, normal to area dA . We have made explicit the dependence of I_ν on position in space, direction and time. The evolution of the specific intensity in time and space is dependent upon the opacity χ_ν and the emissivity η_ν which are defined below (see Figure 2.4):

- The energy of a beam of radiation travelling through a length ds , of cross-sectional area dA , of some source having an opacity χ_ν is reduced in proportion to the incident specific intensity and the distance travelled through the material; this differential energy loss is defined as $dE = \chi_\nu I_\nu dA ds d\omega d\nu dt$.
- Similarly the differential energy gained if the beam travels through a source of emissivity η_ν is given by $dE = \eta_\nu dA ds d\omega d\nu dt$.

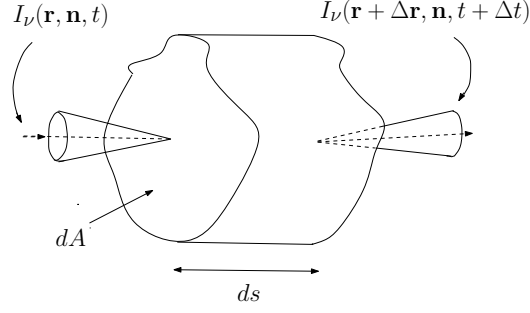


Figure 2.6: Transfer of radiation through some source of opacity and/or emissivity.

Now we need to specify the opacity and emissivity for the resonance scattering process. The former can be deduced reasonably straightforwardly; energy is lost due to ‘absorption’ when photons are removed from the incident beam to excite a scattering atom. The opacity is the product of the density of scattering atoms in the lower state, n_l , and the absorption cross section of the atoms, $\sigma_\nu \equiv \sigma\varphi(\nu)$. Note that σ_ν is the physical cross section, i.e. it has units of m^2 , while σ is the integrated ‘total cross section’ and has units m^2Hz . The total cross section is related to the oscillator strength of the transition f_{lu} by $\sigma = f_{lu} \times (4\pi\epsilon_0)^{-1}\pi e^2/(m_e c)^1$. Thus the opacity is given by:

$$\chi_\nu = n_l \sigma \varphi(\nu). \quad (2.25)$$

The dimensions of χ_ν are m^{-1} . Note that technically this opacity does not account for stimulated emission, which is really a negative contribution to the opacity rather than a contribution to the emissivity, but this is typically assumed unimportant for the purpose of the radiative transfer calculation under circumstances in which the photon occupation number of the excited state is small.

The emissivity arises from photons that have been ‘fully’ scattered in that they have been absorbed and re-emitted; subsequently it is dependent on the actual redistribution function rather than just the absorption profile. The form for η_ν is still dependent on the product $n_l \sigma$ but the frequency dependence is more complicated; we can deduce this dependence from the definition of $R(\nu', \mathbf{n}'; \nu, \mathbf{n})$, see e.g. Ch.2 of Mihalas [1978]. The

¹Ly α has oscillator strength $f_\alpha = 0.416$.

result can be written:

$$\eta_\nu = n_1 \sigma \int R(\nu', \nu) J_{\nu'} d\nu' \quad (2.26)$$

where it is assumed I_ν is locally isotropic (as we are generally more interested in redistribution in frequency than in angle) and the angle-averaged ‘mean’ intensity $J_\nu(\mathbf{r}, t) = (4\pi)^{-1} \oint d\omega I_\nu(\mathbf{r}, \mathbf{n}, t)$. We can justify this in outline by noting that photons are scattered from frequency ν' to frequency ν at a rate proportional to $R(\nu', \nu) J_{\nu'}$ and the rate emitted at ν is given by integrating this over all ν' . Note that the limits on the integral are not specified explicitly, but it should extend over the effective width in frequency for which photons interact with the resonance line.

Now that we have established the opacity and emissivity in resonance line scattering we can use them to write the appropriate equation of radiative transfer. Throughout the remainder of this section we will specify some particular cases of the transfer equation derived from Eq. (2.24) under different circumstances.

2.4.1 Homogeneous Medium

We start by looking at time-dependent scattering in a homogeneous medium; the radiation field is independent of position in space and hence the spatial derivative of I_ν on the LHS of Eq. (2.24) vanishes. We can average the equation over solid angle to make the replacement $I_\nu \rightarrow J_\nu$; we then switch variable from J_ν to $n(\nu)$, where the specific photon number density $n(\nu)$ is given by $n(\nu) = 4\pi/(ch_P \nu) J_\nu \simeq 4\pi/(ch_P \nu_0) J_\nu$:

$$\frac{\partial n(\nu, t)}{\partial t} = n_1 \sigma c \left[-\varphi(\nu) n(\nu, t) + \int R(\nu', \nu) n(\nu', t) d\nu' \right] + S(\nu) \quad (2.27)$$

or, equivalently,

$$\frac{\partial n(\nu, t)}{\partial t} = n_1 \sigma c \int [R(\nu', \nu) n(\nu', t) - R(\nu, \nu') n(\nu, t)] d\nu' + S(\nu) \quad (2.28)$$

and we have included on the RHS a source term $S(\nu)$ defined s.t. $S(\nu) d\nu$ is the rate at which photons are added to the system in frequency range $\nu \rightarrow \nu + d\nu$ per unit volume. The medium is infinite in spatial extent (photons do not leave the system spatially) and the frequency integral extends over the effective width of the resonance

line. Note that this width can be treated as extending from negative to positive infinity for mathematical purposes but physically it is assumed sufficiently narrow that any frequency ν at which photons will interact with the line will satisfy $\nu/\nu_0 \simeq 1$ (previously assumed in changing variable from $J_\nu \propto \nu n(\nu)$ to $n(\nu)$). If we take either form above and integrate over all frequencies, we can show:

$$\frac{\partial}{\partial t} \int n(\nu, t) d\nu = \int S(\nu) d\nu. \quad (2.29)$$

For $S(\nu) = 0$, the total number of photons across all frequencies is conserved. This is expected as the only interaction occurring in the system is scattering, which is a conservative process.

We wish to write the time-dependent radiative transfer equation for a homogeneous medium in a dimensionless form. We switch frequency variable from ν to x , the offset from line centre in Doppler widths, and define a new dimensionless time variable $\tau = t/t_s$ where $t_s = \Delta\nu_D/(n_l \sigma c) \simeq 3.2[n_l/\text{cm}^{-3}]^{-1}(T/\text{K})^{1/2} \text{ s}$ for Ly α . The timescale t_s is directly related to the photon mean-free time between scatters at line centre and is referred to as the ‘scattering time’. The change of variables in the transfer equation yields:

$$\frac{\partial n(x, \tau)}{\partial \tau} = -\phi(x)n(x, \tau) + \int_{-\infty}^{\infty} R(x', x)n(x', \tau) dx' + \tilde{S}(x) \quad (2.30)$$

where $n(x) = (\Delta\nu_D)n(\nu)$ and we have introduced a rescaled source term $\tilde{S}(x) = [(\Delta\nu_D)^2/(n_l \sigma c)]S(\nu)$.

2.4.2 Homogeneous Expanding Universe

The equations in the previous section apply to a static medium. Here we consider the expanding universe as an example of a non-static medium; the universe is homogeneous and isotropic, and undergoes a uniform expansion described by the scale factor $a(t) = R(t)/R_0$. Particles recede from each other with a (spatially constant) velocity gradient $dv/dr = H \equiv \dot{a}/a$. The comoving frequency of a photon scales with the expansion of the universe as the inverse of the scale factor, $\nu \propto [a(t)]^{-1}$ (also affecting the frequency bandwidth); as a result the photon number density per comoving frequency interval is seen to decline as $n(\nu, t) \propto [a(t)]^{-3} \times a(t) = [a(t)]^{-2}$. Accounting for these effects in the

transfer equation requires us to write a total time derivative on the LHS of Eq. (2.27) which subsequently becomes (Peebles [1993]):

$$\begin{aligned} \frac{\partial n(\nu, t)}{\partial t} + 2(\dot{a}/a)n(\nu, t) - (\dot{a}/a)\nu \frac{\partial n(\nu, t)}{\partial \nu} \\ = n_1 \sigma c \left[-\varphi(\nu)n(\nu, t) + \int R(\nu', \nu)n(\nu', t) d\nu' \right] + S(\nu). \end{aligned} \quad (2.31)$$

We now rescale the photon density and source terms according to $n \times a^2 \rightarrow n$ and $S \times a^2 \rightarrow S$ such that we are now working with quantities affected only by direct redshifting of the frequency ν ; the total time derivative on the LHS can now be written as:

$$\begin{aligned} \frac{Dn(\nu, t)}{Dt} &\equiv \frac{\partial n(\nu, t)}{\partial t} + 2(\dot{a}/a)n(\nu, t) - (\dot{a}/a)\nu \frac{\partial n(\nu, t)}{\partial \nu} \\ &\rightarrow \frac{\partial n(\nu, t)}{\partial t} - (\dot{a}/a)\nu \frac{\partial n(\nu, t)}{\partial \nu}. \end{aligned} \quad (2.32)$$

After a change of variables to (x, τ) we obtain the following transfer equation analogous to Eq. (2.30):

$$\frac{\partial n(x, \tau)}{\partial \tau} - \gamma \frac{\partial n(x, \tau)}{\partial x} = -\phi(x)n(x, \tau) + \int_{-\infty}^{\infty} R(x', x)n(x', \tau) dx' + \tilde{S}(x) \quad (2.33)$$

where $\gamma = \nu_0 H / (n_1 \sigma c)$ is called the ‘Sobolev parameter’ - we note that $\gamma = (c/b) \times [t_s/t_{\text{exp}}]$, where t_s is the previously defined scattering time and $t_{\text{exp}} = H^{-1}$ is the expansion timescale of the medium (thus large γ implies the expansion becomes increasingly important in its effect on the scattering process). Eq. (2.33) applies to general expanding/contracting media in the limit of a uniform velocity gradient with the identification $H \rightarrow dv/dr$ in the definition of γ ; in a contracting medium in which the photons seen by the scattering atoms are being blueshifted, we will have $\gamma < 0$.

2.4.3 Plane-Parallel Static Medium

We consider the simple example of a one-dimensional plane-parallel medium. Such a model can describe a finite slab of scattering material or a semi-infinite atmosphere in which the medium is considered to extend to an infinite depth in one direction, a good approximation for transfer in a stellar atmosphere. The coordinate z is defined

along the normal to the plane and the direction $\mathbf{n}$ of a beam of radiation is described by $\mu = \mathbf{n} \cdot \mathbf{e}_z$; the directional dependence of the radiation field at any depth within the medium is a function of μ alone from azimuthal symmetry. If the problem is assumed time-independent then the transfer Eq. (2.24) reduces to the form:

$$\mu \frac{\partial I_\nu(z, \mu)}{\partial z} = -\chi_\nu(z) I_\nu(z, \mu) + \eta_\nu(z) \quad (1 \geq \mu \geq -1) \quad (2.34)$$

where the opacity and emissivity are assumed isotropic. As in the case of a homogeneous medium, it is possible to recast the equation in terms of the angle-averaged intensity J_ν , equivalently described as the zeroth order angular moment, $J_\nu = (1/2) \int_{-1}^1 I_\nu d\mu$. If we take the angle-average of Eq. (2.34) and the angle-average of the same equation multiplied by μ we obtain the following equations for the angular moments of the radiation field:

$$\frac{\partial H_\nu(z)}{\partial z} = -\chi_\nu(z) J_\nu(z) + \eta_\nu(z), \quad (2.35)$$

$$\frac{\partial K_\nu(z)}{\partial z} = -\chi_\nu(z) H_\nu(z) \quad (2.36)$$

where we have introduced the first and second order angular moments, $H_\nu = (1/2) \int_{-1}^1 \mu I_\nu d\mu$ and $K_\nu = (1/2) \int_{-1}^1 \mu^2 I_\nu d\mu$ respectively. It is necessary to utilise an additional relation satisfied by the moments in order to close this system. A very useful simplifying assumption often made is the ‘Eddington approximation’ $K_\nu = (1/3) J_\nu$. This relation holds exactly for an isotropic radiation field and the more general case of the diffusion limit, in which the radiation field has an angular dependence $I_\nu(\mu, z) = a(z) + \mu b(z)$; trivially we find $J_\nu = a$, $H_\nu = b/3$ and $K_\nu = a/3 = J_\nu/3$. We make use of the Eddington approximation to eliminate K_ν and substitute Eq. (2.36) into Eq. (2.35) to eliminate H_ν from the equations above; if we also make the change of variable to the optical depth $d\tau_\nu = -\chi_\nu dz$ and introduce the source function $S_\nu \equiv \eta_\nu/\chi_\nu$, we obtain:

$$\frac{\partial^2 J_\nu}{\partial \tau_\nu^2} = 3(J_\nu - S_\nu). \quad (2.37)$$

This equation is solved together with boundary conditions at the ends of the medium (or at infinite optical depth for one side of a semi-infinite atmosphere). In finding a solution for J_ν following the steps described we sacrifice a full picture of the angular dependence

of the radiation field; it is alternatively possible to attempt a formal solution using the Eq. (2.34) with a known source function.

2.4.4 Spherically Symmetric Non-Static Medium

Here we consider the transfer equation for a time-independent problem with spherical symmetry. Referring to Eq. (2.24), we see that the time-derivative term may be dropped while the $\mathbf{n} \cdot \nabla$ term should be rewritten in our chosen coordinate system. As the problem involves spherical symmetry we may write $I_\nu(\mathbf{r}, \mathbf{n})$ as $I_\nu(r, \mu)$ where $\mu = \mathbf{n} \cdot \mathbf{e}_r$. We write:

$$\mathbf{n} \cdot \nabla = \mu \frac{\partial}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial}{\partial \mu}. \quad (2.38)$$

We consider a medium that is undergoing some radial motion determined by a general law for the radial velocity described by $V(r)$. Under such conditions a photon that is determined to have a frequency ν by some observer in the laboratory frame will be seen to have the Doppler-shifted frequency $\nu_c = \nu - (\nu_0/c)\mu V(r)$ in the frame locally comoving with the medium at r . In order to avoid having to incorporate this dependence into the opacity and emissivity terms it is necessary to work with a radiative transfer equation formulated in the local comoving frame. The derivatives with respect to r and μ in Eq. (2.38) are evaluated at constant lab frame frequency ν and can be related to derivatives evaluated at constant ν_c as follows (Mihalas [1978]):

$$\left. \frac{\partial}{\partial r} \right|_\nu \rightarrow \left. \frac{\partial}{\partial r} \right|_{\nu_c} + \left. \frac{\partial \nu_c}{\partial r} \right|_\nu \left. \frac{\partial}{\partial \nu_c} \right|_r = \left. \frac{\partial}{\partial r} \right|_{\nu_c} - \frac{\mu \nu_0}{c} \frac{dV}{dr} \left. \frac{\partial}{\partial \nu_c} \right|_r, \quad (2.39)$$

$$\left. \frac{\partial}{\partial \mu} \right|_\nu \rightarrow \left. \frac{\partial}{\partial \mu} \right|_{\nu_c} + \left. \frac{\partial \nu_c}{\partial \mu} \right|_\nu \left. \frac{\partial}{\partial \nu_c} \right|_\mu = \left. \frac{\partial}{\partial \mu} \right|_{\nu_c} - \frac{\nu_0}{c} V(r) \left. \frac{\partial}{\partial \nu_c} \right|_\mu. \quad (2.40)$$

The LHS of the desired transfer equation is given by these operators, combined as in Eq. (2.38), acting on the comoving intensity. The final result, with all quantities evaluated in the comoving frame, is given by:

$$\mu \frac{\partial I_\nu}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial I_\nu}{\partial \mu} - (\nu_0/c) \frac{V(r)}{r} \left[1 - \mu^2 + \mu^2 \left(\frac{d \ln V}{d \ln r} \right) \right] \frac{\partial I_\nu}{\partial \nu} = -\chi_\nu I_\nu + \eta_\nu. \quad (2.41)$$

Similarly to the transfer equation in a plane parallel medium considered previously, this equation (together with boundary conditions at the outer and inner boundaries of the system) can be solved by taking angular moments and assuming relations between moments to close the system, or a formal solution that proceeds ray-by-ray.

2.4.5 Diffusion Approximation for Frequency Redistribution

The sum of the opacity and emissivity terms on the RHS of the transfer equation, assuming an isotropic radiation field, is of the form:

$$F(x) \equiv -\phi(x)n(x) + \int R(x', x)n(x') dx' \quad (2.42)$$

where we have omitted any reference to time or position in the argument of the photon density but such dependencies are allowed. A common approximation is often made that replaces the opacity and emissivity terms in the transfer equation with a differential operator. This method is called the ‘diffusion approximation’: we assume $n(x')$ is sufficiently smooth across the region where $R(x', x)$ is non-zero that we can Taylor expand $n(x')$ about $x' = x$, within the integrand of the emissivity term. The emissivity becomes:

$$\begin{aligned} \int dx' R(x', x)n(x') &= \int dx' R(x', x) \left[n(x) + (x' - x) \frac{\partial n}{\partial x} + \frac{1}{2} (x' - x)^2 \frac{\partial^2 n}{\partial x^2} + \dots \right] \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} A_k(x) \frac{\partial^k n}{\partial x^k} \end{aligned} \quad (2.43)$$

where

$$A_k(x) \equiv \int dx' R(x', x) (x' - x)^k \quad (2.44)$$

i.e. we get a series of derivatives of the photon density multiplied by moments of the redistribution function. We do not discuss the details of evaluating the moments $A_k(x)$ beyond noting that they are more easily obtained by working in Fourier space (see Rybicki and dell’Antonio [1994]); the results are written (implicitly) below:

$$\begin{aligned} F(x) &\approx -\phi(x)n(x) + A_0(x)n(x) + A_1(x) \frac{\partial n}{\partial x} + \frac{1}{2} A_2(x) \frac{\partial^2 n}{\partial x^2}, \\ &= \left[\frac{1}{2} \frac{d\phi}{dx} \right] \frac{\partial n}{\partial x} + \frac{1}{2} \left[\phi(x) + \frac{1}{3} \frac{d^2 \phi}{dx^2} \right] \frac{\partial^2 n}{\partial x^2} \end{aligned} \quad (2.45)$$

i.e. $A_0(x) = \phi(x)$, $A_1(x) = (1/2)d\phi/dx$ etc. and we have truncated the expansion after the second order term. We now see a problem with this expansion; the exact equation has the property of conserving photons as can be seen by taking the integral over x of $F(x)$ as given by Eq. (2.42), which reduces to zero, while the finite truncation given in

Eq. (2.45) does not preserve this important property. Rybicki and dell’Antonio consider this problem and propose enforcing the constraint

$$A_1(x) = \frac{1}{2}A_2'(x) \quad (2.46)$$

such that the RHS of the transfer equation reduces to

$$F(x) = \frac{1}{2} \frac{\partial}{\partial x} \left[A_2(x) \frac{\partial n(x)}{\partial x} \right] \quad (2.47)$$

i.e. a divergence, ensuring adherence to the particle conservation property $\int F(x)dx = 0$. Rybicki and dell’Antonio suggest enforcing Eq. (2.46) by leaving $A_1(x)$ untouched but approximating $A_2(x)$ by its first term:

$$A_2(x) = \phi(x) + \frac{1}{3} \frac{d^2\phi}{dx^2} \approx \phi(x) \quad (2.48)$$

$$\implies F(x) = \frac{1}{2} \frac{\partial}{\partial x} \left[\phi(x) \frac{\partial n(x)}{\partial x} \right]. \quad (2.49)$$

We see that this scattering term represents diffusion in frequency with diffusion coefficient $D(x) = \phi(x)$ (up to a factor of a half), hence the ‘diffusion approximation’ description. Such an approximation was first made in the case of scattering in the wings where $\phi(x) = a/(\pi x^2)$ (Harrington [1973], Basko [1978]). The validity of the Eq. (2.48) is assured out in the wings of the line where $\phi''/3\phi \simeq 2/x^2$, but the possibility of a non-negligible error in the core cannot be ruled out. As such the diffusion approximation should not be assumed without justification.

There exists an alternative approximation for $F(x)$ in which the full product $R(x', x)n(x')$ is expanded as a Taylor series, resulting in a transfer equation with manifest Fokker-Planck form, see Meiksin [2006]. This approach conserves photons without making any approximations of the form of Eq. (2.48). However, in the test problems looked at by Meiksin, the results obtained using this approximation are less accurate than those obtained in the diffusion approximation; this could be seen as a suggestion that the subject of the Taylor expansion is not sufficiently smooth. It should be noted that the transfer equation with RHS given by Eq. (2.49) can be written as a Fokker-Planck equation (see e.g. Krolik [1990]) and is referred to as such by some authors.

Basko looked at the redistribution function accounting for the atomic recoil velocity, Eq. (2.23), and suggested an extended diffusion approximation accurate to first-order in the recoil parameter ϵ (Basko [1981]):

$$F_\epsilon(x) \approx \frac{1}{2} \frac{\partial}{\partial x} \left[\phi(x) \frac{\partial n(x)}{\partial x} + 2\epsilon \phi(x) n(x) \right]. \quad (2.50)$$

The resulting transfer equation can be classified as a diffusion equation with a drift term representing the redshifting effect of atomic recoil; this term becomes significant for $\epsilon \gtrsim 1/|x|$ or $\epsilon|x| \gtrsim 1$.

2.5 Monte Carlo Method for Ly α scattering

An alternative approach to solving the transfer problem that does not make use of the radiative transfer equation directly is provided by Monte Carlo methods. A Monte Carlo solution to the Ly α transfer problem amounts to a record of the properties of a photon as it interacts with the scattering medium until it escapes, and the subsequent repetition of this process for many photons in order to determine the radiation field solution from the data. Such methods generally assume the system is in a steady state but may be extended to a time-dependent problem. Monte Carlo methods have the advantage of being easier to apply for a spatially complex system than formulating and solving the transfer equation. An analysis of resonance line scattering in a finite slab using Monte Carlo techniques was undertaken by Avery and House [1968]. They specify the basic principles behind their photon-by-photon simulation in detail, and we summarise the main steps here to give an introduction to the method.

Initially, a photon is generated at a frequency and position obtained from the frequency and depth distributions associated with the source. Upon emission and after any subsequent scattering events the photon is taken to propagate in a particular direction $\mu = \cos \theta$, where θ is the angle from the normal, determined by sampling the directional redistribution function $g(\mathbf{n}', \mathbf{n})$. For a system of large optical depth it is assumed many scatterings will render the result independent of the form of $g(\mathbf{n}', \mathbf{n})$ and it is typical to treat photon emission as isotropic; directions are therefore distributed equally in solid angle. Under such circumstances the probability of emission at an angle in the interval

$[\theta, \theta + d\theta]$ is $p(\theta) d\theta = (1/2) \sin \theta d\theta$. The associated cumulative probability function is evaluated and equated to a random number R obtained from a uniform distribution on $[0, 1]$ - the appropriate angle is given by:

$$P(\theta) \equiv \int_0^\theta p(\theta') d\theta' = \frac{1}{2}(1 - \cos \theta) = R, \quad (2.51)$$

thus we can say $\mu = 1 - 2R$ or equivalently:

$$\mu = 2R - 1. \quad (2.52)$$

Every time that a new direction is required, a new random number R is generated and Eq. (2.52) is used to obtain the corresponding direction.

Another important step amounts to finding the outgoing photon frequency upon scattering. This can be obtained from knowledge of the appropriate redistribution function via $p(x | x') \equiv R(x', x)/\phi(x')$ by solving the following equation for x :

$$P(x) \equiv \int_{-\infty}^x p(y | x') dy = R. \quad (2.53)$$

This last equality typically cannot be inverted to determine $x(R)$ analytically, and its application requires some numerical integration and interpolation as Avery and House indicate. An alternative approach is to sample the components of the thermal velocity of the scattering atom, $\mathbf{v}$, and deduce the outgoing frequency from the (non-relativistic) Doppler shifts (Zheng and Miralda-Escudé [2002]).

After the direction and frequency are found, the distance that the photon travels until it next scatters is determined. This requires the use of the probability distribution for optical depth, $p(\tau) \equiv \exp(-\tau)$, as above to determine the optical depth traversed by the photon:

$$P(\tau) \equiv \int_0^\tau p(\tau') d\tau' = 1 - \exp(-\tau) = R, \quad (2.54)$$

thus we see that $\tau = -\ln(1 - R)$ or equivalently:

$$\tau = -\ln R. \quad (2.55)$$

The optical depth is then converted into a distance traversed prior to the next scattering event, l , given knowledge of the comoving opacity χ_ν encountered by the photon along

its path:

$$\tau = \int_0^l \chi_\nu(l') dl'. \quad (2.56)$$

For an expanding or contracting medium it is necessary to account for the redshift/blueshifting of the comoving photon frequency as it travels between scattering events, typically done in the non-relativistic case by taking $\nu \rightarrow \nu - (\nu_\alpha/c)V_r$ or equivalently $x \rightarrow x - V_r/b$, where V_r is the velocity of the medium projected along the direction of the photon (Bonilha et al. [1979]).

Photon positions and frequencies are updated and are generally binned in frequency and depth (or radius in a spherical system). These steps are repeated for successive scattering events until the photon escapes the boundaries of the medium (or crosses a critical boundary in frequency space for an infinite medium) and the entire process starting from emission at the source is repeated for as many photons as are needed to achieve the desired signal-to-noise in the output.

Many different outputs can be obtained from such a Monte Carlo simulation, including the properties of the escaping radiation in the form of frequency histograms of escaped photons, and the mean number of scatterings of a single photon prior to escape, N_s , estimated directly from counting scattering events. For comparison it is possible to estimate the mean number of scatters per photon before escaping given an analytical or numerical form for the radiation field solution, as N_s is given by the ratio of the total rate at which photons are scattered to the rate at which photons escape the system (or the rate at which photons enter the system, both being equal in the steady state). In the simplest case of a homogeneous system we write (Field [1959b]):

$$N_s = \frac{n_l P_\alpha}{\dot{n}_\alpha} \quad (2.57)$$

where n_l is the number density of hydrogen atoms in the lower state, $P_\alpha = 4\pi\sigma \int J_\nu \varphi(\nu) d\nu$ is the rate at which Ly α photons are scattered by one such atom, and the new quantity $\dot{n}_\alpha$ is the rate at which Ly α photons are created within the system per unit volume and is found from the frequency-integrated source term in the transfer equation. A similar relation can be assumed for a non-homogeneous scattering medium by averaging the RHS over the scattering volume.

For a Monte Carlo treatment seeking to obtain a full solution for the mean intensity of the radiation field, we can record the frequencies and depths / radii at which every scattering event occurs. This is done by keeping number counts binned in the appropriate variable(s) to obtain histograms. If we are interested in finding the frequency dependence of J_ν in a homogeneous medium from $N(\nu)$, the number of scattering events in the frequency range $[\nu, \nu + d\nu]$, we note that $N(\nu) \propto J_\nu \varphi(\nu) d\nu$ and therefore:

$$J_\nu \propto N(\nu) / [\varphi(\nu) d\nu]. \quad (2.58)$$

To establish the dependence of the mean intensity on spatial position, e.g. radius in a spherically symmetric system, we note that the number of scattering events in frequency range $[\nu, \nu + d\nu]$ and radius range $[r, r + dr]$, $N(\nu, r)$, is proportional to the product of $J_\nu(r) \varphi(\nu, r) d\nu$ with the number of scattering atoms in the given radius range and therefore

$$J_\nu(r) \propto \frac{N(\nu, r)}{4\pi r^2 n_1(r) \varphi(\nu, r) d\nu dr}. \quad (2.59)$$

After following enough photons and binning their scatters in ν and r we construct the ‘shape’ of the mean intensity as described. We can obtain a normalisation condition by making use of a suitable integral constraint or a condition relating the number of photons followed to the source strength.

2.6 Ly α Spectrum Properties

We have discussed in detail the physics necessary to quantify the Ly α scattering radiative transfer, namely the physics that specify the form of the redistribution function. We have also discussed the formulation of the transfer equation itself in specific geometries and provided some insight into how these equations might be solved. To reconnect with the significance of the Ly α scattering process for the Wouthuysen-Field process and the 21cm signature of the Epoch of Reionisation, we need to obtain the Ly α scattering rate from the transfer equation solution. This is obtained by integrating the product of the radiation intensity and the scattering cross section in frequency across the line: at a given point in space, we calculate the scattering rate of Ly α photons by a single

H I atom as (Madau et al. [1997]):

$$P_\alpha \equiv \oint d\Omega \int I_\nu(\mathbf{\Omega}) \sigma(\nu) d\nu \quad (2.60)$$

where the specific intensity I_ν is defined in terms of photon number and not energy, in keeping with the conventions of the literature. We can make use of the following equivalent forms (similarly defining the mean intensity J_ν in terms of photon number, $n(\nu) = (4\pi/c)J_\nu$, and $n(x) = (\Delta\nu_D)n(\nu)$):

$$P_\alpha = 4\pi\sigma \int J_\nu \varphi(\nu) d\nu = \sigma c \int n(\nu) \varphi(\nu) d\nu = \frac{\sigma c}{\Delta\nu_D} \int n(x) \phi(x) dx. \quad (2.61)$$

We see that the scattering rate depends critically on the Ly α spectrum across the line centre, as $\phi(x)$ is sharply peaked at $x = 0$. If the spectrum is sufficiently flat across line centre then $P_\alpha \propto J_{\nu_\alpha}$.

While the scattering rate is of most direct significance, there are other physical quantities of interest that can be obtained from the radiative transfer solution for the Ly α spectrum. The spectrum at any particular frequency defines a specific radiation colour temperature such that locally the spectrum matches the shape of the black body spectrum for that temperature. In the Wein limit $h_P\nu \gg k_B T$, we have $n(\nu) \propto \exp[-h_P\nu/(k_B T)]$ and thus:

$$T_n(\nu) = -\frac{h_P}{k} \left[\frac{d \ln n(\nu)}{d\nu} \right]^{-1} \implies T_n(x) = -\frac{h_P \Delta\nu_D}{k} \left[\frac{d \ln n(x)}{dx} \right]^{-1}. \quad (2.62)$$

As this description applies only at a specific frequency we describe the Ly α colour temperature by an appropriate average over the resonance line, weighted by the product $n(x)\phi(x)$ as follows:

$$T_\alpha = [\langle T_n^{-1}(x) \rangle]^{-1} = \frac{\int n(x)\phi(x) dx}{\int n(x)\phi(x) \frac{1}{T_n(x)} dx} = \frac{h_P \Delta\nu_D}{k} \left[\frac{\int n(x)\phi(x) dx}{\int n(x) \frac{d\phi(x)}{dx} dx} \right] \quad (2.63)$$

where in the last equality we have applied Eq. (2.62) and used integration by parts (Meiksin [2006]). This allows a direct computation of the colour temperature of the Ly α spectrum as required to compute the hydrogen spin temperature in the Wouthuysen-Field effect, see Eq. (1.32). Wouthuysen argued that the Ly α colour temperature should tend towards the H I gas kinetic temperature after a sufficiently large

number of scatters - this equilibrium is established through the transfer of energy between the radiation field and the gas via e.g. the recoil effect. This energy transfer is quantified by the (time-dependent) gas heating rate per unit volume Γ , resulting from the net difference between the rate at which energy is injected into the system and the rate at which the total energy of the photons changes (Meiksin [2006]):

$$\Gamma = \int (h_P \nu) \left[S(\nu) - \frac{Dn(\nu, t)}{Dt} \right] d\nu. \quad (2.64)$$

The quantity $Dn(\nu, t)/Dt$ is the total time rate of change of the specific photon number density, including the effects of expansion etc., and is substituted for the RHS of the transfer equation to obtain a suitable form to allow computation from the time-dependent solution. A full description of the energy transfer requires adherence to detailed balance in the transfer equation, see Rybicki [2006], which we have implicitly violated by writing our transfer equation assuming $\nu/\nu_0 \simeq 1$.

2.7 Ly α RT Solutions for Infinite Homogeneous Media

The radiative transfer problem of an isotropic radiation field in an infinite homogeneous medium, described by Eq. (2.30), has been studied in some depth by various authors. Here we summarise some results and solutions with an emphasis on the treatment of the frequency redistribution and additional effects such as recoil and expansion.

2.7.1 Time Dependent Scattering in Frequency

A time-dependent analytic solution in the case of R_I redistribution was found by Field (Field [1959a]); the method utilised properties of the R_I redistribution function to obtain an exact solution to the problem. In the case of no source and a non-zero initial condition (taken by Field to be proportional to the Doppler profile, $\sim e^{-x^2}$) the solution is found to be approximately flat across a frequency range $|x| < x_c(\tau) \simeq (\log \tau)^{1/2}$. The range described spreads out with time and the solution drops off exponentially for $|x| > x_c(\tau)$. As the photon spectrum spreads out in frequency, the value across $[-x_c, x_c]$ drops; this is given by $n(0, \tau) \sim (\log \tau)^{-1/2}$.

Basko extended this study to a rough treatment of the effects of full type-II redistribution (Basko [1978]); assuming a delta-function initial condition, the redistribution at early times while all photons are trapped in the Doppler core is given by R_I , while at some later time it is assumed that the wings begin to dominate and R_{II} reduces to the form of Eq. (2.17). This suggests that initially the photon distribution develops as in Field's analytic solution (Basko's Eq.17) while eventually transitioning to the analytic solution given by the diffusion approximation with $\phi(x) = a/(\pi x^2)$ (his Eq.20); the latter solution is found to spread out fairly smoothly over a wide range in frequency, with a half-width $\sim (a\tau)^{1/4}$.

Rybicki and dell'Antonio solve the time-dependent radiative transfer equation for a static, infinite homogeneous medium in the diffusion approximation numerically (Rybicki and dell'Antonio [1994]). They examine the case with $n(x, 0) = 0$ and a constant creation rate $\sim \phi(x)$, and compare their solutions assuming type I redistribution (and therefore $\phi(x) \rightarrow \phi_D(x)$ in the diffusion term) with Field's corresponding analytic solution. They find agreement near the line core where both solutions adopt, within a short time $\tau \sim 10$, a flat spectrum that grows and widens with τ , though there is some disagreement further out from line centre. They also examine a similar case using the full Voigt profile for $\phi(x)$ (i.e. type II redistribution) with $a = 10^{-3}$; their solution is initially similar, near line centre, to the solution in the $a = 0$ case, before the effect of the wings is felt and significant broadening occurs in the core region; the profile also displays growing 'wings' at large $|x|$ due to the source emission from the Lorentz wings. Another comparison against a constant source analytic solution, analogous to Basko's solution for scattering in the wings, is provided; they find good agreement after the effect of the wings of $\phi(x)$ in the diffusion term begins to dominate, though discrepancies persist in the wings as Basko's solution assumes photon injection at line centre only.

2.7.2 Effect of Recoil

The atomic recoil velocity has a redshifting effect at the level of a single scattering event, as the scattered photon loses energy to the recoiling atom, and one might expect this to have a systematic redshifting effect on the developing photon spectrum. However, it

is also true that Doppler effects from the thermal velocity of the atom ensure a bias in scattering towards line centre (Osterbrock [1962]); it is not obvious to what extent this effect will ‘wash out’ any systematic redshifting from recoil.

Field examined the time-dependent solution in an infinite homogeneous medium accounting for recoil, assuming type-I redistribution with the redistribution function given by Eq. (2.23) in the limit $a \rightarrow 0$. By assuming a perturbation of the form $n = n_0 + \epsilon n_1$, where $n_0(x, \tau)$ is the analytic solution in the absence of recoil, he showed the profile at large τ obeys the approximate relation $n(x, \tau) = n_0(x, \tau) \times (1 - 2\epsilon x)$ across the core, with n_1 negligible outside this region. As the recoil parameter ϵ is small we see that this approximates a profile varying across line centre as $\exp(-2\epsilon x) = \exp[-h_P(\nu - \nu_0)/k_B T]$, proportional to the Planck function in the Wien limit $h_P \nu \gg k_B T$. This is expected as the radiation field eventually comes into thermal equilibrium with the scattering medium (Wouthuysen [1952]). More generally, Basko’s form of the diffusion approximation given in Eq. (2.50), accurate to first order in ϵ and a good approximation in the wings, suggests a solution in equilibrium of the form $n(x) \propto \exp(-2\epsilon x)$, in agreement with Field’s result.

2.7.3 Expanding Medium

The resulting photon spectrum for Ly α scattering in a homogeneous expanding medium is given by the solution of Eq. (2.33). Chugai found an analytic steady-state solution in the diffusion approximation (Chugai [1980]); such a steady state is the result of the rate at which photons redshift to $x = -\infty$ matching the rate at which new photons are injected into the system as described by the source term. Using the wing approximation $\phi(x) = a/(\pi x^2)$, assuming a delta function source at line centre $\tilde{S}(x) = C\delta_D(x)$, and a boundary condition² $n \rightarrow C/\gamma$ for $x \rightarrow -\infty$, the solution obtained is:

$$n(x) = C\gamma^{-1} \times \begin{cases} 1 & ; \quad x \leq 0 \\ \exp\left(-\frac{2\pi\gamma x^3}{3a}\right) & ; \quad x > 0 \end{cases}. \quad (2.65)$$

²This is required by photon conservation as the integrated source term C must equal $n(-\infty) \times |dx/d\tau| \rightarrow \gamma n(-\infty)$ as seen in the time-dependent solution.

The photon spectrum is flat redward of line centre while it extends only to $x_{\text{cut}} \simeq (a/\gamma)^{1/3}$ for $x > 0$. The validity of this solution requires the cutoff on the blue side to occur outside of the Doppler core to ensure $\phi(x) = a/(\pi x^2)$ applies; equivalently, $x_{\text{cut}} \gg 1$ or $\gamma \ll a$. Hummer and Rybicki found numerical solutions to the steady-state problem using the R_{II} redistribution function and a source term $\tilde{S}(x) = G\phi(x)$ (Hummer and Rybicki [1992]). They obtain profiles that are qualitatively similar to the Chugai solution.

Rybicki and dell’Antonio examined the time development of a resonance line in an expanding universe, using the diffusion approximation (Rybicki and dell’Antonio [1994]). They found that the time-dependent solution, after an initial period of developing similarly to the static solution for the given source term, developed asymmetrically in frequency and extended redward. This asymmetry develops into a front that propagates with a constant ‘speed’ in frequency of $dx/d\tau = -\gamma$; for an infinite medium, the steady state solution is technically attained in the limit $\tau \rightarrow \infty$. Motivated by the physical significance of the photon spectrum across the line centre, Rybicki and dell’Antonio defined a ‘relaxation time’ τ_r after which the time-dependent solution at line centre is equal to the steady-state value to within some tolerance, $n(0, \tau_r)/n(0, \infty) = (1 - f)$ for some $f \ll 1$. For conditions matching those of the Chugai solution, i.e. $\phi(x) = a/(\pi x^2)$ and $\tilde{S}(x) = C\delta_D(x)$, they observed the scaling $\tau_r = Kx_{\text{cut}}/\gamma = Ka^{1/3}\gamma^{-4/3}$. The proportionality constant K depends on f ; for $f = 0.1$, $K = 3.35$. They found this scaling was also a good match for the relaxation time of their numerical solutions with $\gamma \ll a$.

2.7.4 Expanding / Contracting Medium with Recoil

Solutions for $\text{Ly}\alpha$ scattering in an infinite homogeneous medium with a uniform velocity gradient characterised by the appropriate Sobolev parameter γ , and accounting for atomic recoil as characterised by the recoil parameter ϵ , have been examined by numerous authors including Chen and Miralda-Escudé [2004], Chuzhoy and Shapiro [2006], Hirata [2006] and Furlanetto and Pritchard [2006]. As a particular example we quote the resulting solution for an expanding medium in the form found by Furlanetto and Pritchard, in the ‘continuous’ case in which photons redshift into resonance from large

frequencies. The result is given in terms of $\delta_J(x) \equiv (J_\infty - J)/J_\infty$, where J_∞ is the intensity for $x \rightarrow \infty$, and has the form:

$$\delta_J(x) = 2\epsilon \int_0^\infty dy \exp \left[-2\epsilon y - 2\gamma \int_{x-y}^x \frac{dx'}{\phi(x')} \right]. \quad (2.66)$$

For a sufficiently large value of γ the solution is constant in frequency with a decrement below J_∞ across the line centre. This feature, given by δ_J , is caused by the recoil effect (clearly $\delta_J = 0$ if $\epsilon = 0$) and ensures the spectrum adheres to the required Planck limit near line centre. The decrement corresponds to an increase in the rate at which photons are redshifted across line centre due to the added redshifting from the recoil effect. Furlanetto and Pritchard describe the effect on the Ly α scattering rate by defining a suppression factor S_α that specifies the fraction by which the recoil feature across the line centre reduces the scattering rate:

$$S_\alpha \equiv \int_{-\infty}^\infty [J(x)/J_\infty] \phi(x) dx. \quad (2.67)$$

Clearly for $\epsilon = 0$, $J(x) \equiv J_\infty$ and $S_\alpha = 1$, while in general $S_\alpha < 1$. As the line profile $\phi(x)$ is sharply peaked with respect to the feature $\delta_J(x)$ it is possible to make the simplifying assumption $S_\alpha \simeq 1 - \delta_J(0)$. The quantity $\delta_J(0)$ in Eq. (2.66) takes the following form in the wing approximation for $\phi(x)$ (found to be an excellent approximation for all realistic temperatures):

$$\delta_J(0) = 2\epsilon \int_0^\infty dy \exp \left[-2\epsilon y - \frac{2\pi\gamma}{3a} y^3 \right] \quad (2.68)$$

$$= 2 \int_0^\infty dt \exp [-2t - (t/\alpha)^3], \quad (2.69)$$

where

$$\alpha \equiv \epsilon \left(\frac{3a}{2\pi\gamma} \right)^{1/3} \simeq 0.717 (T/\text{K})^{-2/3} [\gamma/10^{-6}]^{-1/3}. \quad (2.70)$$

Thus the suppression of the scattering rate is a function of the parameter α alone. The authors provide a series expansion for $\delta_J(0)$ in powers of α ; when α is small, the reduction in the scattering rate from the no-recoil result has the simple dependence $(1 - S_\alpha) \propto \alpha$. Chuzhoy and Shapiro present similar solutions for a contracting medium ($\gamma < 0$) in which an increment above the base value is observed across line centre; this is caused by a reduction in the effectiveness of blueshifting of photons across the line centre due to redshifting of scattered photons by the recoil effect.

2.8 Ly α RT Solutions for Finite 1D Systems

The vast majority of astrophysical problems involving resonance-line scattering cannot be approached by assuming an infinite homogeneous medium. A homogeneous model with a uniform expansion velocity gradient might be appropriate to study resonance scattering in the very early universe during cosmological hydrogen recombination for example (as attempted by Rybicki and dell’Antonio [1994]), but in the more typical applications e.g. scattering in a nebula, we need to account for the physical structure of the scattering medium. Most analytic treatments limit this structure to a 1D slab or spherical system.

2.8.1 Scattering in Frequency and Space

Osterbrock looked at resonance-line radiation escaping from an optically thick nebula, modelled as a static 1D uniform spherical system (Osterbrock [1962]). The optical depth through the system is given as $\tau(x) = \int \chi_\nu dr = \pi^{1/2} \tau_0 \phi(x)$, where τ_0 is the optical depth through the system at line centre. Photons are assumed to escape the system by diffusion in frequency to some x_1 such that $\tau(x) < 1$ for $|x| > x_1$; for type I redistribution with $\phi(x) = \phi_D(x)$, this frequency is given as:

$$x_1 = (\ln \tau_0)^{1/2}. \quad (2.71)$$

This limit also applies for photons escaping directly from the core in type-II redistribution, possible if $x_1 < x_m$ where the latter is defined as the outermost crossover between the core and wing forms of $\phi(x)$ (see Eq. (2.11)). Osterbrock adopted the time-dependent analytic solution for Doppler scattering found by Field to estimate the number of scatterings undergone by a photon prior to escape, N_s , and its dependence on τ_0 , for type-I redistribution. Field suggested his homogeneous medium solution could describe the transfer of photons in a nebula of large optical depth until the solution ‘width’ meets the frequency boundaries for escape from the medium, x_1 (Field [1959a]), whereafter the profile would remain flat across the range $[-x_1, x_1]$ but would decay in amplitude as the initial influx of photons escapes through the boundaries. Osterbrock estimated the escape probability per scattering, p_{esc} , by using the distribution of output

frequencies obtained assuming complete redistribution, $p(x|x') = \phi(x)$:

$$p_{\text{esc}} = 2 \int_{x_1}^{\infty} \phi(x) dx = \text{erfc}(x_1) \simeq \frac{e^{-x_1^2}}{\pi^{1/2} x_1} \quad (2.72)$$

where in the last equality an asymptotic expansion valid for large x_1 has been applied. The mean number of scatterings undergone by one photon prior to escaping with $|x| > x_1$ is estimated as the inverse of this probability:

$$N_s = p_{\text{esc}}^{-1} = \pi^{1/2} x_1 e^{x_1^2} = (\pi \ln \tau_0)^{1/2} \tau_0 \sim \tau_0. \quad (2.73)$$

This result reflects that Doppler redistribution allows photons to escape the system faster than a strictly coherent scattering process in which photons escape by a random walk and scatter N_s times before escape, where $\tau_0 \propto \sqrt{N_s}$ and thus $N_s \propto \tau_0^2$.

Photons can only escape from core frequencies in type II redistribution for low-to-moderate values of the optical depth. Osterbrock also examined the high optical depth limit in which photons escape from frequencies in the wings of the profile. The average and mean-squared frequency shift per scattering event are computed from the redistribution function valid in the wings given by Eq. (2.17):

$$\langle x - x' \rangle \equiv \frac{1}{\phi(x')} \int (x - x') R(x', x) dx = -\frac{1}{x'}, \quad (2.74)$$

$$\langle (x - x')^2 \rangle \equiv \frac{1}{\phi(x')} \int (x - x')^2 R(x', x) dx = 1. \quad (2.75)$$

Note that the first result here is a statement of the bias towards line centre found in the scattering process. Osterbrock approximated the effects of the frequency redistribution in the wings by a 1D random walk in frequency with a mean-free-path chosen so as to recover the correct RMS frequency shift, and an asymmetry in the probabilities for scattering to larger/smaller frequencies chosen to reproduce the bias towards line centre (a ‘not-quite-random walk’). Osterbrock estimated N_s by using the results for R_{I} redistribution to estimate the number of scatterings required to escape from the core regime $|x| < x_m$, and following photons reaching the wings according to the method described until they returned to the core or escaped. He found a dependence that roughly continued the low optical depth core-scattering limit, $N_s \propto \tau_0$. Assuming photons escape with frequencies in the wings beyond which the optical depth is less

than unity and the photons can free-stream out of the system, the escape frequency analogous to Eq. (2.71) is:

$$x_1 = \pi^{-1/4}(a\tau_0)^{1/2}. \quad (2.76)$$

Osterbrock acknowledged that photons in the wings are alternatively able to escape the medium for $|x| < x_1$ due to the non-negligible spatial mean-free-path. He suggested that photons escape in the high- τ_0 limit by multiple passages through the wings, each of which amounting to a single step in a 3 dimensional spatial random walk of step size independent of τ_0 , recovering the dependence found in coherent scattering of $N_s \propto \tau_0^2$ - however, he could not obtain results to confirm this hypothesis due to the effort required to apply his Monte Carlo approach for such excessive numbers of scattering events.

Adams followed up on the results of Osterbrock, looking at the escape of resonance-line radiation from a finite slab (Adams [1972]). He employed the Eddington approximation and solved discretised moment equations by the Feautrier method³. He obtained results confirming the study of the low optical depth core-scattering limit studied by Osterbrock. In the high optical depth limit, he found the number of scatterings per photon prior to escape followed $N_s \propto \tau_0$, contradicting Osterbrock's hypothesis of photon escape by many 'excursions' into the wings; this was explained by a 'single largest excursion' scenario in which a photon reaches the wings but the distance travelled before it returns to the core is comparable to the size of the medium. The results of this hypothesis were probed by the following argument; a photon at some starting frequency $x \gg 1$ lying in the wings will return to the core in $\sim x^2$ scatters, from the RMS frequency shift Eq. (2.75); meanwhile the physical mean-free-path $\lambda(x) \propto 1/\phi(x)$ and thus the RMS distance moved varies as $\langle \tau \rangle = N^{1/2}/\phi(x) \simeq x/\phi(x)$. The photon escapes from a frequency x_* satisfying $\langle \tau \rangle|_{x_*} = \tau_0$, and thus Adams derived the escape frequency:

$$x_* = \pi^{-1/6}(a\tau_0)^{1/3}. \quad (2.77)$$

The solutions obtained displayed an emissivity with frequency dependence $\sim \phi(x)$, equivalent to a frequency probability distribution for photons having undergone a single

³See Chapter 5 for an introduction to this approach and its application.

scattering, and thus the probability for a given photon to reach frequency x in a single scattering is $[\phi(x)/x^2] dx$. Adams subsequently estimated the escape probability per scattering, p_{esc} , as:

$$p_{\text{esc}} = 2 \int_{x_*}^{\infty} \left[\frac{\phi(x)}{x^2} \right] dx = \frac{2a}{3\pi x_*^3}. \quad (2.78)$$

This probability is again the inverse of the number of scatterings undergone by a single photon prior to escape:

$$N_s = p_{\text{esc}}^{-1} = \frac{3\pi x_*^3}{2a} = 1.5\pi^{1/2}\tau_0. \quad (2.79)$$

Thus the model of a photon escaping in a single largest excursion into the wings recovers the correct high- τ_0 limit of N_s and also predicts the correct escape frequency seen in Monte Carlo and analytic solutions in this limit, $x \simeq \pm(a\tau_0)^{1/3}$.

In a separate but closely related paper, Adams looked at the significance of the effect of atomic recoil in terms of his model for photon escape (Adams [1971]). In the wings, the mean frequency shift per scattering $\langle \Delta x \rangle$ is $-1/x$; clearly the aforementioned bias towards line centre becomes negligible very far out in the wings and we would expect the systematic redshifting effect of recoil to have a greater impact on the final solution for the line spectrum. Adams argued that photons reaching a maximum frequency x_{max} during their excursions into the wings would return to line centre in $\sim x_{\text{max}}^2$ scatterings and therefore experience a redwards frequency shift due to recoil of $x_{\text{max}}^2 \epsilon$. If this is comparable to the total frequency shift in returning to line centre, then recoil is important; the condition is then $\epsilon x_{\text{max}}^2 \gtrsim x_{\text{max}}$ or $\epsilon x_{\text{max}} \gtrsim 1$, where we note that the value adopted for x_{max} should be the relevant escape frequency out of x_1 or x_* . This criterion matches that described previously for solutions to the scattering problem accounting for recoil in a homogeneous medium.

2.8.2 Analytic Solutions in Static Media

Unno examined the radiative transfer of He II Ly α in a planetary nebula, approximated as a finite slab (Unno [1955]). Unno assumed Eddington's approximation and solved the combined moment equation, Eq. (2.37), to obtain analytic solutions for $J(x, z)$. We will not make use of Unno's particular results however his solution method, in which

$J(x, z)$ is expanded in a series of eigenfunctions of a differential equation in z satisfying appropriate boundary conditions, has been used by many subsequent authors to obtain analytic solutions in the Eddington approximation.

Harrington sought solutions for scattering in a finite slab of large optical depth, including a source term distributed as $\phi(x)$ in frequency with a general spatial distribution (Harrington [1973]). Harrington treated the frequency redistribution in a self-consistent manner by assuming the approximate redistribution function in the wings found by Unno, see Eq. (2.17), and performing a Taylor expansion of $J(x, \tau)$ under the integral in the scattering emissivity term before utilising the frequency moments given by Equations (2.74) and (2.75), essentially the diffusion approximation (see section 2.4.5). He applied boundary conditions requiring that the photon intensity at each surface is independent of angle, except that photons are only scattered ‘outwards’ i.e. $I_\nu(\tau, \mu)$ is only non-zero for $\mu > 0$ at $\tau = +\tau_0$ and $\mu < 0$ at $\tau = -\tau_0$, giving:

$$H_\nu(\tau)|_{\pm\tau_0} = \pm \frac{1}{2} J_\nu(\tau)|_{\pm\tau_0} . \quad (2.80)$$

Such a boundary condition is commonly assumed for the outer surface in an analytic problem and is known as the second Eddington approximation. Using Unno’s eigenfunction expansion method and assuming photons escape from optical depths greater than unity (as shown to occur in the high- τ_0 limit by Adams), Harrington obtained series solutions for the mean intensity $J(x, \tau)$. He found that the number of scatters per photon required for escape obeyed $N_s \propto \tau_0$, while the solution at the boundaries showed maxima at $x_{\text{peak}} \simeq \pm 0.8(a\tau_0)^{1/3}$: the emergent photons escape from frequencies tightly distributed about $\pm x_*$, as predicted by Adams in this limit.

Dijkstra, Haiman and Spaans obtained an analytic solution in the high optical depth limit for a static uniform sphere analogous to that found by Harrington for a plane-parallel slab (Dijkstra et al. [2006]). They looked at a system of radius R and line centre opacity κ_0 , with a unit-strength source term of frequency distribution $\phi(x)$ and arbitrary radial distribution $j(r)$, with outer boundary condition analogous to Eq. (2.80):

$$H_\nu(R) = \frac{1}{2} J_\nu(R). \quad (2.81)$$

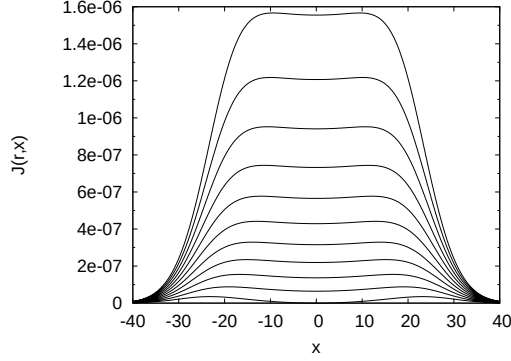


Figure 2.7: Plot of the solution $J(r, x)$ of Dijkstra et al. [2006] for Ly α scattering in a static uniform sphere in the Eddington approximation for $T = 10$ K, $\kappa_0 = 10^4$ and a uniform source of radius $r_S = 5$. Frequency profiles are given from $r = 50$ (highest values of J) to the outer boundary at $r = 100$ (lowest values of J) in steps of 5.

They found the solution

$$J(r, x) = \frac{\sqrt{6\pi}\kappa_0}{16\pi^2 R} \sum_{n=1}^{\infty} Q_n \frac{\sin(\lambda_n r)}{\lambda_n r} \exp \left[-\sqrt{\frac{2\pi}{27}} \frac{\lambda_n}{a\kappa_0} |x^3| \right], \quad (2.82)$$

where the factors $\{Q_n\}$ are related to the radial distribution of the source $j(r)$ by:

$$Q_n \equiv \int_0^R 4\pi r^2 \frac{\sin(\lambda_n r)}{r} j(r) dr, \quad (2.83)$$

and the radial ‘eigenvalues’ $\{\lambda_n\}$ are constrained by the outer boundary condition to the frequency-dependent values:

$$\lambda_n(x) \approx \frac{n\pi}{R} \left[1 - \frac{1}{1 + 1.5\pi^{1/2}\kappa_0 R\phi(x)} \right]. \quad (2.84)$$

An example of this solution is given in Figure 2.7, where we have assumed a uniform source of radius R_S , i.e. $j(r) = 3/(4\pi^{3/2}\kappa_0 R_S^3)$ for $r < R_S$. Note that the presence of a flat frequency profile throughout most of the system gives way to two peaks at the outer boundary, distributed about the spatial diffusion escape frequency $x_* \sim (a\tau_0)^{1/3}$; these same characteristics were found in Harrington’s slab solutions. Analytic solutions of this type have been examined by many authors, in particular Neufeld [1990], who looked at a variety of source configurations in a static plane parallel medium and included line absorption and continuum radiation.

2.8.3 Ly α Point Source in Homogeneous Expanding Universe

In this section we describe a solution found by Rybicki and Loeb for Ly α scattering resulting from a Ly α point source in a zero-temperature, uniform-density, spherically symmetric expanding H I medium (Loeb and Rybicki [1999]). Rybicki and Loeb were interested in the spectrum of scattered photons created around a Ly α source in the universe before reionisation. They took the transfer equation in the comoving frame to be Eq. (2.41) with an extra source term $S(\nu, r)$ on the RHS to model a point source of Ly α photons at the origin:

$$S(\nu, r) = \dot{N}_\alpha \delta(\nu - \nu_\alpha) \frac{\delta(r)}{(4\pi r)^2}, \quad (2.85)$$

where $\dot{N}_\alpha$ is the rate of emission of Ly α photons. In the idealised $T = 0$ limit, atoms have zero thermal velocity and type II redistribution becomes coherent in the observer's frame, while the line profile is that of natural broadening alone. Coherent scattering in an expanding medium means photons emitted at $\nu = \nu_\alpha$ can only get redder, so Loeb and Rybicki dealt only with photons lying in the red wing of the line profile with the wing form of the opacity given by $\chi_\nu = \beta(\nu - \nu_\alpha)^{-2}$ where $\beta \equiv n_{\text{I}} \sigma \Gamma_\alpha / (4\pi^2)$, while the emissivity reduces to $\eta_\nu = \chi_\nu J_\nu$. They assumed a velocity profile for the H I medium given by the Hubble expansion, $V(r) = Hr$; note that for this linear scaling the expression in square brackets in Eq. (2.41) reduces to unity and the expansion term has the form $\alpha(\partial I_\nu / \partial \nu)$ where $\alpha \equiv (\nu_\alpha / c)H$.

Loeb and Rybicki introduced a frequency scale given by $\tilde{\nu} = (\nu_\alpha - \nu) / \nu_*$ where $\nu_* = \beta / \alpha$, the characteristic frequency at which photons accumulate an optical depth of unity in redshifting from the source to an observer at infinity. A characteristic radius and intensity were also defined for the problem, given respectively by $r_* = \nu_* / \alpha = \beta / \alpha^2$ (the radius at which photons redshift to frequency ν_*) and $I_* = \dot{N}_\alpha / (r_*^2 \nu_*)$. Subsequently the transfer equation was non-dimensionalised using the new variables $\tilde{\nu}$, $\tilde{r} = r / r_*$ and $\tilde{I} = I_\nu / I_*$ (and similarly for other radiation field quantities e.g. S , J_ν); the moment equations were taken and a solution was attempted in the Eddington approximation $\tilde{K} = \tilde{J} / 3$. By making further approximations to obtain a combined moment equation analogous to a 3-dimensional diffusion equation with $t \rightarrow \tilde{\nu}^3$, they were able to derive

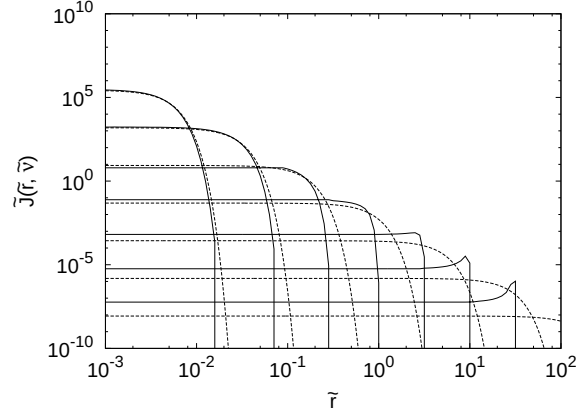


Figure 2.8: Plot of Loeb and Rybicki’s approximate analytic solution for a Ly α halo (dashed line), as given by Eq. (2.86), compared to (our reproduction of) their full Monte Carlo solution (solid line); profiles of $\tilde{J}(\tilde{r}, \tilde{\nu})$ are given for $\log \tilde{\nu} = -1.5, -1.0, -0.5, 0.0, 0.5, 1.0, 1.5$ in order of decreasing value of $\tilde{J}$ at $\tilde{r} = 10^{-3}$.

the following expression for $\tilde{J} = J_\nu/I_*$:

$$\tilde{J}(\tilde{r}, \tilde{\nu}) = \frac{1}{4\pi} \left(\frac{9}{4\pi\tilde{\nu}^3} \right)^{3/2} \exp \left[-\frac{9\tilde{r}^2}{4\tilde{\nu}^3} \right]. \quad (2.86)$$

The solution is plotted in Figure 2.8; the spectrum is localised at the source, spreading out to larger radii at redder frequencies but simultaneously dropping in intensity.

Loeb and Rybicki also looked at the validity of their approximate solution by finding a Monte Carlo solution for the same problem, an improvement in that the method does not require resorting to the Eddington approximation etc. They utilised the steps described in section 2.5 to follow many photons from emission until escape. Note that one must account for redshifting when calculating the optical depth along photon paths between scatters, as $\tilde{\nu}$ increases and the opacity drops; assuming a homogeneous Hubble flow, the frequency along any path length l changes as $\tilde{\nu} \rightarrow \tilde{\nu} + \tilde{l}$, where $\tilde{l} = l/r_*$. A photon re-emitted sufficiently redward of resonance will never scatter again if the optical depth from the opacity integrated redwards of the starting frequency is less than the selected optical depth from Eq. (2.55), and it escapes to infinity; this is the only mechanism by which photons ‘escape’ in this problem, as the medium is spatially infinite.

Loeb and Rybicki obtained their Monte Carlo solution using the radial dependence given in Eq. (2.59) together with the following normalisation constraint found from the zeroth order angular moment equation:

$$(4\pi)^2 \int_0^\infty \tilde{r}^2 \tilde{J} d\tilde{r} = 1. \quad (2.87)$$

The two solutions found by Rybicki and Loeb are compared in Figure 2.8. They show good agreement for small radii and frequencies near line centre, where the diffusion regime assumed in the analytic solution applies; at large radii and far from line centre, the Monte Carlo solution shows peaks corresponding to free streaming photons at $\tilde{\nu} \simeq \tilde{r}$.

CHAPTER 3

Ly α Scattering in a Locally Homogeneous IGM Clump

We examine the case of Ly α scattering far from a source in the homogeneous, expanding Intergalactic Medium prior to both the Epoch of Reionisation and the establishment of any large-scale diffuse radiation field of Ly α photons. We find that the high optical depth of the IGM requires that photons free streaming from the source are received by distant H I gas at frequencies typically hundreds to thousands of Doppler widths blueward of line centre, giving a negligible scattering rate. Using a model that neglects the spatial diffusion of the photons, but treats the photon transport in frequency within a locally homogeneous system we show that a significant steady-state scattering rate can be built up at a scattering site sufficiently optically thick to trap the received photons, corresponding to an overdense ‘clump’ in the IGM:

- Our model yields simple analytic solutions that allow us to readily explain the role of various physical effects on the Ly α scattering rate. We find that the steady-state scattering rate can be significantly reduced by the effects of atomic recoil and the redshifting/blueshifting effect of a locally uniform expansion/contraction.

Additionally, the presence of a bulk peculiar velocity away from the source could redshift the received photons into the line centre, increasing the scattering rate.

- We examine the time-dependence of the scattering within the locally homogeneous system to establish the validity of assuming a steady state given the finite lifetime of the source. We find that the time required to reach the steady state will in many cases exceed realistic source lifetimes, however the fraction of the steady-state scattering rate achieved in a fixed source lifetime can be estimated from our results.

The effects discussed have significant consequences for the 21cm signature of the IGM induced by the Wouthuysen-Field effect due to a source of UV photons in isolation during the early stages of the Epoch of Reionisation. The contents of this chapter are based on the results in Higgins and Meiksin [2009].

3.1 Ly α Optical Depth in a Homogeneous IGM

We consider the Ly α optical depth in a homogeneous, isotropic expanding IGM for a photon emitted by a source at redshift z_S and received at redshift z , $z < z_S$:

$$\tau_\nu = \sigma \int_z^{z_S} n_I(z') \varphi_V \left(a, \nu \frac{1+z'}{1+z} \right) \left| \frac{dl_p}{dz'} \right| dz' \quad (3.1)$$

where $\sigma \simeq 0.011 \text{ cm}^2 \text{ Hz}$ is the total frequency-integrated cross section for the Ly α transition, $n_I \simeq n_{\text{HI}}$ is the number density of atomic hydrogen in the lower level and l_p is the proper path length. For an entirely neutral IGM such that $n_{\text{HI}}(z') \simeq n_{\text{H}}(z')$ for all $z < z' < z_S$, $n_I(z') \simeq n_{\text{H}}(z') = n_{\text{H}}(0)(1+z')^3$ where the present epoch hydrogen density is $n_{\text{H}}(0) = (1-Y)\Omega_b\rho_c(0)/m_{\text{H}} \simeq 0.17 \text{ m}^{-3}$. The proper path length evolves as $|dl_p/dz'| = c/[H(z')(1+z')] \simeq (c/H_0)\Omega_m^{-1/2}(1+z')^{-5/2}$ for a matter-dominated universe, a good approximation over the redshift range associated with the EoR. The argument of the Voigt line profile φ_V accounts for the redshifting of the photon; a photon received at redshift z with frequency ν has been redshifted from a frequency $\nu' = \nu(1+z')/(1+z)$ at redshift $z' > z$. We intend to use the optical depth of photons traversing the IGM from the source at z_S to estimate the scattering rate at some distant site at z .

We consider photons emitted from the source across three separate regimes in the emission frequency, ν_{em} :

- (a) Photons emitted with a frequency $\nu_{\text{em}} \gtrsim \nu_0(1 + z_S)/(1 + z)$ will have $\nu \gtrsim \nu_0$ at redshift z ; these photons will scatter in the blue wing of the local line profile, $x > 0$.
- (b) Photons emitted with $\nu_0 \lesssim \nu_{\text{em}} \lesssim \nu_0(1 + z_S)/(1 + z)$ will redshift into line centre at some intermediate redshift, $\nu' = \nu_0$ at z' , $z_S > z' > z$. These photons would need to survive a significant optical depth to reach z without scattering, essentially the Gunn-Peterson optical depth¹, and are scattered out of the line of sight en route.
- (c) Finally, we note that photons emitted sufficiently redward of line centre at the source, $\nu_{\text{em}} \lesssim \nu_0$, would redshift to frequencies $x < -x_0$ at redshift z where:

$$x_0 = \frac{c}{b_{\text{IGM}}} \frac{z_S - z}{1 + z_S} \simeq 2.3 \times 10^6 (T_{\text{IGM}}/\text{K})^{-1/2} \left[\frac{z_S - z}{1 + z_S} \right], \quad (3.2)$$

for a mean line-of-sight IGM temperature T_{IGM} . These photons thus arrive sufficiently redward of line centre at z that they contribute negligibly to any scattering there. They are, however, capable of scattering in the red wing of the line profile close to the source as in Loeb and Rybicki [1999].

It is clear that any photons reaching redshift z that are sufficiently close to line centre in frequency to scatter at z are of type (a), and they scatter in the blue wing with $\nu \gtrsim \nu_0$. The Voigt line profile $\varphi_V(a, \nu) = (\Delta\nu_D)^{-1} \phi_V(a, x)$ can be assumed to have the dimensionless form $\phi_V(a, x) \simeq a/(\pi x^2)$. We compute the optical depth for such a photon according to Eq. (3.1):

$$\begin{aligned} \tau_\nu &= \frac{\sigma a(\Delta\nu_D)}{\pi} \frac{cn_{\text{H}}(0)}{H_0 \Omega_{\text{m}}^{1/2}} \frac{(1 + z)^{3/2}}{\nu_0^2 y^{3/2}} \int_y^u \frac{t^{1/2}}{(t - 1)^2} dt \\ &= \frac{\sigma a(\Delta\nu_D)}{\pi} \frac{cn_{\text{H}}(0)}{H_0 \Omega_{\text{m}}^{1/2}} \frac{(1 + z)^{3/2}}{\nu_0^2 y^{3/2}} \left\{ \left[\frac{y^{1/2}}{y - 1} - \frac{u^{1/2}}{u - 1} \right] + \frac{1}{2} \ln \left[\frac{(1 - u^{1/2})(1 + y^{1/2})}{(1 - y^{1/2})(1 + u^{1/2})} \right] \right\} \end{aligned} \quad (3.3)$$

where $t(z') = (\nu/\nu_0)(1 + z')/(1 + z)$ and $y \equiv t(z)$, $u \equiv t(z_S)$. This expression is plotted in Figure 3.1 for photons received at redshift $z = 7$ from a source at redshift $z_S = 8$.

¹A calculation of the optical depth according to Eq. (3.1) for photons redshifting through the entire line profile, as given by the piecewise approximation for ϕ described in Eq. (2.11), is given in Higgins and Meiksin [2009].

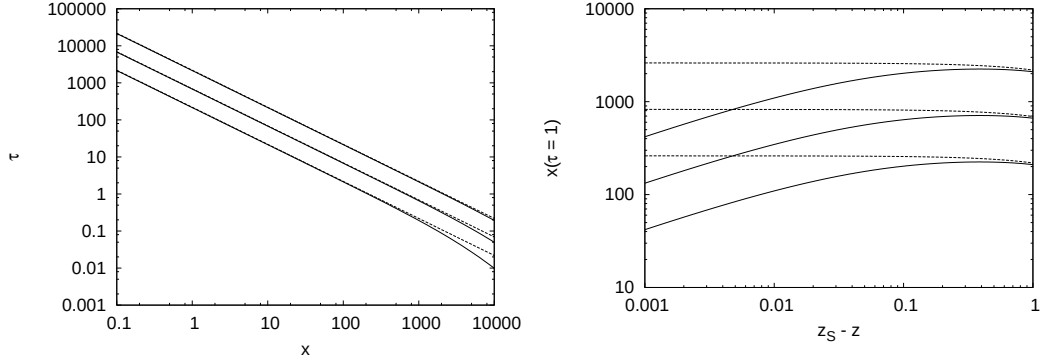


Figure 3.1: Left panel: Ly α optical depth for photons received in the blue wing of the line profile for $T = 10$ K, 100 K and 1000 K (solid lines, from top). Also shown is the approximate form $\tau(x) = x_1/x$ (dashed lines).

Right panel: Value of x at which the optical depth is equal to unity for photons received at redshift z , $z_s > z > (z_s - 1)$, for $T = 10$ K, 100 K and 1000 K (solid lines, from top). Also shown is $x_1(z)$ from Eq. (3.5) (dashed lines).

The optical depth is insurmountable for all photons but those received well blueward of line centre. In the regime $0 < (b/c)x \ll (z_s - z)/(1 + z) \ll 1$, corresponding to photons received in the blue wing that have undergone some non-negligible redshifting to $x \ll x_{\text{em}}$ where x_{em} describes the emitted frequency, the form of $\tau(x)$ is well approximated by the power law:

$$\tau(x) \simeq \frac{x_1}{x}, \quad (3.4)$$

where

$$\begin{aligned} x_1 &= \frac{a\sigma c}{\pi\nu_0} \frac{n_{\text{H}}(0)}{H_0\Omega_{\text{m}}^{1/2}} (1+z)^{3/2}, \\ &\simeq 214h^{-1}(1+z)^{3/2}T_{\text{IGM}}^{-1/2} \end{aligned} \quad (3.5)$$

for values $\Omega_{\text{m}} = 0.27$ and $\Omega_{\text{b}}h^2 = 0.022$. The result can be obtained more straightforwardly if we can assume constant $H(z) = H$ and $n_{\text{H}}(z) = n_{\text{H}}$ along the photon path length, giving $\tau(x) = \frac{1}{\gamma} \int_x^{x_{\text{em}}} \phi(u) du = \frac{a}{\pi\gamma} \left[\frac{1}{x} - \frac{1}{x_{\text{em}}} \right]$, i.e. $\tau(x) = x_1/x$ with $x_1 = \frac{a}{\pi\gamma}$ for $x \ll x_{\text{em}}$. This form for the optical depth is also shown in Figure 3.1 and is found to be a close match over much of the frequency range. The optical depth also depends on the redshift of observation; in the right panel of Figure 3.1 we show the variation

with redshift of x_1 , defined such that $\tau(x) \leq 1$ for all $x \geq x_1$. Far from the source we can see that Eq. (3.5) is a good approximation.

We are interested in the effect that the depletion of the source spectrum by the intervening IGM will have on the scattering rate. The incident spectrum of free-streaming photons, originating from a source of constant specific luminosity L_ν and arriving at redshift z without scattering, is:

$$n(\nu) = \frac{1}{(h_P \nu) c} \frac{L_\nu}{4\pi r_L^2} \exp(-\tau_\nu), \quad (3.6)$$

where r_L is the luminosity distance between the source at z_S and the gas at redshift z while τ_ν is the optical depth of the intervening IGM. The scattering rate at z is computed by integrating the incident photon spectrum across the line profile, see Eq. (2.61). For the case in which we ignore the IGM optical depth i.e. all photons are allowed to free stream, the scattering rate is:

$$P_\alpha(\tau_\nu = 0) = \sigma \frac{L_\nu / h_P \nu}{4\pi r_L^2}. \quad (3.7)$$

This is to be compared with the scattering rate resulting from the inclusion of the IGM optical depth for photons along the line of sight to the scattering site. Such a comparison, assuming scattering in the blue wing and the corresponding optical depth given in Eq. (3.4), gives

$$\begin{aligned} \frac{P_\alpha(\tau_\nu)}{P_\alpha(0)} &\equiv \frac{\sigma c}{P_\alpha(0)} \int_{-\infty}^{\infty} \phi(x) n(\nu) dx, \\ &\simeq \frac{a}{\pi} \int_0^{\infty} x^{-2} \exp(-x_1/x) dx = \frac{a}{\pi x_1}, \\ &\simeq 7.0 \times 10^{-5} h(1+z)^{-3/2} \left[\frac{T_{\text{IGM}}}{T_a} \right]^{1/2} \end{aligned} \quad (3.8)$$

where T_a is the temperature of the scattering H I gas. Clearly the IGM results in a significant reduction in the strength of Ly α scattering far from the source and superficially casts doubt on the effectiveness of the Wouthuysen-Field effect as a means of decoupling the spin temperature of the gas from the CMB during the era of first light in the universe. However, these calculations neglect rescatterings and fail to account for the inhomogeneous nature of the IGM, which is somewhat clumpy at the redshifts of interest for the expected 21cm signal (Tozzi et al. [2000], Gnedin and Shaver [2004]).

3.2 Homogeneous Absorber

We wish to quantify the scattering of Ly α photons from a single, distant source within some discrete, overdense H I clump in the IGM. We consider our clump to be a homogeneous system and refer to it as the ‘absorber’ for simplicity. Photons from the source that arrive at the system with a sufficiently short mean-free path will be effectively confined by the system and scatter within it, undergoing diffusion in both frequency and space. The mean-free path of a photon of frequency x in the wings of the line profile is given by

$$\lambda_{\text{mfp}}(x) = \frac{\Delta\nu_{\text{D}}}{n_1\sigma\phi(x)} \simeq \frac{\pi\Delta\nu_{\text{D}}}{n_1\sigma a}x^2. \quad (3.9)$$

A minimal requirement to halt the immediate escape of photons from our system is given by $\lambda_{\text{mfp}} < L_{\text{a}}$, where L_{a} is the lengthscale of the absorption system. Equivalently we can write $\tau_{\nu} = L_{\text{a}}/\lambda_{\text{mfp}} > 1$, where $\tau_{\nu} = \pi^{-1/2}(a\tau_0)x^{-2}$ is the optical depth across the system for photons in the wings and $\tau_0 = \pi^{-1/2}n_1L_{\text{a}}\sigma/(\Delta\nu_{\text{D}})$ is the optical depth at line centre. We can give a more robust condition for photon escape by defining a factor f such that escape can occur from a frequency $|x| > x_{\text{esc}}$ for which the mean-free path is a fraction f of the absorber lengthscale, i.e. $\lambda_{\text{mfp}}(x_{\text{esc}}) = f \times L_{\text{a}}$. We see that the resulting escape frequency has the form:

$$\begin{aligned} x_{\text{esc}} &= \pi^{-1/4}f^{1/2}(a\tau_0)^{1/2} \\ &\simeq 395(10f)^{1/2}N_{19}^{1/2}(T_{\text{a}}/\text{K})^{-1/2} \end{aligned} \quad (3.10)$$

where the column density is given as N_{19} , defined as N_{HI} in units of 10^{19} cm^{-2} . It must be noted that this condition applies to photons escaping by diffusion in frequency; in the limit of large τ_0 , random walk arguments suggest that photons escape through spatial diffusion from frequencies $|x| > x_* = \pi^{-1/6}f^{1/3}(a\tau_0)^{1/3}$ (see section 2.8.1). Such a limit can be accounted for if necessary by taking $x_{\text{esc}} \rightarrow x_*$ in the results from the radiative transfer solutions presented later in this chapter, though we will make limited use of this result. We suggest that a solution of the transfer problem including the spatial dependence might be necessary to circumvent any ambiguity involved in specifying the escape frequency in cases where its value is critical in determining the Ly α spectrum across the line centre.

The meaning of x_{esc} within our model is simple; photons are only able to scatter within the absorption site across the frequency range $[-x_{\text{esc}}, x_{\text{esc}}]$ - outwith this range, the photons escape. In order for any photons to scatter in the first place, we require that the incident Ly α spectrum from the source overlaps in frequency with this range. An approximate constraint is $x_{\text{esc}} > x_1$; as the IGM optical depth only drops below unity for $x > x_1$ from Eq. (3.4), this condition is necessary at the very least to ensure the required overlap. By taking $x_1 = x_{\text{esc}}$, using the definitions in Eqs. (3.5) and (3.10), and solving for the absorber column density, we obtain:

$$N_{19, \text{crit}} \simeq 0.29 h^{-2} (10f)^{-1} (1+z)^3 \left(\frac{T_a}{T_{\text{IGM}}} \right). \quad (3.11)$$

For $N_{19} > N_{19, \text{crit}}$ the escape frequency of the absorber is sufficient to allow it to intercept and confine photons from the source; such a system will build up a scattering rate greater than that found in the single-scattering limit, as the photons scatter multiple times within the system.

3.2.1 Injection of Source Photons

The absorber is subject to an incident photon spectrum given by Eq. (3.6). We describe the rate at which photons from the source are scattered by the system to a given frequency by an emissivity (rate per unit volume, per unit frequency):

$$S(\nu) = n_1 c \sigma \int_0^\infty R(\nu', \nu) n(\nu') d\nu' \quad (3.12)$$

where the notation $S(\nu)$ is adopted as the emissivity acts as a source term for the system, describing the frequency distribution of ‘injected’ photons; we anticipate the need for such a quantity in describing the radiative transfer of the Ly α scattering within the system. As the incident photon spectrum is only non-zero in the blue wing (where τ_ν is small) we can assume an approximate form for the redistribution function appropriate in the far wings, namely coherent redistribution: $R(\nu', \nu) \simeq \varphi(a, \nu') \delta_D(\nu' - \nu)$. Subsequently the source term becomes:

$$\begin{aligned} S(\nu) &= n_1 c \sigma \varphi(a, \nu) n(\nu), \\ &\simeq \frac{n_1 \sigma a}{\pi(\Delta\nu_D)} \frac{L_\nu / (h_P \nu)}{4\pi r_L^2} x^{-2} \exp(-x_1/x). \end{aligned} \quad (3.13)$$

The functional dependence on x results in a somewhat sharp peak at $x = x_1/2$. It will be useful to represent the source term by a delta function centred on some generalised injection frequency x_{inj} , i.e.

$$\begin{aligned}\tilde{S}(x) &\simeq \frac{a}{\pi c} \frac{\Delta\nu_{\text{D}}}{x_1} \frac{L_{\nu}/(h_{\text{P}}\nu)}{4\pi r_{\text{L}}^2} \delta_{\text{D}}(x - x_{\text{inj}}), \\ &= A \delta_{\text{D}}(x - x_{\text{inj}})\end{aligned}\tag{3.14}$$

where a factor $\int_0^\infty x^{-2} \exp(-x_1/x) dx = x_1^{-1}$ has been inserted to recover the correct normalisation after integrating over frequency. The normalisation factor A is given by:

$$\begin{aligned}A &\equiv \frac{\Gamma_{\alpha}}{4\pi^2 c x_1} [(L_{\nu}/h_{\text{P}}\nu)/4\pi r_{\text{L}}^2], \\ &\simeq 2.5 \times 10^{-6} h(1+z)^{-3/2} (T_{\text{IGM}}/\text{K})^{1/2} [(L_{\nu}/h_{\text{P}}\nu)/4\pi r_{\text{L}}^2]\end{aligned}\tag{3.15}$$

where all quantities are in CGS units and we have used $\Gamma_{\alpha} = 6.26 \times 10^8$ Hz. Clearly A is independent of the properties of the absorber.

It is important to note that the best value to take for x_{inj} is also dependent on other important factors including the depth within the absorber. The absorber is subject to free streaming source photons at frequencies $x \gtrsim x_1$, set by the properties of the intervening IGM; these photons are scattered at a given depth within the absorber corresponding to a summed optical depth from the IGM and the absorber of order unity. Photons of frequency x_1 scatter near the surface, while photons blueward of x_1 see a reduced cross section for scattering within the absorber and will penetrate to greater depth or exit the absorber completely. If we want to model source photons intercepted at deeper layers within the absorber we should account for a blueward shift in the peak of the emissivity.

Another important factor in specifying the injected frequency is any peculiar velocity of the absorber. For scattering near the surface of an absorber in the absence of any peculiar velocity we adopt a delta-function source centred on an injection frequency $x_{\text{inj}} = x_1/2$. A peculiar motion along the line of sight from the source will cause the incident photon spectrum to be redshifted/blueshifted, for motion away from/towards the source, respectively. If the absorber has a peculiar velocity v_{pec} away from the source then our delta-function model of the emissivity is shifted to the absorber-frame frequency $x_{\text{inj}} \rightarrow (x_{\text{inj}} - v_{\text{pec}}/b_{\text{a}})$ where $b_{\text{a}} = (2k_{\text{B}}T_{\text{a}}/m_{\text{H}})^{1/2}$.

3.3 Ly α RT Steady State in the Diffusion Approximation

In the previous section we introduced our model for the scattering of Ly α photons in a homogeneous absorber in which source photons scattered by the system are captured and scatter within the system until escape. A key consequence is that the absorber acts as a photon ‘bucket’ as its stored energy density builds up and subsequently a steady state photon spectrum will be achieved when the rate of photon escapes matches the rate at which photons are ‘injected’ from the source. This buildup is in contrast to the single-scattering limit assumed in deriving Eq. (3.8). To solve for such a steady state photon distribution, we need to construct the equation of radiative transfer for the system. We assume isotropic scattering within our homogeneous absorber; the appropriate equation of radiative transfer is:

$$\frac{1}{2} \frac{d}{dx} \left[\phi(x) \frac{dn}{dx} \right] + \tilde{S}(x) = 0 ; \quad n(\pm x_{\text{esc}}) = 0. \quad (3.16)$$

Here we describe several important points of note about this formulation:

- The resonance-line scattering absorption and emissivity terms involving the re-distribution function are taken to reduce to the differential form found in the diffusion approximation, see section 2.4.5.
- The source term $\tilde{S}(x)$ represents the photons injected into the system by the source, and will be assumed to have the form of Eq. (3.14); the fiducial value $A = 1$ is assumed for all solutions displayed in figures.
- The scattering medium in question only interacts with photons in the frequency range $[-x_{\text{esc}}, x_{\text{esc}}]$. For frequencies outwith this range, the medium is optically thin and the photon density drops to zero as the frequency boundaries are approached. Consequently we impose the boundary condition that $n(x)$ is equal to zero for $x = \pm x_{\text{esc}}$.

The above points apply to all of the solutions we will seek in this section, however the specific equation shown above is valid for a static scattering medium and ignores the effect of atomic recoil; we will modify Eq. (3.16) to allow for such considerations later.

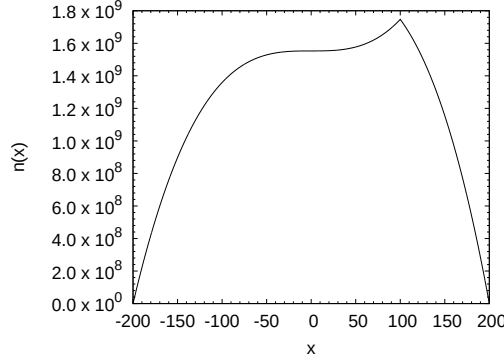


Figure 3.2: Steady-state frequency distribution of Ly α resonance-line photons. Obtained by solving Eq. (3.16) with $\tilde{S}(x) = \delta_D(x - x_{\text{inj}})$ for $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$ and an absorber temperature $T_a = 100$ K.

The radiative transfer equation (3.16) is solved with the delta-function source term $\tilde{S}(x) = A\delta_D(x - x_{\text{inj}})$ and the wing form for the line profile, $\phi(x) = a/(\pi x^2)$. The solution is easily obtained analytically and can be written:

$$n(x) = \frac{\pi}{3a}A \times \begin{cases} \left[1 - x_{\text{inj}}^3/x_{\text{esc}}^3\right] (x_{\text{esc}}^3 + x^3) & ; \quad -x_{\text{esc}} < x < x_{\text{inj}} \\ \left[1 + x_{\text{inj}}^3/x_{\text{esc}}^3\right] (x_{\text{esc}}^3 - x^3) & ; \quad x_{\text{inj}} < x < x_{\text{esc}}. \end{cases} \quad (3.17)$$

The solution is shown in Figure 3.2. Although it could be argued that the solution is not trustworthy in the core region because of the wing approximation used for the line profile, it was found that numerical integration of the ODE using the full Voigt profile function $\phi_V(x)$ produced a solution nearly identical to Eq. (3.17).

The most physically important property of the solution described by Eq. (3.17) is the resulting Ly α scattering rate. As the steady-state solution has a dependence on the strength of the source (via the factor A), we look at a scaled scattering rate that depends on $A^{-1}n(x)$; such a quantity is provided by determining the steady-state scattering rate relative to that found in the free-streaming, single-scattering limit of Eq. (3.7), as follows:

$$\frac{P_{\alpha, \text{ss}}}{P_{\alpha}(0)} \equiv \frac{1}{A} \frac{a}{\pi x_1} \int_{-\infty}^{\infty} \phi(x) n(x) dx \simeq \frac{1}{3x_1} \left(1 - \frac{x_{\text{inj}}^3}{x_{\text{esc}}^3}\right) x_{\text{esc}}^3, \quad (3.18)$$

$$\simeq 9.6 \times 10^4 h \left[\frac{(10f)N_{19}}{(1+z)T_a} \right]^{3/2} T_{\text{IGM}}^{1/2} \left(1 - \frac{x_{\text{inj}}^3}{x_{\text{esc}}^3}\right). \quad (3.19)$$

Thus as expected our model predicts a Ly α scattering rate significantly higher than the single scattering limit. As a more specific example, if we take our absorber to have the critical column density required to trap photons i.e. $N_{19} = N_{19,\text{crit}}$, Eq. (3.19) reduces to $P_{\alpha,\text{ss}}/P_{\alpha}(0) \simeq 1.5 \times 10^4 h^2 (1+z)^3 T_{\text{IGM}}^{-1} (1 - x_{\text{inj}}^3/x_{\text{esc}}^3)$ which implies that even a warm IGM temperature of $T_{\text{IGM}} = 1000 \text{ K}$ will give a significant boost in the scattering rate.

3.3.1 Effect of Atomic Recoil

The effect of atomic recoil on our steady-state solution can be examined by solving the approximate radiative transfer equation that accounts for recoil to first order in ϵ , the recoil parameter; $\epsilon \equiv h_P \nu_0 / (2k_B T_a m_H c^2)^{1/2} \simeq 0.025 T_a^{-1/2}$ (see section 2.3.2). This radiative transfer equation is just the steady-state case of Eq. (2.50), and can be written:

$$\frac{1}{2} \frac{d}{dx} \left[\phi(x) \frac{dn}{dx} + 2\epsilon \phi(x) n(x) \right] + \tilde{S}(x) = 0 ; \quad n(\pm x_{\text{esc}}) = 0. \quad (3.20)$$

Once again, a piecewise analytic solution is obtained by taking the source term to be a delta-function centred on the injection frequency and assuming the Lorentz-wing form for the line profile. This solution is:

$$n(x) = \begin{cases} g_{\epsilon}(x, -x_{\text{esc}}) & ; \quad -x_{\text{esc}} < x < x_{\text{inj}} \\ g_{\epsilon}(x, -x_{\text{esc}}) - g_{\epsilon}(x, x_{\text{inj}}) & ; \quad x_{\text{inj}} < x < x_{\text{esc}} \end{cases} \quad (3.21)$$

where

$$g_{\epsilon}(x, y) = \frac{\pi}{2\epsilon^3 a} A \exp(-2\epsilon x) \times \frac{[f_{\epsilon}(x) - f_{\epsilon}(y)][f_{\epsilon}(x_{\text{esc}}) - f_{\epsilon}(x_{\text{inj}})]}{[f_{\epsilon}(x_{\text{esc}}) - f_{\epsilon}(y)]} \quad (3.22)$$

and

$$f_{\epsilon}(x) = (1 - 2\epsilon x + 2\epsilon^2 x^2) \exp(2\epsilon x). \quad (3.23)$$

The solution is plotted for two different temperatures in Figure 3.3, together with the corresponding no-recoil solution in each case. For high temperatures, the solution is broadly similar to that obtained in the no-recoil case. The most apparent difference is the deviation from a flat spectrum across the line centre; a non-zero gradient is induced near $x = 0$ by the recoil effect corresponding to a radiation colour temperature $T_{\alpha} = T_a$, as required by thermodynamic arguments and found in existing solutions accounting

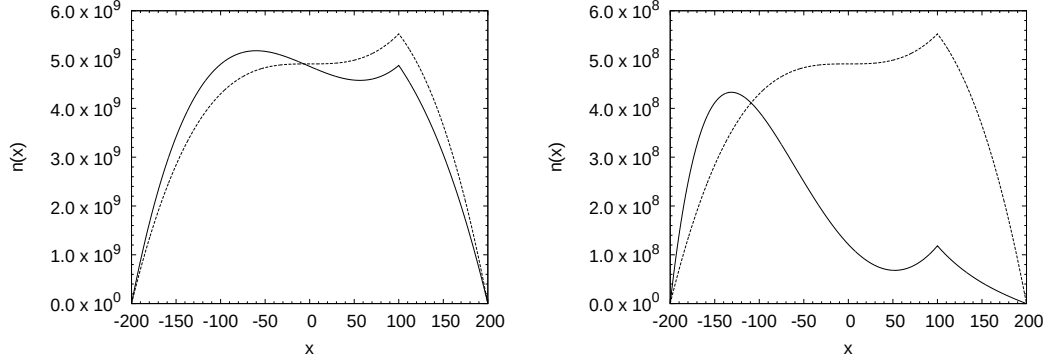


Figure 3.3: Steady-state frequency distribution of Ly α resonance-line photons, accounting for the effect of atomic recoil (solid lines). Obtained by solving the radiative transfer Eq. (3.20) with $\tilde{S}(x) = \delta_D(x - x_{\text{inj}})$, $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$, and a temperature of 1000 K (left) and 10 K (right). The dashed lines in each case are the corresponding solutions found without accounting for recoil.

for recoil (Field [1959b]). If we take the limit of even higher temperatures, the gradient at $x = 0$ tends to zero and the solution reverts to that obtained in the absence of the recoil effect. In contrast to this, at lower temperatures for which photon scattering is able to give rise to a stronger atomic recoil effect, a significant deviation is seen upon accounting for recoil - the value of $n(x)$ across the line centre is significantly reduced.

From the solution Eq. (3.21) we can obtain an approximate expression for the Ly α scattering rate relative to that found in the free-streaming limit, similarly to that found for the solution ignoring recoil in Eq. (3.18). We find:

$$\frac{P_{\alpha, \text{ss}}}{P_{\alpha}(0)} \simeq \frac{1}{2\epsilon^3 x_1} \left[\frac{f_{\epsilon}(x_{\text{esc}}) - f_{\epsilon}(x_{\text{inj}})}{f_{\epsilon}(x_{\text{esc}}) - f_{\epsilon}(-x_{\text{esc}})} \right] [1 - f_{\epsilon}(-x_{\text{esc}})]. \quad (3.24)$$

We examine the dependence of this steady state scattering rate on temperature in Figure 3.4 - note that the y-axis is given by the relative scattering rate multiplied by x_1 to give a quantity solely dependent on the properties of the absorber. We see that the scattering rate at high temperatures assumes the value found in the absence of the recoil effect, as expected, while at increasingly lower temperatures the rate drops as $T_{\text{a}}^{1.5} \sim \epsilon^{-3}$. It is clear that the boost to the scattering rate allowed by the trapping of photons within the absorber is significantly diminished at low temperatures by the recoil effect.

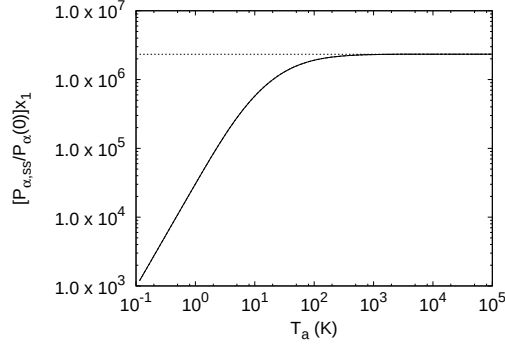


Figure 3.4: Ly α scattering rate, relative to free-streaming limit and multiplied by x_1 , as a function of absorber temperature T_a for a system with $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$; the rate is computed numerically for the recoil solution (solid line) and in the case without recoil (dashed line). The rate found according to Eq. (3.24) is coincident with the solid line.

We have discussed the effect of temperature on the steady state Ly α spectrum but we could also achieve a strong effect by varying the column density of the absorber. From the form of Eq. (3.21), we see that the ‘shape’ of the spectrum in frequency is a function of ϵx and thus the deviation from the no-recoil solution is characterised by ϵx_{esc} . For $\epsilon x \ll 1$ we obtain $f_\epsilon(x) \simeq 1 + 4/3\epsilon^3 x^3$; in this limit, the solution $n(x)$ reduces to Eq. (3.17). In the left and right panels of Figure 3.3, $\epsilon x_{\text{esc}} \simeq 0.16$ and $\epsilon x_{\text{esc}} \simeq 1.61$ respectively; this is consistent with Adams’ assertion that recoil is increasingly important for $\epsilon x_{\text{esc}} \gtrsim 1$ (Adams [1971], see section 2.8.1). It is clear that the estimated Ly α scattering rate within the system can be heavily dependent on the column density through x_{esc} and thus the results for the Ly α scattering rate from these solutions will be strongly dependent on whether photons escape by diffusion in frequency - in a single longest flight - or diffusion in space in e.g. Adams’ single longest excursion.

3.3.2 Expanding / Contracting medium

Here we consider the extension to the case where the absorber is undergoing some internal expansion or contraction. We assume this motion is characterised by a constant velocity gradient $dv/dr = H_a$, which is in general distinct from the Hubble parameter $H(z)$. The radiative transfer equation in the diffusion approximation is given by the

steady-state form of Eq. (2.33):

$$\frac{1}{2} \frac{d}{dx} \left[\phi(x) \frac{dn}{dx} + 2\gamma n(x) \right] + \tilde{S}(x) = 0 ; \quad n(\pm x_{\text{esc}}) = 0 \quad (3.25)$$

where $\gamma = \nu_0 H_a / (n_l \sigma c)$ is the Sobolev parameter introduced in section 2.4.2, although it is not specific to the expansion of the universe and is negative for a contracting medium. The transfer equation is solved straightforwardly assuming the same forms for $\tilde{S}(x)$ and $\phi(x)$ to give the solution:

$$n(x) = \begin{cases} g_\gamma(x, -x_{\text{esc}}) & ; \quad -x_{\text{esc}} < x < x_{\text{inj}} \\ g_\gamma(x, -x_{\text{esc}}) - g_\gamma(x, x_{\text{inj}}) & ; \quad x_{\text{inj}} < x < x_{\text{esc}} \end{cases} \quad (3.26)$$

where

$$g_\gamma(x, y) = A\gamma^{-1} \times \frac{f_\gamma(x, y) f_\gamma(x_{\text{esc}}, x_{\text{inj}})}{f_\gamma(x_{\text{esc}}, y)} \quad (3.27)$$

and

$$f_\gamma(x, y) = 1 - \exp \left[-\frac{2\pi\gamma}{3a} (x^3 - y^3) \right]. \quad (3.28)$$

The solution is shown for some examples of an expanding medium with $\gamma = 1.7 \times 10^{-7}$ in Figure 3.5. Photons injected at x_{inj} are subject to the redshifting effect of the expanding medium. The solution is extremely sensitive to $\gamma x_{\text{esc}}^3/a$ and when this quantity is large the spectrum adopts a step-function shape of height $A\gamma^{-1}$ redward of x_{inj} . If we define $\gamma_{\text{crit}} \equiv 3a/(2\pi x_{\text{esc}}^3)$, we see that this step-function spectrum is obtained in the limit $\gamma \gg \gamma_{\text{crit}}$; for the left panel in Figure 3.5 with $T_a = 100$ K and $x_{\text{esc}} = 200$, we find $\gamma_{\text{crit}} \simeq 2.8 \times 10^{-10}$. The Ly α scattering rate relative to that found in the free streaming case in the limit $\gamma \gg \gamma_{\text{crit}}$ is given by:

$$\frac{P_{\alpha, \text{ss}}}{P_\alpha(0)} \simeq \frac{a}{\pi\gamma x_1}, \quad (3.29)$$

which follows from the constant value $n(x) = A\gamma^{-1}$ across the line centre. We note that we can write x_1 generally as $x_1 = a/[\pi\gamma(z)]$; if the internal motion of the absorber matches the expansion of the universe at the redshift z , i.e. $H_a = H(z)$, we find $P_{\alpha, \text{ss}}/P_\alpha(0) = 1$: the strong redshifting effect in such a system prevents any enhancement in the scattering rate.

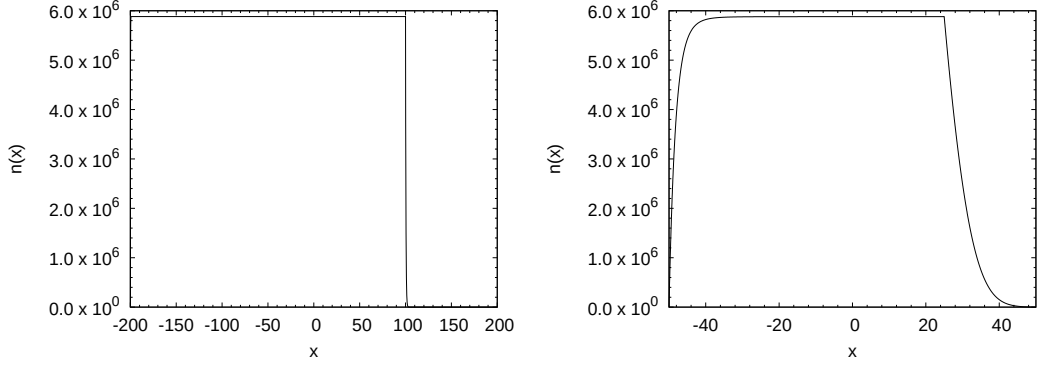


Figure 3.5: Steady-state frequency distribution of Ly α resonance-line photons in an expanding medium with $\gamma = 1.7 \times 10^{-7}$. Given by Eq. (3.26) with a temperature of 100 K and $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$ (left) and $(25, 50)$ (right).

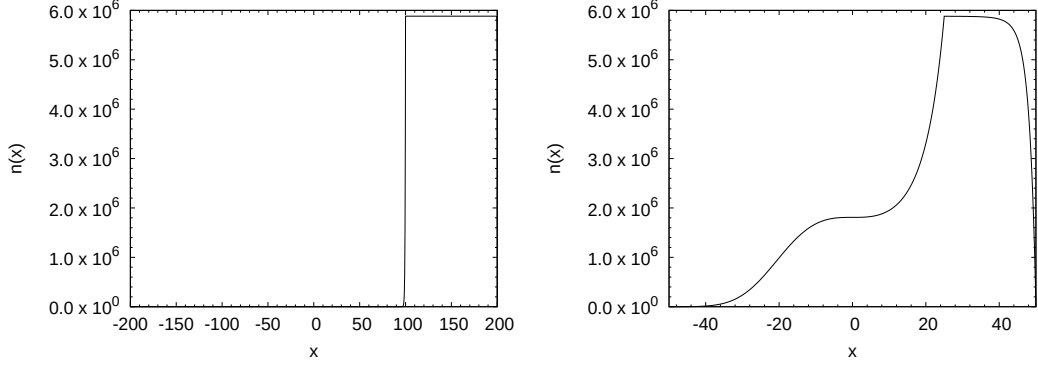


Figure 3.6: Steady-state frequency distribution of Ly α resonance-line photons in a contracting medium with $\gamma = -1.7 \times 10^{-7}$. Given by Eq. (3.26) with a temperature of 100 K and $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$ (left) and $(25, 50)$ (right).

In the case of a contracting medium ($\gamma < 0$) the solution given by Eq. (3.26) still applies, however for $|\gamma| \gg \gamma_{\text{crit}}$ we found that numerical evaluation of the form given is difficult. It is possible to get around this by rewriting the solution in the following equivalent form optimised for the contracting case:

$$n(x) = \begin{cases} h_\gamma(x, x_{\text{esc}}) - h_\gamma(x, x_{\text{inj}}) & ; \quad -x_{\text{esc}} < x < x_{\text{inj}} \\ h_\gamma(x, x_{\text{esc}}) & ; \quad x_{\text{inj}} < x < x_{\text{esc}} \end{cases}, \quad (3.30)$$

$$h_\gamma(x, y) = A|\gamma|^{-1} \times \frac{f_{|\gamma|}(y, x)f_{|\gamma|}(x_{\text{inj}}, -x_{\text{esc}})}{f_{|\gamma|}(y, -x_{\text{esc}})}. \quad (3.31)$$

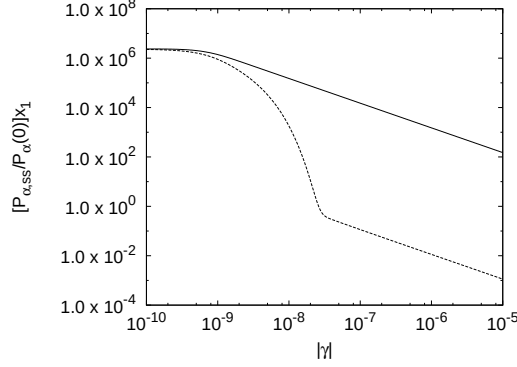


Figure 3.7: Ly α scattering rate, relative to free streaming limit and multiplied by x_1 , as a function of $|\gamma|$ for a system with $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$ and $T_a = 100$ K; the rate is computed numerically for $\gamma > 0$ (expanding medium, solid line) and $\gamma < 0$ (contracting medium, dashed line).

In Figure 3.6, solutions are shown for contracting media with $|\gamma| = 1.7 \times 10^{-7}$. We define a γ_{crit} identically to the expanding case; for the left panel we have $|\gamma| \gg \gamma_{\text{crit}}$ and the solution adopts a steep step-function form with height $A|\gamma|^{-1}$ that extends bluewards of x_{inj} , due to the blueshifting effect of the medium’s velocity gradient. As the photons can physically only be injected bluewards of resonance, such a strong blueshifting effect means that effectively no photons reach the line centre and the Ly α scattering rate is entirely negligible. In the right panel we see that the blueshifting effect does not dominate over the resonance scattering diffusion effect (which has a bias towards line centre) and in this case a significant fraction of the scattering rate found in the corresponding redshift-dominated case, $P_{\alpha,ss}/P_{\alpha}(0) = 1$, is preserved.

As an example of the dependence of the scattering rate on the magnitude of the internal motion for expanding and contracting media, we examine both as a function of $|\gamma|$ in Figure 3.7. Both the expanding and contracting medium have an effectively constant scattering rate for small $|\gamma|$; this corresponds to that found in the static solution. As $|\gamma|$ increases, the scattering rate for the expanding medium transitions to the γ^{-1} dependence found when redshifting dominates, while for the contracting medium the scattering rate drops significantly as blueshifting suppresses the photon density across the core. For sufficiently large $|\gamma|$ the contracting medium also displays the $|\gamma|^{-1}$ de-

pendence due to dominance of the scattering rate by overlap of the cross-section with the non-zero photon spectrum for $x > x_{\text{inj}}$; the rate is reduced relative to that in the corresponding $\gamma > 0$ case by the factor $\int_{x_{\text{inj}}}^{x_{\text{esc}}} \phi(x) dx \simeq (a/\pi)(x_{\text{inj}}^{-1} - x_{\text{esc}}^{-1})$.

3.3.3 Expanding / contracting medium with recoil

Combining the extra terms in the steady-state radiative transfer equation for the case of atomic recoil and an expanding/contracting medium gives the result:

$$\frac{1}{2} \frac{d}{dx} \left[\phi(x) \frac{dn}{dx} + 2(\epsilon\phi(x) + \gamma)n(x) \right] + \tilde{S}(x) = 0 ; \quad n(\pm x_{\text{esc}}) = 0. \quad (3.32)$$

We take the delta-function approximation for the source term and the wing approximation for the line profile and attempt a solution by direct integration followed by an integrating factor. In doing this we find that the solution cannot be expressed in a closed form, but we write it below in terms of integrals that can be computed numerically:

$$n(x) = \begin{cases} \left[1 - \frac{f_{\epsilon,\gamma}(x_{\text{inj}}, x_{\text{esc}})}{f_{\epsilon,\gamma}(x_{\text{esc}}, x_{\text{esc}})} \right] \times f_{\epsilon,\gamma}(x, x) & ; \quad -x_{\text{esc}} < x < x_{\text{inj}} \\ f_{\epsilon,\gamma}(x_{\text{inj}}, x) - \left[\frac{f_{\epsilon,\gamma}(x_{\text{inj}}, x_{\text{esc}})}{f_{\epsilon,\gamma}(x_{\text{esc}}, x_{\text{esc}})} \right] \times f_{\epsilon,\gamma}(x, x) & ; \quad x_{\text{inj}} < x < x_{\text{esc}} \end{cases} \quad (3.33)$$

where

$$f_{\epsilon,\gamma}(x, y) = \frac{2\pi A}{a} \int_{-x_{\text{esc}}}^x t^2 \exp \left[2\epsilon(t - y) + \frac{2\pi\gamma}{3a}(t^3 - y^3) \right] dt. \quad (3.34)$$

Similarly to the case of a contracting medium without recoil, this expression will break down for a medium with sufficiently negative γ . In this case it is necessary to use the following (equivalent) form:

$$n(x) = \begin{cases} d_{\epsilon,\gamma}(x_{\text{inj}}, x) - \left[\frac{d_{\epsilon,\gamma}(x_{\text{inj}}, -x_{\text{esc}})}{d_{\epsilon,\gamma}(-x_{\text{esc}}, -x_{\text{esc}})} \right] \times d_{\epsilon,\gamma}(x, x) & ; \quad -x_{\text{esc}} < x < x_{\text{inj}} \\ \left[1 - \frac{d_{\epsilon,\gamma}(x_{\text{inj}}, -x_{\text{esc}})}{d_{\epsilon,\gamma}(-x_{\text{esc}}, -x_{\text{esc}})} \right] \times d_{\epsilon,\gamma}(x, x) & ; \quad x_{\text{inj}} < x < x_{\text{esc}} \end{cases} \quad (3.35)$$

where

$$d_{\epsilon,\gamma}(x, y) = \frac{2\pi A}{a} \int_x^{x_{\text{esc}}} t^2 \exp \left[2\epsilon(t - y) + \frac{2\pi\gamma}{3a}(t^3 - y^3) \right] dt. \quad (3.36)$$

Examples of the solution for an expanding medium are displayed in Figure 3.8. We find a similar solution as for expanding media without recoil, with some deviation that ensures the required Boltzmann distribution is recovered across line centre. In the

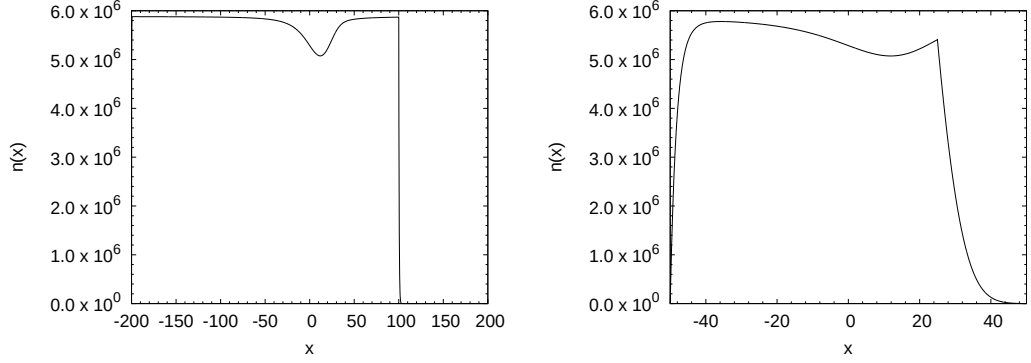


Figure 3.8: Steady-state frequency distribution of Ly α resonance-line photons in an expanding medium with $\gamma = 1.7 \times 10^{-7}$ including the effect of recoil, as given by Eq. (3.33) with a temperature of 100 K and $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$ (left) and $(25, 50)$ (right).

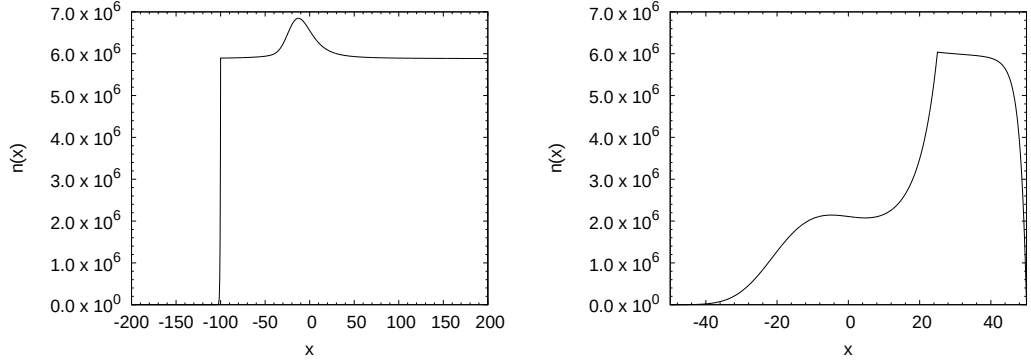


Figure 3.9: Steady-state frequency distribution of Ly α resonance-line photons in a contracting medium with $\gamma = -1.7 \times 10^{-7}$ including the effect of recoil, as given by Eq. (3.35) with a temperature of 100 K and $(x_{\text{inj}}, x_{\text{esc}}) = (-100, 200)$ (left) and $(25, 50)$ (right).

limiting case of a dominant redshifting effect, this deviation becomes a localised decrease below the $A\gamma^{-1}$ value across the line centre, identical to that found by e.g. Furlanetto and Pritchard [2006] who solved Eq. (3.32) with different boundary equations. The scattering rate is given by that found from Eq. (3.29) multiplied by the suppression factor S_α (see section 2.7.4). A similar deviation is found in the contracting case, although in the limit of a dominant blueshifting effect the deviation results from an increase in photons across the line centre, as found by Chuzhoy and Shapiro [2006]. Some examples of our solution for a contracting medium are given in Figure 3.9.

3.4 Time-Dependent Solutions

The solutions derived in the previous section all assume that a steady state has been reached in the balancing of photons arriving from the source and photons escaping the absorbing medium. In application of the solutions we would like to be confident that this steady-state assumption is justified, thus it is of interest to examine the time-dependent radiative transfer problem. The appropriate time-dependent equation in the diffusion approximation is:

$$\frac{\partial n(x, \tau)}{\partial \tau} = \frac{1}{2} \frac{\partial}{\partial x} \left[\phi(x) \frac{\partial n(x, \tau)}{\partial x} \right] + \delta_D(x - x_{\text{inj}}) ; \quad n(\pm x_{\text{esc}}, \tau) = 0 \quad (3.37)$$

where $\tau = t/t_s$ and $t_s = \Delta\nu_D/(n_l \sigma c) \simeq 3.2[n_l/\text{cm}^{-3}]^{-1}(T_a/\text{K})^{1/2} \text{ s}$ is the mean free scattering time for photons at line centre (see section 2.4.1). In order to solve this problem, a Crank-Nicholson finite difference scheme was used. The scheme was tested against Rybicki and dell'Antonio's solution in the diffusion approximation for $J(x, \tau)$ in an infinite homogeneous medium with $\tilde{S}(x) = \phi_D(x)$ (Rybicki and dell'Antonio [1994]).

The solution found after applying this method in solving Eq. (3.37) with a full Voigt function line profile is shown in the left panel of Figure 3.10. After some time the time-dependent photon number density is found to resemble the expected steady-state distribution in shape; it proceeds to increase with time until converging towards the steady state. The right panel shows the time development of the photon density at line centre; the corresponding scattering rate, expressed as a fraction of the steady-state value, is also shown. From the figure we see that the scattering rate traces the line centre photon density after $\tau \sim 10^9$, indicating that the shape of the spectrum across the line centre remains constant during this time, and ultimately a significant number of scattering events, $\tau \sim 10^{12}$, is required to establish the steady state. Clearly if a source has been active only for a small fraction of the time required to achieve a steady state, the scattering rate at the absorber may be negligibly small compared with the final result.

It is worthwhile to examine the variation of τ_{ss} , the time required to reach a steady state in units of the line-centre scattering time, with properties of the absorber. In the left panel of Figure 3.11 we examine the variation with x_{esc} for $x_{\text{inj}} = x_{\text{esc}}/2$;

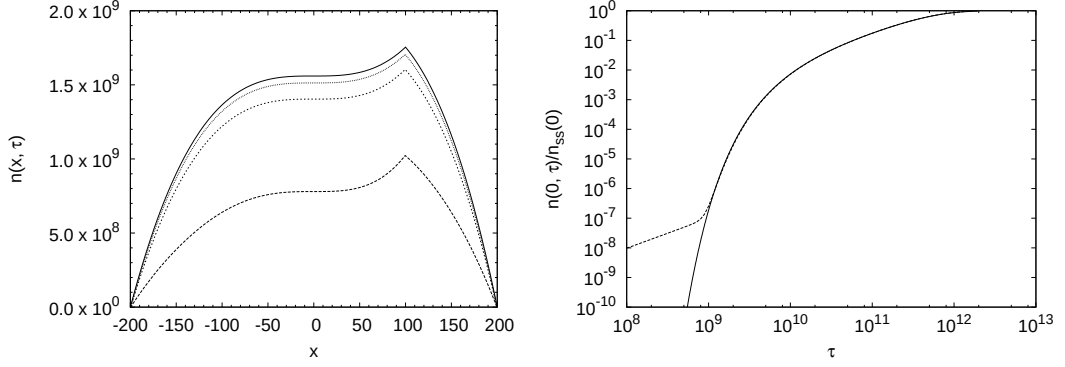


Figure 3.10: Left panel: snapshots of time-dependent solution $n(x, \tau)$ to Eq. (3.37) with temperature $T_a = 100$ K and $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$, taken at $\tau = 3.38 \times 10^{11}$ (long-dashed line), 1.11×10^{12} (short-dashed line) and 1.95×10^{12} (dotted line) for which $n(0, \tau)$ is equal to 50%, 90% and 97% respectively of the line centre value of $n_{ss}(x)$ (solid line). Right panel: time evolution of $n(0, \tau)$ (solid line), expressed as a fraction of $n_{ss}(0)$. Also shown is the scattering rate expressed as a fraction of its steady-state value (dashed line).

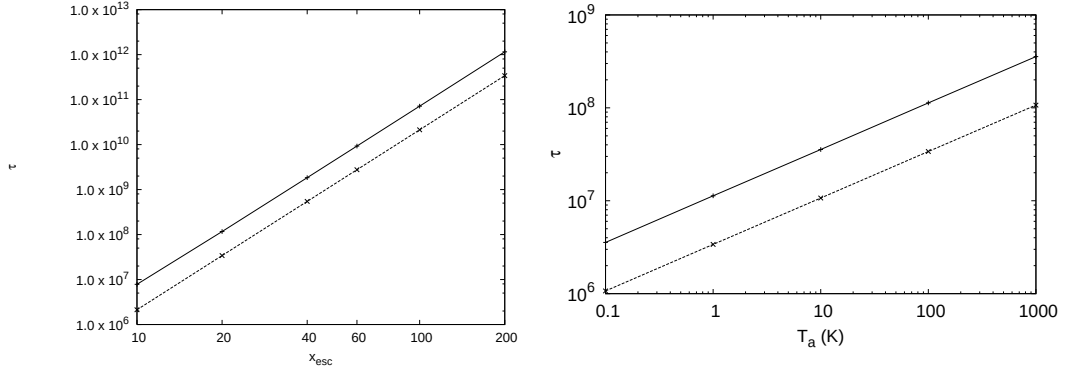


Figure 3.11: Left panel: time in units of t_s required to achieve 50% (dashed line) and 90% (solid line) of $n_{ss}(x)$ at line centre as a function of x_{esc} where $x_{\text{inj}} = x_{\text{esc}}/2$ and $T_a = 100$ K. Right panel: scattering times, defined as in left panel, as a function of absorber temperature T_a with fixed values $x_{\text{esc}} = 20$ and $x_{\text{inj}} = 10$.

a simple power law relation of the form $\tau_{ss} \sim x_{\text{esc}}^4$ is apparent. We also examine the variation of τ_{ss} with the temperature of the absorber, T_a ; this is shown in the right panel of Figure 3.11 for the fixed values $(x_{\text{esc}}, x_{\text{inj}}) = (20, 10)$. A power law dependence of the form $\tau_{ss} \sim T_a^{1/2}$ is found. From the information in the plots we infer

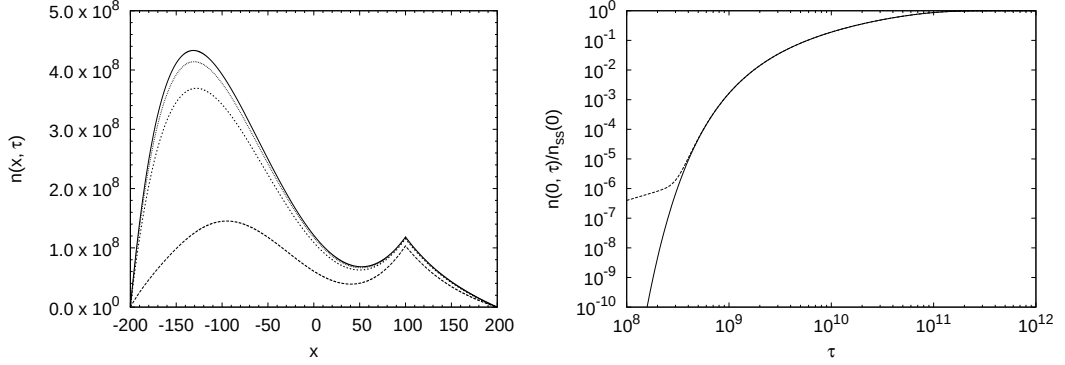


Figure 3.12: Left panel: snapshots of $n(x, \tau)$ accounting for recoil with temperature $T_a = 10$ K and $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$, taken at times $\tau = 3.16 \times 10^{10}$ (long-dashed line), 1.14×10^{11} (short-dashed line) and 1.77×10^{11} (dotted line) for which $n(0, \tau)$ is equal to 50%, 90% and 97% respectively of the line centre value of $n_{\text{ss}}(x)$ (solid line). Right panel: time evolution of $n(0, \tau)$, expressed as a fraction of $n_{\text{ss}}(0)$. Also shown is the scattering rate expressed as a fraction of its steady-state value (dashed line).

that the steady-state convergence times for 50% and 90% of the steady state obey the approximate relations $\tau_{\text{ss},50} \simeq 21T_a^{1/2}x_{\text{esc}}^4$ (50%) and $\tau_{\text{ss},90} \simeq 71T_a^{1/2}x_{\text{esc}}^4$ (90%). These scaling relations are consistent with dimensional analysis of Eq. (3.37) which suggests $\tau \sim x^2/\phi(x) \simeq (\pi/a)x^4$; thus we expect $\tau_{\text{ss}} \propto T_a^{1/2}x_{\text{esc}}^4$.

It is also possible to examine the time-dependent solution in a case that accounts for atomic recoil and allows for a uniformly expanding / contracting medium. The transfer equation is the time-dependent extension of Eq. (3.32):

$$\frac{\partial n(x, \tau)}{\partial \tau} = \frac{1}{2} \frac{\partial}{\partial x} \left\{ \phi(x) \frac{\partial n(x, \tau)}{\partial x} + 2[\epsilon \phi(x) + \gamma]n(x, \tau) \right\} + \delta_D(x - x_{\text{inj}}); \quad n(\pm x_{\text{esc}}, \tau) = 0. \quad (3.38)$$

This equation can be solved by the same finite-difference scheme applied to Eq. (3.37). A time-dependent solution for a static medium with recoil (i.e. $\gamma = 0, \epsilon \neq 0$) is given in the upper left panel of Figure 3.12. The solution is seen to converge to the steady-state solution given in Eq. (3.21). We find that the time required to reach a steady state is generally less than that found in the absence of the recoil effect; in the example shown in Figure 3.12, the values of $\tau_{\text{ss},50}$ and $\tau_{\text{ss},90}$ are about one third of the values we would estimate in the absence of recoil using our scaling relations. This effect can be

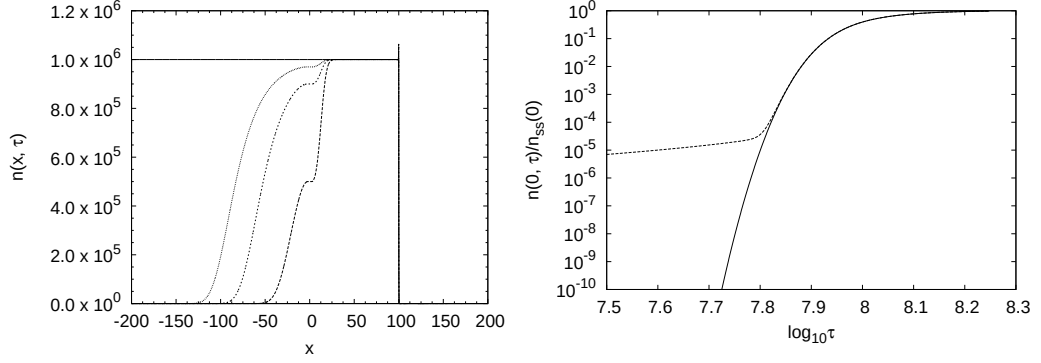


Figure 3.13: Left panel: snapshots of $n(x, \tau)$ for an expanding medium with temperature $T_a = 100$ K, $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$ and $\gamma = 10^{-6}$, taken at times $\tau = 1.05 \times 10^8$ (long-dashed line), 1.47×10^8 (short-dashed line) and 1.77×10^8 (dotted line) for which $n(0, \tau)$ is equal to 50%, 90% and 97% respectively of the line centre value of $n_{\text{ss}}(x)$ (solid line). Right panel: time evolution of $n(0, \tau)$, expressed as a fraction of $n_{\text{ss}}(0)$. Also shown is the scattering rate expressed as a fraction of its steady-state value (dashed line).

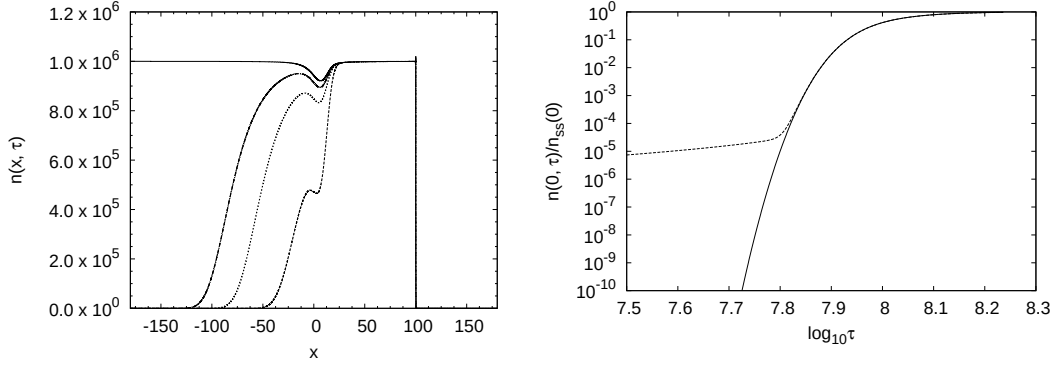


Figure 3.14: Left panel: snapshots of $n(x, \tau)$ in an expanding medium including recoil with temperature $T_a = 100$ K, $(x_{\text{inj}}, x_{\text{esc}}) = (100, 200)$ and $\gamma = 10^{-6}$, taken at times $\tau = 1.04 \times 10^8$ (long-dashed line), 1.43×10^8 (short-dashed line) and 1.72×10^8 (dotted line) for which $n(0, \tau)$ is equal to 50%, 90% and 97% respectively of the line centre value of $n_{\text{ss}}(x)$ (solid line). Right panel: time evolution of $n(0, \tau)$, expressed as a fraction of $n_{\text{ss}}(0)$. Also shown is the scattering rate expressed as a fraction of its steady-state value (dashed line).

understood by noting that atomic recoil systematically redshifts photons and reduces the time required for a photon to escape the system compared with that found without recoil, for which photons traverse the frequency space in an approximate random-walk.

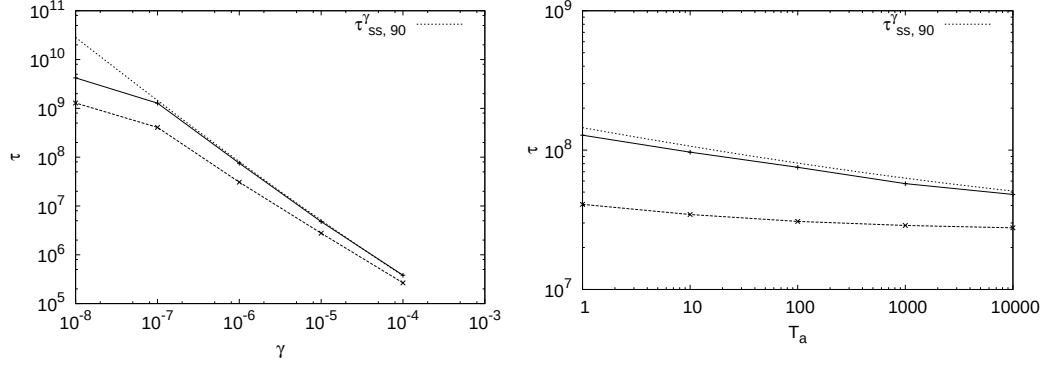


Figure 3.15: Left panel: scattering times required to achieve 50% (dashed line) and 90% (solid line) of steady-state photon density at line centre as a function of γ for an expanding medium with $(x_{\text{esc}}, x_{\text{inj}}) = (50, 25)$ and $T_a = 100$ K; the estimated value from Eq. (3.39) is also displayed (short-dashed line).

Right panel: scattering times, defined as in left panel, as a function of absorber temperature T_a with $(x_{\text{esc}}, x_{\text{inj}}) = (50, 25)$ and $\gamma = 10^{-7}$; again, the estimate from Eq. (3.39) is also given (short-dashed line).

We give an example of a time-dependent solution for scattering in an expanding medium in Figure 3.13; for the parameters given (i.e. $\gamma = 10^{-6}$, $T_a = 100$ K and $x_{\text{esc}} = 200$) we find $\gamma/\gamma_{\text{crit}} \simeq 3.5 \times 10^3$ and thus the solution is dominated by the effect of expansion. We also look at an identical system with the added inclusion of atomic recoil; this is shown in figure 3.14 and the time-evolution is seen to be negligibly affected. After looking at a number of solutions in the limit $\gamma \gg \gamma_{\text{crit}}$, the time-dependent solution is seen to build up at $x = x_{\text{inj}}$ before levelling off at the steady-state value (i.e. A/γ). This feature subsequently extends redwards in frequency before crossing the line centre where it behaves in a more complicated manner as diffusion becomes a stronger effect. Similarly to the solutions of Rybicki and dell’Antonio [1994], away from line centre the solution resembles a ‘front’ that redshifts with the approximately constant rate $dx/d\tau \simeq -\gamma$ (see section 2.7.3). Note that a key difference from Rybicki and dell’Antonio’s study and our own is that we inject our photons at some frequency $x_{\text{inj}} \gg 0$. We can use these properties to suggest a lower limit to the time required to reach the steady state scattering rate: the photon front requires a time $\tau \simeq x_{\text{inj}}/|dx/d\tau| = x_{\text{inj}}/\gamma$ to reach

the line centre. We can account for the diffusion through the line centre by utilising Rybicki and dell’Antonio’s result that the time required to build up the steady-state photon density across the line centre satisfies $\tau = Ka^{1/3}\gamma^{-4/3}$. In particular, if the steady state is required to an accuracy of 10% the proportionality constant is given as $K = 3.35$; thus, we estimate the number of line centre scattering times required to attain a photon density across the line centre equal to 90% of the steady-state value as:

$$\tau_{\text{ss},90}^\gamma = x_{\text{inj}}/\gamma + 3.35(a/\gamma^4)^{1/3} \quad (3.39)$$

i.e. the total time is comprised of the time required to redshift photons from the injection frequency to line centre, and the time required to build up to the steady state solution at the line centre. This estimate is tested against numerical calculations of $\tau_{\text{ss},90}$ for a variety of values of γ and absorber temperature T_{a} in Figure 3.15. We find Eq. (3.39) to be a good approximation for values of γ and T_{a} consistent with the limit $\gamma/\gamma_{\text{crit}} \gg 1$.

3.5 Ly α RT Steady State using R_{II}

In section 3.3, we assumed the diffusion approximation for the scattering in frequency to find analytic solutions. To verify the validity of these solutions we seek steady-state solutions that treat the frequency redistribution exactly. The full radiative transfer equation describing the steady state photon number density $n(x)$ in a homogeneous scattering medium that confines photons within a frequency range $[-x_{\text{esc}}, x_{\text{esc}}]$ and subject to a delta function source at $x = x_{\text{inj}}$ is given by the integro-differential equation:

$$\gamma \frac{dn(x)}{dx} - \phi(x)n(x) + \int_{-x_{\text{esc}}}^{x_{\text{esc}}} R(x', x)n(x') dx' + \delta_{\text{D}}(x - x_{\text{inj}}) = 0 \quad (3.40)$$

where the terms represent (left-to-right): the effect of a uniform velocity gradient; the absorption of photons of frequency x , equivalent to scattering from x to any other frequency; the scattering of photons from anywhere in the range $[-x_{\text{esc}}, x_{\text{esc}}]$ to x , and the photons received from the source. Photons scattered outside the range $[-x_{\text{esc}}, x_{\text{esc}}]$ escape the medium and are lost; they cannot be scattered back. The redistribution function appropriate for the Ly α scattering problem has the form given by Eq. (2.15) or, if we are accounting for the effect of atomic recoil, Eq. (2.23).

It is useful to use the normalisation property $\phi(x) = \int_{-\infty}^{\infty} R(x, x') dx'$ to rewrite the radiative transfer equation, Eq. (3.40), in the following way:

$$\gamma \frac{dn(x)}{dx} + \int_{-x_{\text{esc}}}^{x_{\text{esc}}} [R(x', x)n(x') - R(x, x')n(x)] dx' - E(x)n(x) + \delta_D(x - x_{\text{inj}}) = 0, \quad (3.41)$$

where

$$E(x) \equiv \int_{-\infty}^{-x_{\text{esc}}} R(x, x') dx' + \int_{x_{\text{esc}}}^{\infty} R(x, x') dx' \quad (3.42)$$

i.e. we have used the normalisation of $R(x', x)$ to break the absorption term into constituents corresponding to scattering within the range $[-x_{\text{esc}}, x_{\text{esc}}]$ and scattering outside this range. The former is grouped under the integral with the emission term, while the latter is written separately; it functions as an effective photon loss rate by redistribution across the frequency boundaries of the medium.

The function $E(x)$ can be evaluated by numerical integration of $R_{\text{II}}(x, x')$ or we can use the approximate form valid in the wings, see Eq. (2.17); in this limit we can write the form of the emitted frequency probability distribution as:

$$\begin{aligned} p(x|x') &= \left(\frac{x+x'}{2x'} \right)^{-2} \text{ierfc} \left(\frac{|x-x'|}{2} \right) \\ &\simeq \left[1 - \frac{x-x'}{x'} \right] \text{ierfc} \left(\frac{|x-x'|}{2} \right). \end{aligned} \quad (3.43)$$

Note that this is an excellent approximation as long as x_{esc} is far out in the wings; if this is the case then clearly x' lies in the wings over the ranges of integration in Eq. (3.42), while x is necessarily close to x' if $R(x', x)$ is to be non-zero. Thus we obtain:

$$\begin{aligned} E(x) &= \phi(x) \left[\int_{-\infty}^{-x_{\text{esc}}} p(x'|x) dx' + \int_{x_{\text{esc}}}^{\infty} p(x'|x) dx' \right] \\ &= 2\phi(x) \left[\int_{(x_{\text{esc}}-x)/2}^{\infty} \text{ierfc}(\Delta) d\Delta + \int_{(x_{\text{esc}}+x)/2}^{\infty} \text{ierfc}(\Delta) d\Delta \right. \\ &\quad \left. - \frac{2}{|x|} \int_{(x_{\text{esc}}-|x|)/2}^{(x_{\text{esc}}+|x|)/2} \Delta \text{ierfc}(\Delta) d\Delta \right] \end{aligned} \quad (3.44)$$

where we have changed variables to $\Delta \equiv |x - x'|/2$ in the integrals. Note that the first two terms here represent the rate of photon escape provided by symmetric redistribution far from line centre, while the last term reflects that the escape rate is reduced at smaller

$|x|$ in accordance with the bias towards line centre. The integrals can be evaluated analytically to provide an accurate estimate of the photon escape function $E(x)$ to be used in Eq. (3.41).

We solve Eq.(3.41) by means of an expansion of the photon number density in a basis of cubic splines. The appropriate expansion given a series of discrete gridpoints $\{x_j\} = \{x_1, x_2, \dots, x_N\}$ is written (see Adams et al. [1971]):

$$n(x) \rightarrow \sum_{j=1}^N n(x_j) \psi_j(x), \quad \psi_j(x_k) = \delta_{j,k}. \quad (3.45)$$

The cubic splines ψ_j are ‘natural’ (they have zero second-derivative at the boundaries of the grid) and ‘cardinal’ (they vanish at all but one of the gridpoints) and can be calculated by standard numerical methods (see Press et al. [1992]). We work on a uniform grid spanning the range $[-x_{\text{esc}}, x_{\text{esc}}]$; evaluation of the various terms in Eq. (3.41) at $x = x_i$ results in the following replacements:

$$\int_{-x_{\text{esc}}}^{x_{\text{esc}}} R(x', x) n(x') dx' \rightarrow \sum_{j=1}^N R_{ij} n(x_j); \quad R_{ij} \equiv \int_{-x_{\text{esc}}}^{x_{\text{esc}}} R(x', x_i) \psi_j(x') dx', \quad (3.46)$$

$$\int_{-x_{\text{esc}}}^{x_{\text{esc}}} R(x, x') n(x) dx' \rightarrow n(x_i) \sum_{j=1}^N \bar{R}_{ij}; \quad \bar{R}_{ij} \equiv \int_{-x_{\text{esc}}}^{x_{\text{esc}}} R(x_i, x') \psi_j(x') dx', \quad (3.47)$$

$$\gamma \frac{dn(x)}{dx} \rightarrow \gamma \sum_{j=1}^N D_{ij} n(x_j); \quad D_{ij} \equiv \left. \frac{d\psi_j(x)}{dx} \right|_{x=x_i}. \quad (3.48)$$

These quantities are easily evaluated from the forms of the spline functions and the redistribution function; in particular, for a frequency grid of constant spacing Δx , the first derivatives of the splines needed for the D_{ij} coefficients are related to the known spline properties by $\psi'_j(x_i) = [\psi_j(x_{i+1}) - \psi_j(x_i)]/\Delta x - \psi''_j(x_i)\Delta x/3 - \psi''_j(x_{i+1})\Delta x/6$.

The resulting representation of Eq. (3.41) can be written, defining $S_i \equiv \delta_D(x_i - x_{\text{inj}})$, as:

$$\sum_{j=1}^N M_{ij} n(x_j) = S_i \quad (3.49)$$

where

$$M_{ij} \equiv \left[E(x_i) + \sum_{j=1}^N \bar{R}_{ij} \right] \delta_{i,j} - R_{ij} - \gamma D_{ij}. \quad (3.50)$$

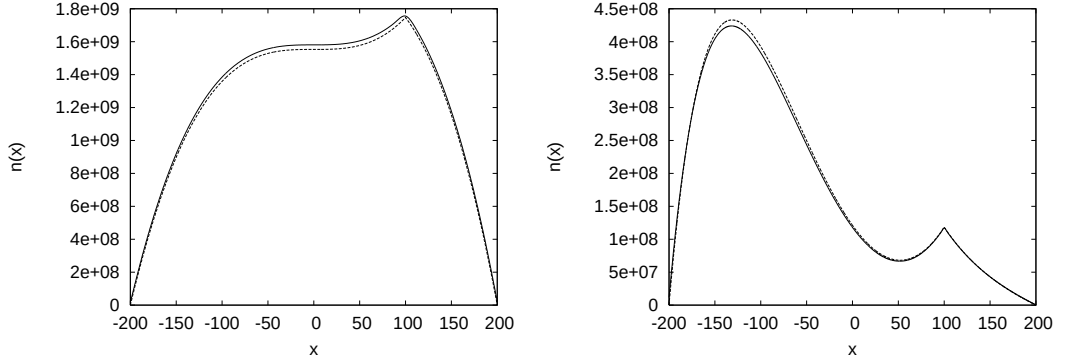


Figure 3.16: Left panel: solution resulting from spline solution of Eq. (3.41) (solid line) and diffusion approximation solution (dashed line) for $T = 100$ K, $x_{\text{esc}} = 200$, $x_{\text{inj}} = 100$ and $R = R_{\text{II}}$.

Right panel: solution resulting from spline solution of Eq. (3.41) (solid line) and diffusion approximation solution (dashed line) for $T = 10$ K, $x_{\text{esc}} = 200$, $x_{\text{inj}} = 100$ and $R = R_{\text{II},\epsilon}$.

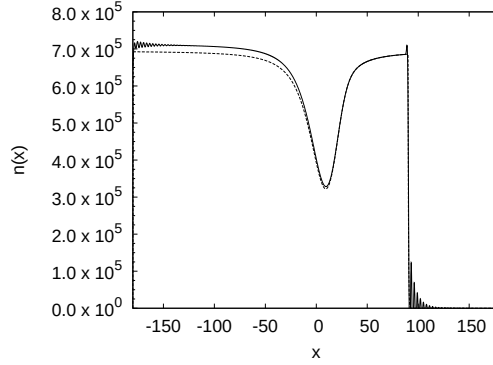


Figure 3.17: Solution resulting from spline solution of Eq. (3.41) (solid line) and diffusion approximation solution (dashed line) for $T = 2.65$ K ($\epsilon = 0.016$), $\gamma = 1.44 \times 10^{-6}$, $x_{\text{esc}} = 180$, $x_{\text{inj}} = 90$ and $R = R_{\text{II},\epsilon}$.

Thus the integro-differential equation is reduced to an $N \times N$ matrix equation, solvable by standard methods. Note that the sum of quantities in the square brackets here is formally equal to $\phi(x_i)$, as expected from a straightforward discretisation of Eq. (3.40); we do not make this substitution as we found it necessary to ensure symmetry in our treatment of emission and absorption and the associated numerical errors. Figure 3.16 displays solutions obtained by this method in a static medium ($\gamma = 0$) for cases with

and without recoil. The solutions agree extremely well with those obtained analytically in the diffusion approximation. Figure 3.17 shows good agreement for a medium with a uniform velocity gradient.

3.6 Discussion

In this section we utilise some of the results obtained throughout this chapter in a series of applications. Consider a region around a bright QSO with a specific luminosity at the Lyman edge of $10^{31} \text{ erg s}^{-1} \text{ Hz}^{-1}$ preheated by soft X-rays ahead of an ionisation front to a mean temperature $T_{\text{IGM}} \simeq 1800 \text{ K}$ (Madau et al. [1997]). At a redshift $z = 8$, according to Eq. (3.5), we find the optical depth through the intervening IGM is characterised by the frequency $x_1 \simeq 200$. Now consider a static structure 250 kpc across with a moderate overdensity $n_{\text{HI}}/n_{\text{HI}}(z) = 3$ and internal temperature $T_{\text{a}} = 120 \text{ K}$ at $z = 8$, a distance 10 Mpc from the QSO. Such a structure has a neutral hydrogen column density $N_{\text{HI}} \simeq 3 \times 10^{20} \text{ cm}^{-2}$ and a corresponding frequency for escape $x_{\text{esc}} \simeq 200$, from Eq. (3.10) (assuming the value $f = 0.1$). Assuming a power-law spectrum varying as $\nu^{-1.5}$ and applying Eq. (3.7) we find that the $\text{Ly}\alpha$ scattering rate in the free-streaming limit is $P_{\alpha}(0) \simeq 8.7 \times 10^{-13} \text{ s}^{-1}$; this is roughly an order of magnitude smaller than the thermalisation rate required to decouple the hydrogen spin temperature from the CMB, $P_{\text{th}} \simeq 6.8 \times 10^{-12} \text{ s}^{-1}$ from Eq. (1.35). The steady state value from Eq. (3.19), however, gives $P_{\alpha, \text{ss}} \simeq 10^{-8} \text{ s}^{-1}$, well in excess of P_{th} .

It is necessary, however, to consider the time required to reach the steady state. The $\text{Ly}\alpha$ scattering time within the structure is given by $t_{\text{s}} \simeq 8.5 \times 10^4 \text{ s}$ and thus, using $\tau_{\text{ss}, 90} \simeq 71 T_{\text{a}}^{1/2} x_{\text{esc}}^4$, we find the time required to be about 10^{17} s or 3 Gyr. This greatly exceeds the expected lifetime of the QSO. We assume the QSO illuminates the structure for a time 0.1 Gyr; noting that the timescales involved vary weakly with absorber temperature we can assume the time variation of the scattering rate displayed in Figure 3.10 and thus the scattering rate reached is $P_{\alpha}(\tau) \simeq 0.05 \times P_{\alpha, \text{ss}}$. This scattering rate is still in excess of P_{th} . Note that if the structure happens to have a peculiar velocity with a non-zero radial component away from the source then the

received photon spectrum, and thus x_{inj} , will be shifted redwards; if x_{inj} is closer to line centre then the steady-state scattering rate will be increased and it will also be reached in a shorter time. We note that the optimum scattering rate, achieved when x_{inj} is shifted to line centre, is found for a radial velocity away from the QSO of $v_{\text{pec}} \simeq \frac{1}{2}x_1b_a \simeq 140 \text{ km s}^{-1}$, a plausible value.

Discounting any peculiar velocity, the scattering rate attained would also be boosted significantly for a much more overdense structure acting as our absorber. A virialised structure 35 kpc across with an overdensity of 200 and a temperature $T_a \simeq 1000 \text{ K}$ would have a neutral hydrogen column density $N_{\text{HI}} \simeq 3 \times 10^{21} \text{ cm}^{-2}$ and an escape frequency $x_{\text{esc}} \simeq 220$. The time for such a structure to reach a steady state would then be about 0.6 Gyr, a plausible lifetime for the QSO.

By contrast we find that it may be quite difficult to achieve a steady state in a void. For a mean IGM temperature $T_{\text{IGM}} \simeq 100 \text{ K}$, we find $x_1 = 825$ at $z = 8$. Consider a region 3 Mpc across with a temperature $T_a = 10 \text{ K}$, underdense by a factor of 3; the resulting neutral hydrogen column density is $N_{\text{HI}} = 4 \times 10^{20} \text{ cm}^{-2}$ and the escape frequency is $x_{\text{esc}} \simeq 800$. The scattering time at line centre is $t_s \simeq 2.2 \times 10^5 \text{ s}$ and the time required to reach a steady state is about 640 Gyr. Even if the void is illuminated for as long as the age of the universe, the radiation field will be negligibly small compared with its steady state value. Since the void will expand, however, the incident radiation field will be redshifted across the line centre in significantly less time. Voids expand somewhat faster than the mean Hubble expansion; if we adopt the Hubble constant at $z = 8$ for $h = 0.7$, we find $\gamma \simeq 5 \times 10^{-6}$. As $\gamma \gg \gamma_{\text{crit}} \simeq 1.4 \times 10^{-11}$, the steady-state scattering rate reduces to the free-streaming value - $P_{\alpha, \text{ss}} = P_{\alpha}(0)$ - and the steady state is reached in a time $t \gtrsim \tau_{\text{ss}, 90}^{\gamma} t_s \simeq 6 \times 10^5 \text{ yrs}$; the effect of the expansion may then be adequate to produce a 21cm signature in the presence of sufficient sources.

The preceding results are based on the solutions presented in our locally homogeneous absorber model in the absence of atomic recoil. If we apply the criterion for a static medium that recoil becomes significant for $\epsilon x_{\text{esc}} \gtrsim 1$ we find that it could have a significant effect in the void discussed above; for $T_a = 10 \text{ K}$ and $x_{\text{esc}} = 800$, we find $\epsilon x_{\text{esc}} \simeq 6.3$. Comparison of the scattering rate found in the static solution accounting

for recoil, Eq. (3.24), with that found without recoil tells us that, in the limit $\epsilon x_{\text{esc}} \gtrsim 1$, we have a reduction by a factor of $3/(2\epsilon^3(x_{\text{esc}}^3 - x_{\text{inj}}^3)) \simeq 6.5 \times 10^{-3}$. However, it is quite possible that the value found for the escape frequency is a significant overestimate and any such real system would be sufficiently optically thick as to allow escape by spatial diffusion, in which case the escape frequency is replaced by that of Adams, x_* , and recoil has less impact. Of course, any such considerations become academic when the expansion of the medium is accounted for. We can include the effect of recoil in the expanding void by using the results of Furlanetto and Pritchard [2006] for the suppression factor, S_α ; recoil induces a decrease in the photon density across the line centre in a system dominated by redshifting and the scattering rate is reduced by a factor $S_\alpha < 1$ relative to that found in the absence of recoil. We can compute the suppression factor from the approximation $S_\alpha \approx 1 - \delta_J(0)$ and Equations (2.69) and (2.70); we find $1 - S_\alpha \simeq 1.8 \times 10^{-2}$, and thus the scattering rate for the expanding void is negligibly affected by recoil. We also expect the time required to reach a steady state to be unaffected.

These applications show that the results obtained in this chapter can give estimates of the effectiveness of the Wouthuysen-Field effect in providing 21cm coupling in the IGM for H I structure scattering Ly α photons from some distant, isolated source. Assumptions and approximations were made in deriving our results and we have attempted to assess the impact of such where possible; in particular, we have demonstrated the validity of the diffusion approximation made in treating the photon scattering in frequency. The biggest potential limitation of the utility of our results is the reduction of the Ly α scattering radiative transfer problem to a one-dimensional problem in frequency, a consequence of our model of a locally homogeneous scattering medium. In subsequent chapters we will look at solving related problems of Ly α scattering in a less limited formulation of the associated radiative transfer, namely a spherically symmetric medium in which the transfer of photons in both frequency and space can be treated.

CHAPTER 4

Ly α Scattering by Monte Carlo Methods

In this chapter we adopt the approach of Monte Carlo methods in solving Ly α scattering radiative transfer. In particular:

- We describe a Monte Carlo treatment of type II frequency redistribution that makes direct use of the frequency redistribution function $R(x', x)$ and its limiting form far from line centre. We test our method and compare it with the widely-applied method of Zheng and Miralda-Escudé [2002] based on modelling the scattering off individual atoms, and find it to be faster by a factor of ~ 3 .
- We describe in detail an implementation of Monte Carlo methods for a spherically symmetric scattering medium subject to a radial velocity field. We examine some simple applications of our methods and find that they give results in agreement with pre-existing solutions.

These methods can in principle be extended to treat a scattering medium with any spatial configuration, as might be required to predict the Wouthuysen-Field coupling of sources arising from cosmological simulations

4.1 Monte Carlo Redistribution using R_{II}

In this section we describe a Monte Carlo method intended to calculate the effect of type II frequency redistribution on an ensemble of Ly α photons. From the definition of $R(x', x)$, the probability distribution of scattered photon frequencies x given an incident photon frequency x' is given by $p(x | x') \equiv R(x', x)/\phi(x')$. Thus, the cumulative probability distribution function describing the scattered frequency is:

$$P(x | x') = \frac{1}{\phi(x')} \int_{-\infty}^x R(x', y) dy. \quad (4.1)$$

This is the same function as that given in Eq. (2.53); $P(x | x')$ gives the probability that the photon is scattered to any frequency $y < x$ and its value is uniformly distributed between zero and unity. As stated in section 2.5, by calculating $P(x | x')$ and inverting to find $x(P)$ we are able to select output frequencies distributed accordingly - explicitly, we solve for x the equation $P(x | x') = R$ where R is a uniformly distributed random number lying in the range $[0, 1]$.

4.1.1 Scattering by Lookup Tables

The integration involved in the computation of the cumulative probability of Eq. (4.1) for a given input frequency x' is accomplished by the composite Simpson rule applied to the R_{II} redistribution function [see Eq. (2.15)]. The integral is calculated as a sum of smaller integrals between grid-values $\{x_i\}$, where $i = 0, 1, 2, \dots, I$ and $x_0 = x_{\min} < x_1 < \dots < x_I = x_{\max}$. For $i \geq 1$ we write:

$$P(x_i | x') = \frac{1}{\phi(x')} \sum_{j=1}^i \int_{x_{j-1}}^{x_j} R(x', y) dy. \quad (4.2)$$

Note that the values $x_{\min}$ and $x_{\max}$ are chosen such that $p(x | x')$ is effectively zero outside of the enclosed frequency range and thus $P(x_0 | x') = 0$. Following e.g. Avery and House [1968], we determine the output frequency by selecting a random number R and finding the index i such that $P(x_i) \leq R < P(x_{i+1})$. This process is streamlined by using the values of $P(x_i)$ to obtain values of the inverse function $x(P_j)$ on a grid of J values $\{P_j\}$ spanning $[0, 1]$ with uniform spacing $\Delta P = 1/J$; for each scatter we determine $x(R)$ by interpolation between the values of P_j bracketing R .

This method is only practical for a single input frequency. If we follow a Ly α photon scattering in a static H I medium for example, the photon will scatter with an input frequency given by the output frequency from the previous scatter and generally we have to account for all input frequencies x' lying within the boundaries set by the escape frequency. Though some work is involved, the method described for a single input frequency can be applied by constructing lookup tables of $P(x_i | x'_k)$ and its inverse for a suitable grid of input frequencies $\{x'_k\}$; we found that the greater dependence of $p(x | x')$ upon x' for absorption near line centre demanded a greater density of grid-values x'_k across $x' = 0$, and adopted a Gaussian distribution for the density of points. For some $x'_k < x' < x'_{k+1}$, we compute output frequencies x from the pre-calculated lookup tables applicable at each of x'_k and x'_{k+1} and interpolate x as a function of x' . In this way we can deal with a finite set of lookup tables, but if photons escape large numbers of Doppler widths from line centre, as in the high optical depth case, the number of lookup tables required might become impractical.

4.1.2 Scattering in the Wings

For photons undergoing type II frequency redistribution far from line centre we can assume Unno's approximate form for R_{II} , Eq. (2.17). Dividing by the form of the absorption profile appropriate in the wings, $\phi(x') = a/(\pi x'^2)$, we obtain:

$$p(x | x') = \left(\frac{x + x'}{2x'} \right)^{-2} \text{ierfc} \left(\frac{|x - x'|}{2} \right), \quad (4.3)$$

$$\simeq \left[1 - \frac{x - x'}{x'} \right] f(\Delta) \quad (4.4)$$

where $\Delta \equiv |x - x'|/2$ and $f(\Delta) = \text{ierfc}(\Delta) \equiv \pi^{-1/2} e^{-\Delta^2} - \Delta \text{erfc}(\Delta)$. This approximation applies in the wings where $|x'|$ is large, while $f(\Delta)$ is non-zero for small Δ only; consequently the factor in square brackets is close to unity across this domain and we might expect we can take $p(x | x') = f(\Delta)$, however the prefactor is necessary to preserve the mean frequency shift per scattering responsible for the bias towards line centre [see Eq. (2.74)]. As such we seek to apply the acceptance-rejection method (as described by e.g. Press et al. [1992]), using some multiple of the function $f(\Delta)$ as a comparison distribution in a Monte Carlo treatment for scattering in the wings.

The first step in this method requires us to select frequencies distributed according to the comparison distribution $g(x | x') = A \times f(\Delta)$, where the numerical factor A is chosen to ensure that $g(x | x') > p(x | x')$ for all x . The selection process is independent of the normalisation of the comparison distribution and we can take $g(x | x') \rightarrow f(\Delta)$ for now. We obtain the comparison cumulative probability distribution $C(x | x')$ analytically:

$$\begin{aligned}
C(x | x') &= \int_{-\infty}^{x'} g(y | x') dy + \int_{x'}^x g(y | x') dy, \\
&= 2 \int_0^\infty \text{ierfc}(\delta) d\delta \pm 2 \int_0^\Delta \text{ierfc}(\delta) d\delta, \\
&= \frac{1}{2} \pm \left[\left(\frac{1}{2} + \Delta^2 \right) \text{erf}(\Delta) - \Delta^2 + \frac{1}{\sqrt{\pi}} \Delta e^{-\Delta^2} \right] \quad (4.5)
\end{aligned}$$

where the plus and minus correspond to $x > x'$ and $x < x'$ respectively. Thus we can construct a lookup table of the values of $|C(x | x') - 1/2|$ as a function of Δ and determine the inverse relationship as described for the non-wing-specific case. For a uniform random number R_1 we relate $|R_1 - 1/2|$ to the appropriate Δ and determine the output frequency $x_0 = x' \pm 2\Delta$, where the plus and minus signs are taken for $R_1 > 1/2$ and $R_1 < 1/2$ respectively.

The normalisation of the comparison distribution is important in the main step of the acceptance-rejection method; for a maximum value $\Delta_{\max}$ such that $f(\Delta)$ becomes negligible for $\Delta > \Delta_{\max}$ ($\Delta_{\max} \simeq 5$ for example), we must take $A > \left[1 - \frac{\Delta_{\max}}{|x'|} \right]^{-2}$ to ensure $g(x | x') > p(x | x')$ for all $x \in [x' - 2\Delta_{\max}, x' + 2\Delta_{\max}]$. Given the candidate output frequency x_0 , a new random number R_2 is selected and compared with the ratio:

$$r \equiv \frac{p(x_0 | x')}{g(x_0 | x')} = \frac{1}{A} \left[\frac{x_0 + x'}{2x'} \right]^{-2}, \quad (4.6)$$

the value of which dictates whether x_0 is accepted or rejected for $R_2 < r$ or $R_2 > r$ respectively. Both steps are repeated with new values for R_1 and R_2 until an output frequency determined from $g(x | x')$ is accepted. In this way we ensure that the accepted x_0 are distributed according to $p(x | x')$ as given by Eq. (4.3), the probability distribution for scattering in the wings. This method allows us to account for the redistribution in the wings with the use of only a single lookup table, and no numerical integration is required.

4.2 Alternative: Redistribution using $p(u_{\parallel})$

We briefly summarise the widely-adopted method of Zheng and Miralda-Escudé [2002] for choosing the outgoing frequency of a scattered Ly α photon. Instead of attempting to treat the redistribution function directly, this method works by choosing the thermal velocity of the scattering atom (written $\mathbf{v}$ or $\mathbf{u} = \mathbf{v}/b$) and determining the outgoing frequency from the associated Doppler shifts. The most complicated part of this approach is the selection of the scattering atomic velocity component $u_{\parallel}$, parallel to the incoming photon direction $\mathbf{n}'$, and drawn from the distribution:

$$p(u_{\parallel} | x') = \frac{a}{\pi H(a, x')} \left[\frac{e^{-u_{\parallel}^2}}{(x' - u_{\parallel})^2 + a^2} \right] \quad (4.7)$$

i.e. a Gaussian (Maxwellian thermal velocity distribution) weighted by a Lorentzian centred on the incident frequency x' , due to the requirement that the atomic rest frame frequency $\xi' = 0$ to within the limits set by natural broadening. We assume $x' \geq 0$; if $x' < 0$ we can use the symmetry $p(u_{\parallel} | -x') = p(-u_{\parallel} | x')$ i.e. take $x' \rightarrow |x'|$ and after determining $u_{\parallel}$, switch its sign. Zheng and Miralda-Escudé implemented Eq. (4.7) by applying the acceptance-rejection method to a comparison distribution $g(u_{\parallel} | x')$ given by (suppressing the ‘parallel’ subscript, $u_{\parallel} \rightarrow u$):

$$g(u | x') = \frac{a}{\pi H(a, x')} \times \begin{cases} [(x' - u)^2 + a^2]^{-1} & ; -u_{\max} < u \leq u_0 \\ e^{-u_0^2} [(x' - u)^2 + a^2]^{-1} & ; u_0 < u < u_{\max} \end{cases} \quad (4.8)$$

where the maximum permitted value of $|u|$ is $u_{\max}$ (infinite by default) and u_0 can be chosen to reduce the number of rejections for a given x' . Semelin et al. [2007] suggest the fit:

$$u_0 = \begin{cases} 1.85 - \log a/6.73 + \ln(\ln x') & ; x' > 3 \\ 0 & ; x' \leq 3 \end{cases} \quad (4.9)$$

together with a truncation of the domain to $u_{\max} = 3$ if $x' > 10$. This tactic is motivated by scattering in the wings for which the distribution $p(u | x')$ is Gaussian-dominated and limiting our search to around $u = 0$ (corresponding to the near-coherent scattering limit) is effective in reducing the fraction of rejections.

Zheng and Miralda-Escudé [2002] perform an integration and inversion of the comparison distribution to determine candidate values of u to accept/reject. They determine the fractional area under $g(u | x')$ up to $u = u_0$ to be:

$$\begin{aligned} r(u_0) &\equiv \int_{-u_{\max}}^{u_0} g(u | x') du \Big/ \int_{-u_{\max}}^{u_{\max}} g(u | x') du , \\ &= (\theta_0 + \theta_+) \left[(1 - e^{-u_0^2})\theta_0 + \theta_+ + e^{-u_0^2}\theta_- \right]^{-1} \end{aligned} \quad (4.10)$$

where $\theta_0 \equiv \tan^{-1}[(u_0 - x')/a]$ and $\theta_{\pm} \equiv \tan^{-1}[(u_{\max} \pm x')/a]$ (note that we have altered Zheng and Miralda-Escudé's results to account for finite $u_{\max}$, else $\theta_+ = \theta_- = \pi/2$). Calculation of the cumulative distribution function $r(u)$ tells us the quantity $\theta = a \tan^{-1}[(u - x')/a]$ is uniformly distributed on the range (i) $[-\theta_+, \theta_0]$ if $u \leq u_0$ or (ii) $[\theta_0, \theta_-]$ if $u > u_0$. Thus the selection process can be implemented analytically:

$$u_{\parallel} = x' + \begin{cases} a \tan[-\theta_+ + (\theta_0 + \theta_+)R_2] & ; R_1 \leq r(u_0) \\ a \tan[\theta_0 + (\theta_- - \theta_0)R_2] & ; R_1 > r(u_0) \end{cases} \quad (4.11)$$

where we have introduced two uniformly-distributed random deviates; R_1 is compared with $r(u_0)$ to ascertain if $u_{\parallel}$ will be greater than or less than u_0 , while R_2 sets the value of θ within the range (i) or (ii). Given the candidate $u_{\parallel}$, it is necessary to compute another random number R_3 uniform on $[0, 1]$ and compare with the fraction

$$f \equiv \frac{p(u_{\parallel} | x')}{g(u_{\parallel} | x')} = \begin{cases} e^{-u_{\parallel}^2} & ; u_{\parallel} \leq u_0 \\ e^{-(u_{\parallel}^2 - u_0^2)} & ; u_{\parallel} > u_0 \end{cases} \quad (4.12)$$

where $R_3 < f$ ($R_3 > f$) dictates that we accept (reject) $u_{\parallel}$. This process is repeated for a given scattering event until a value of $u_{\parallel}$ is accepted.

The velocity $\mathbf{u}$ is written in the basis defined by the orthonormal triad $[\mathbf{n}', \mathbf{n}'_{\perp,1}, \mathbf{n}'_{\perp,2}]$ as $\mathbf{u} = u_{\parallel}\mathbf{n}' + u_{\perp,1}\mathbf{n}'_{\perp,1} + u_{\perp,2}\mathbf{n}'_{\perp,2}$. Each of the components perpendicular to $\mathbf{n}'$ is independently Gaussian-distributed according to $p(u_{\perp,(1,2)}) = e^{-u_{\perp,(1,2)}^2}/\sqrt{\pi}$, but we will only need the magnitude of $\mathbf{u}$ projected onto the plane perpendicular to $\mathbf{n}'$, $u_{\perp} \equiv (u_{\perp,1}^2 + u_{\perp,2}^2)^{1/2}$. This quantity has a distribution determined by integrating

$p(u_{\perp,1})p(u_{\perp,2}) du_{\perp,1} du_{\perp,2}$ around an annulus of radius $u_{\perp} \rightarrow u_{\perp} + du_{\perp}$:

$$\begin{aligned} p(u_{\perp}) du_{\perp} &= \int_0^{2\pi} \left[\frac{1}{\pi} e^{-u_{\perp}^2} \right] u_{\perp} du_{\perp} d\phi, \\ &= 2u_{\perp} e^{-u_{\perp}^2} du_{\perp}. \end{aligned} \quad (4.13)$$

We determine appropriately distributed values of $u_{\perp}$ from the corresponding cumulative distribution function $P(u_{\perp})$ as follows:

$$P(u_{\perp}) = 2 \int_0^{u_{\perp}} v e^{-v^2} dv = 1 - e^{-u_{\perp}^2} = R, \quad (4.14)$$

giving

$$u_{\perp} = \sqrt{-\ln R}. \quad (4.15)$$

Finally, we can use the components of $\mathbf{u}$ to write the outgoing frequency for a scattered photon. The scattered frequency x , given the outgoing photon direction $\mathbf{n}$, is related to the pre-scattering frequency x' by:

$$x = x' - \mathbf{u} \cdot \mathbf{n}' + \mathbf{u} \cdot \mathbf{n} - \epsilon(1 - \mathbf{n} \cdot \mathbf{n}') \quad (4.16)$$

which follows by noting that the shift is given by Eq. (2.21) in the rest frame of the atom. Further simplification is allowed if we write the outgoing direction vector as $\mathbf{n} = \mu \mathbf{n}' + (1 - \mu^2)^{1/2} \mathbf{n}'_{\perp}$ where $\mu = \mathbf{n} \cdot \mathbf{n}'$ and $\mathbf{n}'_{\perp} = (\cos \phi_1) \mathbf{n}'_{\perp,1} + (\sin \phi_1) \mathbf{n}'_{\perp,2}$ for some angle ϕ_1 . Writing $u_{\perp,1} = u_{\perp} \cos \phi_2$ and $u_{\perp,2} = u_{\perp} \sin \phi_2$ we find:

$$x = x' - (1 - \mu)(u_{\parallel} + \epsilon) + \left[(1 - \mu^2)^{1/2} \cos \phi \right] u_{\perp} \quad (4.17)$$

where $\mu = 2R_1 - 1$ and $\phi \equiv (\phi_2 - \phi_1) = 2\pi R_2$. Thus the Monte Carlo treatment of the RII frequency redistribution using the scattering atom's thermal velocity amounts to (i) determining a candidate $u_{\parallel}$ from Eq. (4.11) and performing the comparison specified in Eq. (4.12) until an acceptable outcome is achieved, (ii) determining $u_{\perp}$ from Eq. (4.15), and (iii) using the input frequency with the components $u_{\parallel}$ and $u_{\perp}$ to determine the output frequency from Eq. (4.17). All steps are essentially performed analytically, as opposed to the large amount of numerical integration etc. involved in the more direct method (in principle) using the redistribution function.

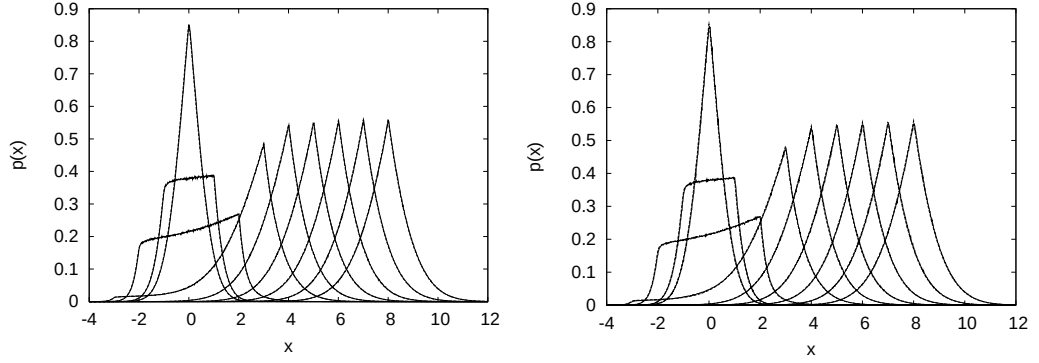


Figure 4.1: Monte Carlo histograms for the output frequency (solid lines) determined from the scattering atom velocity method (left panel) and the redistribution function method (right panel), compared with the analytic form $p(x|x') = R_{\Pi}(x', x)/\phi(x')$ (dashed lines). Histograms correspond to fixed input frequencies $x' = 0, 1, 2, 3, 4, 5, 6, 7, 8$ (peak values from left to right).

4.2.1 Comparison with Redistribution Method

We performed a test consisting of determining the output frequency distribution for a fixed input frequency, the results of which are given in Figure 4.1. The method of Zheng and Miralda-Escudé [2002] produces histograms exactly coincident with $p(x|x')$, as expected in the limit of many scattered photons due to the analytic nature of the method. The redistribution function method was also found to produce the correct result, but only in the limit of high resolution in the grids related to the lookup tables. For each lookup table, we computed $P(x_i|x'_k)$ for $I = 500$ grid values uniformly spaced in frequency from $(x'_k - 10)$ to $(x'_k + 10)$. We then determined inverse values of $x(P_j|x'_k)$ for $J = 10^6$ grid values on $[0, 1]$. We timed the operation of each method in selecting 10^7 scattered frequencies for a series of input frequency values. The redistribution function method required ~ 7 seconds on our machine independent of the input frequency, while we found the scattering atomic velocity method required ~ 20 seconds near line centre (where most scatters occur in any physical problem) and longer at larger $|x'|$. Thus, after some initial setup time constructing the lookup tables, we expect our redistribution function method to require approximately one third of the time required by Zheng and Miralda-Escudé's method, or at least its implementation as described in this section.

4.3 Test Problem: Homogeneous Absorber

Here we return to the problem of Ly α scattering in a locally homogeneous absorber described in Chapter 3. As we have previously obtained solutions to this problem in both the diffusion approximation and using the actual R_{II} function to treat the frequency redistribution exactly, the problem will provide a test of our Monte Carlo approach.

We follow a version of the usual Monte Carlo methodology described in section 2.5, simplified in that the homogeneity of the problem allows us to skip over any steps involving the spatial position and direction of a given photon. We need only account for the frequency of a photon as it scatters within the system. Photons enter the system with frequency x_{inj} ; they are scattered to a new frequency (determined in principle from Eq. (2.53)) by either of the methods described in the last section. In a static system, this new frequency becomes the incident frequency for the next scattering event. If the system undergoes expansion/contraction then the comoving frequency of the photon will be red/blue-shifted as it follows the path between scatterings. This strategy is repeated until the photon escapes beyond the frequency boundaries set by the escape frequency, $|x| > x_{\text{esc}}$, and the process is repeated for a large number of photons.

For a photon (re-)emitted with frequency x_{em} in a non-static medium, an optical depth $\tau = -\ln R$ is selected and used to determine the red/blue-shifted frequency x' reached before the photon is next scattered (we adopt this label to match the label of the absorbed photon frequency upon scattering). If the medium has a uniform velocity gradient H and a corresponding Sobolev parameter γ , the relation between the optical depth and the path length l given by Eq. (2.56) simplifies with the change of variable $x = x_{\text{em}} - Hl/b$ to give:

$$\tau = \frac{1}{\gamma} \int_{x'}^{x_{\text{em}}} \phi(x) dx. \quad (4.18)$$

For the purpose of the current problem we will ignore the effect of redshifting / blueshifting while a photon has a frequency lying in the core of the line i.e. $|x_{\text{em}}| < x_{\text{m}}$ [see Eq. (2.11)] and treat only the case where $|x_{\text{em}}| > x_{\text{m}}$; the shifts in frequency taking place between scattering events near line centre are negligible compared with the effect of redistribution at these frequencies. Performing the integration in Eq. (4.18) with

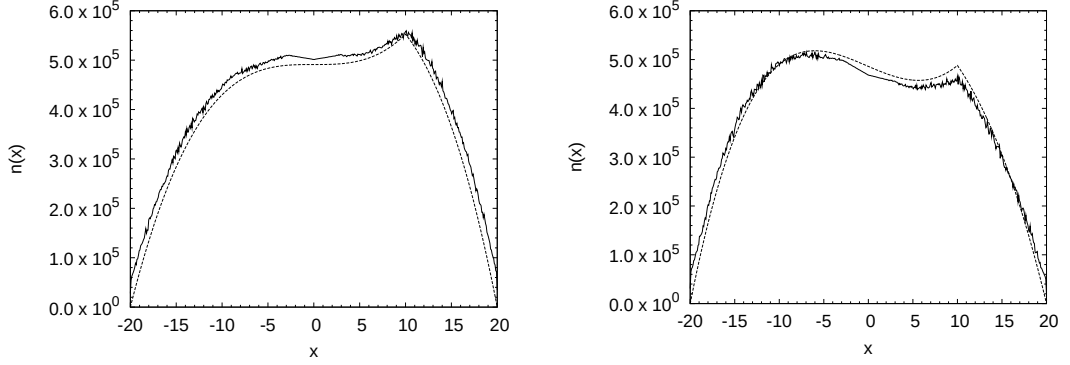


Figure 4.2: Monte Carlo solution (solid line) for scattering of photons in a static homogeneous medium excluding/including atomic recoil (left/right panel respectively) with $x_{\text{esc}} = 20$, $x_{\text{inj}} = 10$ and temperature $T = 10$ K, normalised to $A = 1$, compared with the corresponding analytic diffusion solution (dashed line).

$\phi(x) = a/(\pi x^2)$ and solving for x' we find:

$$x' = \left[\frac{1}{x_{\text{em}}} + \frac{\pi \gamma \tau}{a} \right]^{-1}, \quad |x_{\text{em}}| > x_{\text{m}}. \quad (4.19)$$

While photons will still escape the system when they reach any frequency $|x| > x_{\text{esc}}$, it is also necessary to account for the possibility of photons that escape to infinity if the required optical depth τ exceeds that corresponding to an infinite path length.

The scattering events are binned as a function of frequency to determine $N(x)$, the total number of scattering events resulting from photons scattered from frequencies $x \rightarrow x + \Delta x$. The solution for the radiation field frequency distribution is then obtained according to:

$$n(x) \propto N(x)/\phi(x), \quad (4.20)$$

following from Eq. (2.58) with a constant bin size Δx . To determine the constant of proportionality we need to make use of a normalisation condition for the problem; this is provided by taking the frequency integral of the appropriate transfer equation, Eq. (3.41), to give:

$$A + \gamma \{n(x_{\text{esc}}) - n(-x_{\text{esc}})\} = \int_{-x_{\text{esc}}}^{x_{\text{esc}}} E(x)n(x) dx \quad (4.21)$$

where A is the frequency-integrated source term ($\tilde{S}(x) = A\delta_{\text{D}}(x - x_{\text{inj}})$) and the quantity $E(x)$ is as defined in Eq. (3.42). The RHS of Eq. (4.21) describes the total rate at which

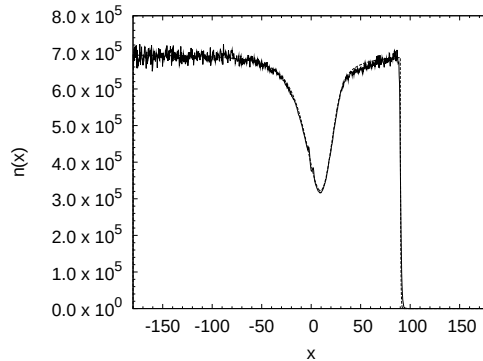


Figure 4.3: Monte Carlo solution (solid line) for scattering of photons in a homogeneous expanding medium with recoil, with $\gamma = 1.44 \times 10^{-6}$, $x_{\text{esc}} = 180$, $x_{\text{inj}} = 90$ and $T = 2.65$ K, normalised to $A = 1$, compared with the analytic solution Eq. (3.33)(dashed line).

photons are scattered across the escape frequency boundaries. $E(x)$ can be evaluated analytically using the form of the redistribution function in the wings, see Eq. (3.44). We construct $\tilde{n}(x) = N(x)/\phi(x)$ and evaluate numerically the integral of $E(x)\tilde{n}(x)$; the constant of proportionality in Eq. (4.20) is then chosen to ensure adherence to the equilibrium between source injection and the net escape rate given in Eq. (4.21).

We computed solutions for a static medium with and without recoil, see Figure 4.2, and a medium undergoing uniform expansion with recoil, see Figure 4.3; the results agree closely with the corresponding analytic solutions in chapter 3. The plotted solutions were obtained using our method described in section 4.1 to treat the frequency redistribution, though the method of Zheng and Miralda-Escudé [2002] summarised in section 4.2 was also applied and found to give near-identical solutions.

For the problem shown in Figure 4.3 we used our lookup table method to treat the frequency redistribution for frequencies $|x'| < 80$, carried out by integrating $R_{\text{II},\epsilon}$ as defined in Eq. (2.23), while the method for scattering in the wings was applied for $80 < |x'| < x_{\text{esc}}$. We constructed 200 lookup tables on $[-80, 80]$, Gaussian-distributed in x' about zero with a standard deviation of 15. Our solution was determined from a run of 20,000 photons in $\simeq 115$ minutes, not including the setup time to compute and invert the lookup tables, while an identical run using the method of section 4.2 required $\simeq 360$ minutes, consistent with our expectations from our earlier test.

4.4 Ly α Intensity in Spherical Symmetry

We seek a means of determining the Ly α radiation field intensity from a Monte Carlo simulation of Ly α photons scattering within a spherically symmetric scattering medium. We will adopt an approach based on the transport of photons that applies the definition of the specific intensity directly, as opposed to the indirect method used to determine the angle-averaged intensity from the distribution of scattering events as in Eq. (2.59). The additional angular information yielded by this method can be used to determine higher order angular moments such as the flux $H_\nu(r)$ which, unlike the average intensity $J_\nu(r)$, cannot be determined from the scattering event distribution. While not important in specifying the scattering rate like the average intensity, the Ly α flux in a non-homogeneous system is physically illuminating.

We consider a spherically symmetric medium divided into a series of shells with boundaries at radii $\{r_d\}$ for $d = 1, 2, \dots, D$ where $r_1 < r_2 < \dots < r_D$. We seek the specific intensity of Ly α photons crossing each spherical boundary as a function of frequency ν and the angle θ to the local normal i.e. $I_\nu(r_d, \mu)$ where $\mu = \cos \theta$. From the definition of specific intensity we write the differential number of photons in frequency range $[\nu, \nu + d\nu]$ crossing the boundary at $\mathbf{r}_d$ within solid angle $d\omega$ about direction $\mathbf{n}$, normal to area dA , in time dt as $dN = I_\nu(\mathbf{r}_d, \mathbf{n}) dA d\omega d\nu dt$. The differential solid angle is simply $d\omega = |d\mu| d\phi$ and the area dA normal to $\mathbf{n}$ is related to the differential area of the boundary dS by $dA = |\mu| dS$. We can then say $N(r_d, \mu, \nu)$, defined as the total number of photons within frequency range $[\nu, \nu + d\nu]$ crossing the boundary of radius r_d within angular range $[\mu, \mu + d\mu]$, is equal to the integral of dN over azimuthal angle and the boundary surface: $N(r_d, \mu, \nu) = I_\nu(r_d, \mu) |\mu| (\oint dS) (\int d\phi) d\mu d\nu dt$, or:

$$I_\nu(r_d, \mu) = \frac{N(r_d, \mu, \nu)}{8\pi^2 r_d^2 |\mu| (\Delta\mu)(\Delta\nu)(\Delta t)} \propto \frac{N(r_d, \mu, \nu)}{r_d^2 |\mu|} \quad (4.22)$$

where $\Delta\mu$ and $\Delta\nu$ are the bin sizes in angle and frequency, assumed constant in the proportionality, and Δt is the time in the Monte Carlo run over which the N crossings are counted. Throughout the remainder of this section we will describe our Monte Carlo method to construct $N(r_d, \mu, \nu)$ for Ly α photons emitted by some source in a generally expanding/contracting, spherically symmetric medium.

4.4.1 Photon Path Geometry

A photon is emitted/scattered at position $\mathbf{r}_{\text{em}}$ in direction $\mathbf{k}$, $|\mathbf{k}| = 1$; in spherical symmetry it is sufficient to designate its radius of emission r_{em} and the angle it makes with the normal θ_{em} , the latter having cosine $\mu_{\text{em}} = \mathbf{k} \cdot \mathbf{r}_{\text{em}} / r_{\text{em}}$. The position vector of the photon after travelling a distance λ along its path is given by:

$$\mathbf{r} = \mathbf{r}_{\text{em}} + \lambda \mathbf{k}. \quad (4.23)$$

Physically the distance travelled along the path λ is positive and has some maximum value corresponding to the distance to the next scattering of the photon, though for the purpose of describing our method we consider a ‘projected photon path’ corresponding to the range $\lambda = -\infty \rightarrow \infty$. An important characteristic of this path is the impact parameter r_{min} , defined as the minimum distance from the origin; $r_{\text{min}} = r_{\text{em}} \sin \theta_{\text{em}} = r_{\text{em}}(1 - \mu_{\text{em}}^2)^{1/2}$. For any boundary of radius $r_d > r_{\text{min}}$ the projected photon path will intersect the sphere at distances along the path $\lambda_{\pm}$ determined from solving $\mathbf{r} \cdot \mathbf{r} = r_d^2$ with $\mathbf{r} = \mathbf{r}_{\text{em}} + \lambda \mathbf{k}$:

$$\begin{aligned} \lambda_{\pm} &= -\mathbf{k} \cdot \mathbf{r}_{\text{em}} \pm [r_d^2 - r_{\text{em}}^2 + (\mathbf{k} \cdot \mathbf{r}_{\text{em}})^2]^{1/2}, \\ &= -\mu_{\text{em}} r_{\text{em}} \pm (r_d^2 - r_{\text{min}}^2)^{1/2}. \end{aligned} \quad (4.24)$$

Solutions satisfying $\lambda_{\pm} > 0$ denote boundary intersections of the potential photon path defined by $\mathbf{r}_{\text{em}}$ and μ_{em} as in Eq. (4.23) with $\lambda = 0 \rightarrow \infty$, and occur in a specific sequence. It is important to record the angle to the local normal made by a photon crossing any sphere, given by $\mu = \mathbf{k} \cdot \mathbf{r}_d / r_d$ where $\mathbf{r}_d = \mathbf{r}_{\text{em}} + \lambda_{\pm} \mathbf{k}$:

$$\begin{aligned} \mu_{\pm} &= (\mu_{\text{em}} r_{\text{em}} + \lambda_{\pm}) / r_d, \\ &= \pm [1 - (r_{\text{min}} / r_d)^2]^{1/2}. \end{aligned} \quad (4.25)$$

We distinguish between photon paths based on the sign of μ_{em} :

- For a photon emitted in an ‘outward’ direction with $\mu_{\text{em}} > 0$, only λ_+ potentially represents a boundary crossing as $\lambda_- < 0$ (see Figure 4.4.1). The photon can potentially cross every boundary with radius $r > r_{\text{em}}$. If we specify d such

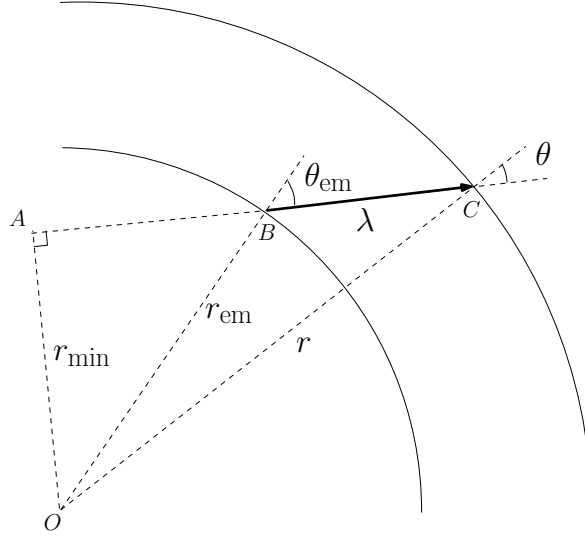


Figure 4.4: Geometry of intersection of photon path, originating from radius $r_{\text{em}} \equiv OB$ in outward direction $\theta_{\text{em}} < \pi/2$, with sphere of radius $r \equiv OC$. The projected photon path has an impact parameter $r_{\text{min}} \equiv OA$. The distance travelled by the photon from the point of emission to the intersection with the sphere of radius r is $\lambda \equiv BC = (r^2 - r_{\text{min}}^2)^{1/2} - r_{\text{em}} \cos \theta_{\text{em}}$.

that $r_d < r_{\text{em}} \leq r_{d+1}$, intersections occur in the sequence $\{r_{d+1}, r_{d+2}, \dots, r_D\}$ at distances along the path given by λ_+ and local angles μ_+ .

- For a photon emitted ‘inwards’ with $\mu_{\text{em}} < 0$, the solution $\lambda_+ > 0$ for all $r > r_{\text{min}}$ and $\lambda_- > 0$ for $r_{\text{min}} < r < r_{\text{em}}$. If we choose d as above and specify d_{min} such that $r_{d_{\text{min}}} < r_{\text{min}} \leq r_{d_{\text{min}}+1}$ then the potential boundary crossings occur in the sequence $\{r_d, r_{d-1}, \dots, r_{d_{\text{min}}+1}\}$ at distances (angles) given by λ_- (μ_-), followed by $\{r_{d_{\text{min}}+1}, r_{d_{\text{min}}+2}, \dots, r_D\}$ at λ_+ (μ_+).

The actual path of the photon is given by following the potential photon path until the photon is scattered after a distance λ_{max} in accordance with the optical depth along the path, as described below in section 4.4.3. After travelling this distance the photon arrives at a new radius r given by applying the cosine rule to the triangle of sides r_{em} , r and λ_{max} :

$$r = (r_{\text{em}}^2 + \lambda_{\text{max}}^2 + 2\mu_{\text{em}}r_{\text{em}}\lambda_{\text{max}})^{1/2}. \quad (4.26)$$

4.4.2 Comoving Photon Frequency Along Path

The spatial transport of the Ly α photons in the Monte Carlo simulation depends on the optical depth τ built up by a photon along its path, which in turn depends on the photon frequency. It is also necessary to record the frequency of a photon as it crosses each boundary, to determine the frequency dependence of $N(r_d, \mu, \nu)$. For a medium subject to some radial velocity field $\mathbf{V}(\mathbf{r}) = V(r)[\mathbf{r}/r]$, we need to consider the comoving photon frequency along the path between scattering events i.e. the photon frequency seen in the frame in which the scattering medium is locally at rest; this frequency is seen redshifted/blueshifted as $\nu \rightarrow \nu - (\nu_0/c)\mathbf{V} \cdot \mathbf{k}$ where $\mathbf{k}$ is the direction of the photon path.

We consider a photon that is emitted or scattered at $\mathbf{r}_{\text{em}}$ with comoving frequency $x(\mathbf{r}_{\text{em}})$. We will assume a uniform temperature medium to allow use of the scaled frequency offset x defined for a unique value of the Doppler width $\Delta\nu_D$, although all equations can be easily formulated with frequency variable ν if dealing with a variable temperature $T(r)$. At any point $\mathbf{r}$ along the photon's path it will have a comoving frequency corresponding to the same lab frame frequency as $x(\mathbf{r}_{\text{em}})$, and thus:

$$\begin{aligned} x(\mathbf{r}) &= x(\mathbf{r}_{\text{em}}) - \mathbf{V}(\mathbf{r}) \cdot \mathbf{k}/b + \mathbf{V}(\mathbf{r}_{\text{em}}) \cdot \mathbf{k}/b, \\ &= x(\mathbf{r}_{\text{em}}) - \mu V(r)/b + \mu_{\text{em}} V(r_{\text{em}})/b \end{aligned} \quad (4.27)$$

where μ describes the angle to the local normal of the sphere at $\mathbf{r}$. For the special case of a Hubble-flow velocity field i.e. $V(r) = Hr$, this reduces to:

$$\begin{aligned} x(\mathbf{r}) &= x(\mathbf{r}_{\text{em}}) - [\mu r - \mu_{\text{em}} r_{\text{em}}] H/b, \\ &= x(\mathbf{r}_{\text{em}}) - \lambda H/b \end{aligned} \quad (4.28)$$

where the contents of the square brackets simplifies following Eq. (4.25); the frequency shift is linearly dependent on the distance travelled along the path, λ .

4.4.3 Optical Depth Along Photon Path

When τ reaches a sufficiently large value, the photon path ends as the photon is scattered. The maximum optical depth is chosen according to a probability distri-

bution $e^{-\tau}$ i.e. $\tau = -\ln R$ for a uniform deviate R . For a Ly α scattering opacity $\chi_\nu = n_{\text{HI}}\sigma\varphi(\nu)$ we can write the differential optical depth accumulated along a length $d\lambda$ as $d\tau = n_{\text{HI}}\sigma[\phi(x)/\Delta\nu_{\text{D}}]d\lambda$ and the total optical depth is the integral along the path as in Eq. (2.56). For a static medium of constant temperature and H I density n_{HI} this integral is trivial and we have the simple relation $\lambda = \tau\Delta\nu_{\text{D}}/[n_{\text{HI}}\sigma\phi(x)]$; however, for a non-static medium the frequency x varies as in Eq. (4.27) and no simple τ -dependence is found for λ .

A less rigid approach is to assume the density, temperature and velocity of the medium are essentially constant across shells, as in the Monte Carlo code of Dijkstra et al. [2006]. Under these circumstances the photon comoving frequency changes in steps as the path crosses shell boundaries and the optical depth between two boundaries behaves as in the uniform static case. We can write the optical depth between boundaries at distances λ_d and λ_{d+1} along the photon path as:

$$\Delta\tau = \frac{\sigma n_{\text{HI}}(r_d)\phi(x_d)}{\Delta\nu_{\text{D}}} |\lambda_{d+1} - \lambda_d| \quad (4.29)$$

where we attach the subscript d to the distances λ and frequency x to denote that they are to be evaluated at the intersection with the boundary of radius r_d , using Equations (4.24) and (4.27) respectively. The photon is permitted to progress along its path until the sum of $\Delta\tau$'s exceeds the selected total optical depth, at which stage it is scattered.

4.4.4 Monte Carlo Implementation

Here we summarise the method developed in this section and how it can be applied within an efficient Monte Carlo approach to determine the intensity in an expanding/contracting, spherically symmetric system. The following steps apply for a single photon and are repeated in the specified sequence until the photon escapes (note: every instance of a uniform random number ' R ' below is drawn from $[0, 1]$ independently).

- (i) A photon is emitted at some radius r_{em} and comoving frequency x_{em} determined from the properties of the source. The photon is assigned a direction described by the cosine μ_{em} of the angle to the local radius vector, typically taken

to be isotropic i.e. $\mu_{\text{em}} = 2R - 1$, and an optical depth $\tau = -\ln R$ after which it will be scattered by a hydrogen atom.

- (ii) We follow the potential path of the photon defined by r_{em} and μ_{em} , originating at $\lambda = 0$, to the first intersection with a shell boundary and compute the distance λ_s and optical depth τ_s from Equations (4.24) and (4.29) respectively.
- (iii) If $\tau_s < \tau$ then the photon will cross the boundary, if not we skip to (iv). We update the position by setting $(\lambda + \lambda_s) \rightarrow \lambda$ and compute μ and ν at the boundary using Equations (4.25) and (4.27) respectively. We bin these values and increment $N(r_d, \mu, \nu)$ for the appropriate boundary. We take $(\tau - \tau_s) \rightarrow \tau$ and determine values of λ_s and τ_s from the current position to the next shell boundary along the path; this step is repeated until $\tau_s > \tau$ indicating the photon scatters before reaching the next boundary. If the photon crosses the boundary at r_D then it escapes the H I medium and cannot be scattered back to $r < r_D$.
- (iv) We assume the photon travels a further distance $\Delta\lambda = (\tau/\tau_s)\lambda_s$ along the path and obtain the total distance travelled by the photon before scattering from $\lambda + \Delta\lambda \rightarrow \lambda$. The radius r is updated according to Eq. (4.26) with λ in place of λ_{max} . The comoving frequency from which the photon is scattered, x' , is determined from Eq. (4.27) using the value of r and the corresponding μ from Eq. (4.25) with r in place of r_d .
- (v) The photon is re-emitted at $r_{\text{em}} = r$ with a comoving frequency $x_{\text{em}} = x_{\text{em}}(x', T)$ determined from the appropriate redistribution treatment (described in detail for R_{II} scattering in section 4.1). We assign an isotropically distributed direction $\mu_{\text{em}} = 2R - 1$ and optical depth to next scatter $\tau = -\ln R$. We return to step (ii).

This sequence of steps is repeated for as many photons as are necessary to reduce the statistical noise in $N(r_d, \mu, \nu)$ to acceptable levels. The intensity $I_\nu(r_d, \mu)$ is determined from Eq. (4.22); normalisation is enforced using an integral constraint or by computing the Monte Carlo Δt from the number of photons followed.

4.5 Test Problem: Static Sphere

We consider the problem of Ly α scattering in a static, uniform sphere of radius R and line centre opacity κ_0 . An analytic solution for the radiation field derived in the diffusion regime was found by Dijkstra et al. [2006] as described in section 2.8.2, specifically Equations (2.81) - (2.84). The equation of radiative transfer for this problem has the form of Eq. (2.41) with $V(r) \equiv 0$ and a general source term $S(\nu, r)$ added to the right-hand side. The equation can be integrated over angle to give the moment equation:

$$\frac{1}{r^2} \frac{\partial}{\partial r} [r^2 H(x, r)] = -\chi(x) J(x, r) + \eta(x, r) + S(x, r) \quad (4.30)$$

where the radiation flux has been written as $H(x, r) = (\Delta\nu_D) H_\nu$. Similar relations hold for the radiation intensity J , opacity χ , emissivity η and the source term S . Upon integrating Eq. (4.30) over frequency, we find:

$$\begin{aligned} \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 \int H(r, x) dx \right] &= \int [\eta(x, r) - \chi(x) J(x, r)] dx + \int S(x, r) dx \\ &= \int S(x, r) dx \end{aligned} \quad (4.31)$$

where in the first equality, the first term on the RHS integrates to zero due to radiative equilibrium¹, as can be confirmed for the forms of the opacity and emissivity given in Equations (2.25) and (2.26). For a source of ‘unit strength’ satisfying $\int dx \int dV \oint d\Omega S(x, r) = 1$, we can use Eq. (4.31) to write:

$$(4\pi r)^2 \int H(r, x) dx = 1. \quad (4.32)$$

This flux conservation relation provides a useful normalisation condition for our attempt to solve the problem using the Monte Carlo approach.

We examine this particular problem with the aim of comparing our solution with the approximate analytic solution of Dijkstra et al. [2006]. In the Eddington approximation assumed by Dijkstra et al. the radiation flux is related to the average intensity by the first order angular moment equation: $H(r, x) = -1/(3\chi_\nu) \partial J(r, x) / \partial r$, where $\chi_\nu = \sqrt{\pi} \kappa_0 \phi(x)$. We can take the solution for the average intensity given by Eq. (2.82),

¹The energy emitted by the medium across all frequencies is equal to that absorbed.

together with the corresponding solution for the flux derived by taking the radial derivative:

$$\begin{aligned} J(x, r) &= \frac{\sqrt{6\pi}\kappa_0}{16\pi^2 R} \sum_{n=1}^{\infty} Q_n \frac{\sin(\lambda_n r)}{\lambda_n r} \exp \left[-\sqrt{\frac{2\pi}{27}} \frac{\lambda_n}{a\kappa_0} |x^3| \right]; \\ H(x, r) &= \frac{\sqrt{6}}{48\pi^2 R\phi(x)} \sum_{n=1}^{\infty} \frac{Q_n}{\lambda_n} \left\{ \frac{\sin(\lambda_n r)}{r^2} - \frac{\lambda_n \cos(\lambda_n r)}{r} \right\} \exp \left[-\sqrt{\frac{2\pi}{27}} \frac{\lambda_n}{a\kappa_0} |x^3| \right]. \end{aligned} \quad (4.33)$$

The source term is written in the form $S(x, r) = \chi_\nu j(r)/(4\pi)$ where the function $j(r)$ describes the radial distribution of the source. Dijkstra et al. suggest a source term describing a thin shell at some source radius r_S with radial distribution:

$$j(r) = \frac{1}{\sqrt{\pi}\kappa_0} \frac{\delta_D(r - r_S)}{4\pi r^2} \quad (4.34)$$

which is seen as a point source in the limit $r_S \rightarrow 0$ or at radii $r \gg r_S$, and the normalisation ensures the condition $\int dx \int dV \oint d\Omega S(x, r) = 1$ is met. If we adopt this form we find from Eq. (2.83) that the coefficients Q_n take the form:

$$Q_n = \frac{1}{\sqrt{\pi}\kappa_0} \frac{\sin(\lambda_n r_S)}{r_S} \quad (4.35)$$

where the $\{\lambda_n\}$ are given by Eq. (2.84).

The analytic solution assumes the Eddington approximation and is theoretically valid only in the limit of high optical depth. We have attempted to solve the problem exactly using our Monte Carlo approach outlined in section 4.4. Photons are generated at a radius and frequency consistent with the source term; thus we take $r_{\text{em}} = r_S$ while x_{em} is distributed according to $\phi(x)$. As the solution is not expected to be particularly sensitive to the frequency distribution of the source it is sufficient to distribute x_{em} according to the Doppler (Gaussian) distribution, e.g. $x_{\text{em}} = \sqrt{-\ln R_1} \cos(2\pi R_2)$ by the Box-Muller method (Press et al. [1992]), or even simply assume source emission with $x_{\text{em}} = 0$. The frequency redistribution can be treated using either of the methods described in sections 4.1 or 4.2. After determining the intensity crossing each spherical boundary we determine the flux and mean intensity by angular integration before scaling all three quantities by a single factor to satisfy the normalisation Eq. (4.32), which will be satisfied at all r by photon conservation.

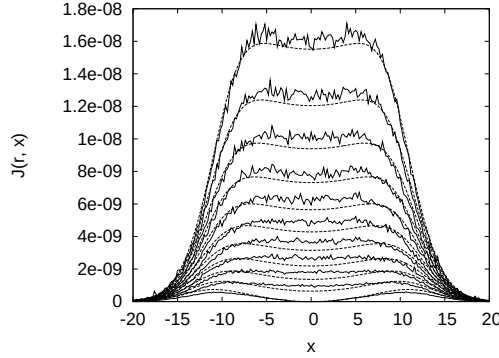


Figure 4.5: Plot of $J(r, x)$ for $\text{Ly}\alpha$ scattering in a static, uniform sphere. We assume a temperature $T = 10$ K, line-centre opacity $\kappa_0 = 100$ and a thin shell source at radius $r_S = 5$. Frequency profiles are given from $r = 500$ (highest values of J) to $R = 1000$ (lowest values of J) in steps of 50. We display our Monte Carlo solution (solid line) together with the analytic solution in the Eddington approximation (dashed line).

Our results for a moderately optically thick system are given in Figure 4.5; our chosen example has line-centre optical depth $\tau_0 = \kappa_0 R = 10^5$. The Monte Carlo solution is close to the analytic solution; however, it does not obviously deviate from a flat spectrum across the core as seen in the relative ‘dip’ of the analytic solution. We suspect the dip is an unphysical result of an approximation made in the derivation of the analytic solution that $\tau_0 \phi(x) \gg 1$ for all x (Harrington [1973]), or equivalently $(a\tau_0)^{1/3} \gg 1$ as seen by noting that the frequency width of the solution scales as $x \sim (a\tau_0)^{1/3}$. The example in Figure 4.5 has $(a\tau_0)^{1/3} \simeq 11.5$ which is probably insufficient to guarantee the accuracy of the analytic solution.

The solution displayed in Figure 4.5 was determined from 2×10^5 photons (in ~ 20 hours) using the method of Zheng and Miralda-Escudé [2002] described in section 4.2 for the frequency redistribution (our lookup table method produced a near-identical solution). The physical mean free path of a photon is given by $l(x) = [\sqrt{\pi} \kappa_0 \phi(x)]^{-1}$; the vast majority of the Monte Carlo code runtime is spent following photons in the core, which move negligible distances $l \sim 1/\kappa_0$ between successive scattering events. Photons in the core can undergo $\sim 10^4$ scatterings, or more at higher temperatures, before reaching the wings where their mean free paths increase and they are able to

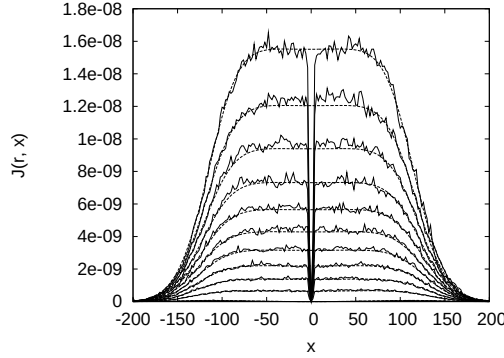


Figure 4.6: Plot of $J(r, x)$ for $\text{Ly}\alpha$ scattering in an optically thick, static, uniform sphere. The solution applies for a temperature $T = 10$ K, line-centre opacity $\kappa_0 = 1.2 \times 10^5$ and a thin shell source at radius $r_S = 5$. Frequency profiles are given from $r = 500$ (highest values of J) to $R = 1000$ (lowest values of J) in steps of 50. We compare our Monte Carlo solution using the core-skipping method (solid line) with the analytic solution in the Eddington approximation (dashed line).

escape the medium by spatial diffusion (Tasitsiomi [2006]). In the next section, we examine how these core scatters may be avoided.

4.5.1 Skipping Core Scatterings

For a system of greater optical thickness we found the time required for all photons to escape increases dramatically. As such we attempt to obtain a Monte Carlo solution for such a system using the ‘core-skipping’ method in which photons in the core are artificially scattered by a fast-moving atom to increase their frequency shift and the likelihood of exiting the core, as suggested by e.g. Ahn et al. [2002], Dijkstra et al. [2006]. The probability distribution for the component of the scattering atom’s thermal velocity perpendicular to the photon direction, $p(u_\perp)$, is given by the distribution of Eq. (4.13) truncated such that $u_\perp > x_c$, where x_c denotes the core boundary at the outermost crossover between the Doppler and Lorentz profiles:

$$p(u_\perp) = \begin{cases} 2u_\perp e^{-(u_\perp^2 - x_c^2)} & ; \quad u_\perp \geq x_c \\ 0 & ; \quad u_\perp < x_c \end{cases}. \quad (4.36)$$

The scattered frequency is determined from Eq. (4.17) with the perpendicular velocity distributed as in Eq. (4.36) to give:

$$u_{\perp} = \sqrt{x_c^2 - \ln R}. \quad (4.37)$$

We have obtained a Monte Carlo solution using this core-skipping method for an optically thick system with $\tau_0 = 1.2 \times 10^8$, shown in Figure 4.6. The mean intensity is again approximately flat in frequency, discounting the depleted contribution from photons in the core, for all radii out to the outer boundary where the double peaked escaping profile is found. The analytic solution of Dijkstra et al. is flatter than in the moderate optical depth case and closer to the Monte Carlo solution, presumably a result of greater accuracy given $(a\tau_0)^{1/3} \simeq 120 \gg 1$.

We note an alternative core-skipping method to that based on the scattering atom velocity. This method is conceptually simpler; when a photon undergoes a core scattering with $|x'| < x_c$, the scattered frequency is selected using the frequency distribution for photons scattered out of the core, given by (Auer [1968]):

$$p(x) \propto \int_{-x_c}^{x_c} J(x') R(x', x) dx' \propto \int_{-x_c}^{x_c} R(x', x) dx', \quad |x| \geq x_c \quad (4.38)$$

where we assume that the mean intensity $J(x)$ is flat in frequency across the core. The distribution can be normalised and integrated to find the cumulative probability distribution and inverted to calculate a lookup table for output frequencies.

4.6 Test Problem: Homogeneous Expanding Universe

We take the problem examined by Loeb and Rybicki [1999] as a simple test of the Monte Carlo method for a non-static, spherically symmetric medium. This problem, the coherent scattering of Ly α photons emitted from a monochromatic point source in an expanding medium, was introduced in section 2.8.3 together with a Monte Carlo solution and analytic solution for the mean intensity (valid in the diffusion regime) obtained by the authors. In the diffusion limit the intensity is written as the Legendre expansion $I_{\nu} = J_{\nu} + 3\mu H_{\nu}$ with $H_{\nu} \ll J_{\nu}$ and thus we neglect the derivative $\partial \tilde{H} / \partial \tilde{\nu}$ in the first order angular momentum equation to write $\tilde{H}(\tilde{r}, \tilde{\nu}) = -1/(3\tilde{\chi}) \partial \tilde{J} / \partial \tilde{r}$, where

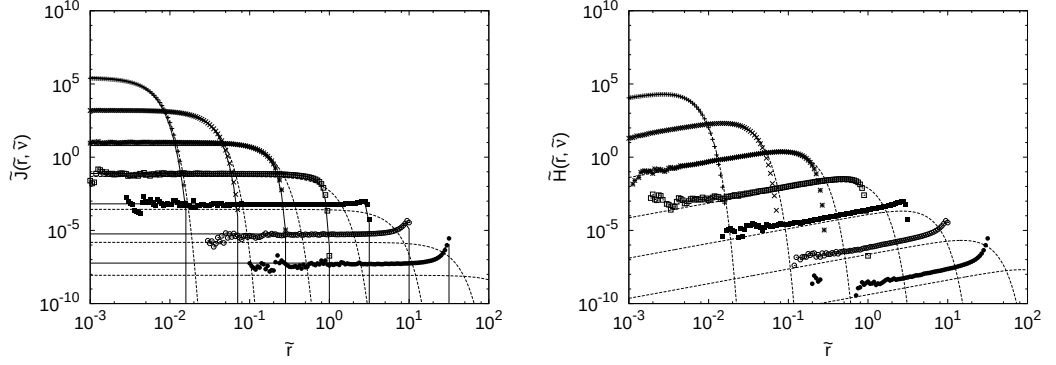


Figure 4.7: Monte Carlo coherent scattering solution (various points) for average intensity (left) and flux (right) arising from a monochromatic Ly α point source in a homogeneous expanding medium, together with Loeb and Rybicki's Monte Carlo solution for the mean intensity (solid line, left panel only) and the diffusion regime analytic solutions (dashed lines); the profiles shown correspond to frequencies $\log \tilde{\nu} = -1.5, -1.0, -0.5, 0.0, 0.5, 1.0, 1.5$ in order of decreasing value of $\tilde{J}$ or $\tilde{H}$ at $\tilde{r} = 10^{-3}$.

$\tilde{\chi} = r_* \chi_\nu = 1/\tilde{\nu}^2$ (all quantities being non-dimensionalised as in section 2.8.3). Thus we can derive the flux from Loeb and Rybicki's solution for the mean intensity, Eq. (2.86):

$$\begin{aligned}\tilde{J}(\tilde{r}, \tilde{\nu}) &= \frac{1}{4\pi} \left(\frac{9}{4\pi\tilde{\nu}^3} \right)^{3/2} \exp \left[-\frac{9\tilde{r}^2}{4\tilde{\nu}^3} \right]; \\ \tilde{H}(\tilde{r}, \tilde{\nu}) &= -\frac{\tilde{\nu}^2}{3} \frac{\partial \tilde{J}}{\partial \tilde{r}} = \frac{3\tilde{r}}{8\pi\tilde{\nu}} \left(\frac{9}{4\pi\tilde{\nu}^3} \right)^{3/2} \exp \left[-\frac{9\tilde{r}^2}{4\tilde{\nu}^3} \right].\end{aligned}\quad (4.39)$$

We compare these analytic solutions, valid in the diffusion regime, with our exact solution to the problem obtained by the Monte Carlo method.

Photons are emitted from the Ly α point source at $r \simeq 0$ with $\nu \simeq \nu_\alpha$. The steps described in section 4.4 are followed with the exception of the frequency redistribution upon scattering, as the problem assumes coherent scattering. As the medium undergoes Hubble expansion the comoving photon frequency redshifts between scatterings according to Eq. (4.28); in the preferred frequency and radius units of Loeb and Rybicki this becomes $\tilde{\nu} \rightarrow \tilde{\nu} + \tilde{\lambda}$. As the medium is technically infinite there is no well-defined outer radius to take for r_D , but a large value such as $\tilde{r} \simeq 100$ was found to be sufficient. After determining $\tilde{I}(\tilde{\nu}, \tilde{r}, \mu)$ we compute the angular moments $\tilde{J}(\tilde{\nu}, \tilde{r})$ and $\tilde{H}(\tilde{\nu}, \tilde{r})$ and normalise each using the constraint Eq. (2.87).

We give results in Figure 4.7. Our solutions agree with the analytic solutions in the diffusion regime, $\tilde{r} \ll \tilde{\nu}$, where photons have undergone many scatterings. Our solution for $\tilde{J}$ agrees everywhere with Loeb and Rybicki's Monte Carlo solution.

4.7 Discussion

In this chapter we have described in detail the methods required to solve Ly α scattering radiative transfer problems in both homogeneous and spherically symmetric scattering media. We developed a method based on lookup tables of the cumulative probability distribution of the $R(x', x)$ function to treat the photon frequency redistribution, and found it to give accurate solutions for problems in both geometries. The results obtained using this method were found to require high resolutions in the grids associated with the pre-calculated lookup tables in order to match the intrinsic accuracy of those obtained using the near-analytic method of Chen and Miralda-Escudé [2004] based on the scattering atom thermal velocity distribution, but our method was found to be faster in its execution within the Monte Carlo runs by a factor of ~ 3 .

The Monte Carlo approach can require a lot of photons to achieve an acceptable signal-to-noise in its output. For systems where frequency redistribution by scattering is the dominant transport mechanism in frequency space (as opposed to e.g. redshifting in an expanding medium), excessive time and effort can be expended in following these scattering events. This can be circumvented somewhat by using some 'core-skipping' method to artificially cut down on core scatters, although in the limit of high optical depth many scatters will still occur outside the core before any given photon will escape the system. As such we believe that, at least for a spherically symmetric system, a method to solve the radiative transfer equation itself might be preferable to the Monte Carlo approach.

CHAPTER 5

Solution of Ray and Moment Equations in Spherical Symmetry

Monte Carlo methods to treat $\text{Ly}\alpha$ scattering can be applied for any general density and velocity structure of the scattering medium, however in Chapter 4 we found a Monte Carlo implementation for spherical symmetry to be inefficient when applied to problems involving large optical depths, for example. In this chapter we use a grid-based method to treat radiative transfer in spherical symmetry:

- We describe two differing approaches to solving the transfer equation in the co-moving frame of a spherically symmetric expanding medium, based on the solution of ray and moment equations. We formulate and solve these equations using strategies presented in a series of papers by Mihalas, Kunasz and Hummer ([1975], [1976]).
- We examine the practical application of these methods to the spherically symmetric $\text{Ly}\alpha$ scattering problems previously examined using Monte Carlo methods. We find the solutions of the moment/ray equations to agree with pre-existing solutions or our own Monte Carlo solutions.

These methods are generally limited in their applicability to simulations of the structure of the IGM preceding reionisation, however they are ideal for examining qualitatively the effects of density and velocity profiles etc. on the Ly α scattering rate.

5.1 Solution of Ray Equations

As derived in section 2.4.4, the radiative transfer equation in the comoving frame for a spherically symmetric scattering medium with radial velocity $V(r)$ is given by:

$$\mu \frac{\partial I_\nu}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial I_\nu}{\partial \mu} - \alpha(r) [1 - \mu^2 + \mu^2 \beta(r)] \frac{\partial I_\nu}{\partial \nu} = -\chi_\nu I_\nu + \eta_\nu, \quad (5.1)$$

where $\alpha(r)$ and $\beta(r)$ are derived from $V(r)$:

$$\alpha(r) \equiv (\nu_0/c) \frac{V(r)}{r}, \quad (5.2)$$

$$\beta(r) \equiv \frac{d \ln V(r)}{d \ln r}. \quad (5.3)$$

In this section we will describe in detail the method of Mihalas et al. [1975] in which the transfer equation is formulated for a series of parallel rays traversing the system, and the corresponding finite-difference equations are solved as a function of distance along each ray for one frequency at a time, ray-by-ray. We limit our study to expanding velocity fields $V(r)$ satisfying $V(r) > 0$ and $V'(r) > 0$ for all r (see section 5.1.2).

For the special case of a spherically symmetric medium, it is possible to recover the specific intensity by integrating Eq. (5.1) along parallel rays with different impact parameters p , the rays' perpendicular distances from the centre of symmetry. A more suitable choice of coordinates is obtained by making the change of variable $(r, \mu) \rightarrow (p, z)$ where z is the distance along the ray from the point of closest approach to the centre of symmetry. The relationships between the two sets of quantities are clear from Figure 5.1; $p = r \sin \theta$ and $z = r \cos \theta$, with inverse relations $r = (p^2 + z^2)^{1/2}$ and $\mu \equiv \cos \theta = z/r$.

In this system of coordinates we describe a radius and direction by first specifying the impact parameter p and then the position along the ray z ; at this position we describe the specific intensity travelling away from the $z = 0$ axis (i.e. towards an external observer at $z = \infty$) as $I_\nu^+(p, z)$ and the specific intensity travelling towards the

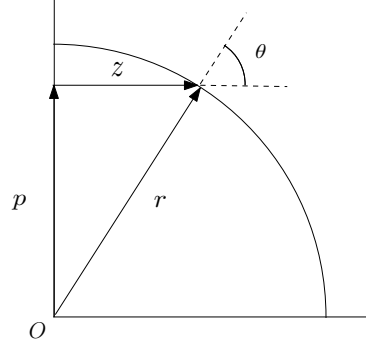


Figure 5.1: Illustration of (r, θ) and (p, z) coordinates: $r = (p^2 + z^2)^{1/2}$ and $\mu \equiv \cos \theta = z/r$.

$z = 0$ axis (i.e. away from the external observer at $z = \infty$) as $I_\nu^-(p, z)$. These quantities can be written as $I_\nu^+(p, z) = I_\nu(r, \mu)$ and $I_\nu^-(p, z) = I_\nu(r, -\mu)$, where $\mu > 0$. Along a specific ray characterised by p , the equation of transfer for the variation of $I_\nu^\pm$ with z is:

$$\pm \frac{\partial I_\nu^\pm(p, z)}{\partial z} - \alpha(r) [1 - \mu^2 + \beta(r)\mu^2] \frac{\partial I_\nu^\pm(p, z)}{\partial \nu} = \eta_\nu(r) - \chi_\nu(r) I_\nu^\pm(p, z). \quad (5.4)$$

There are two separate equations for I_ν^+ and I_ν^- . It is preferable to work with two different dependent variables defined as follows:

$$u_\nu(p, z) \equiv \frac{1}{2} [I_\nu^+(p, z) + I_\nu^-(p, z)], \quad (5.5)$$

$$v_\nu(p, z) \equiv \frac{1}{2} [I_\nu^+(p, z) - I_\nu^-(p, z)]. \quad (5.6)$$

Note that u_ν is an average of intensities like the mean intensity J_ν , while v_ν is a difference of intensities like the flux H_ν . We can recast the two equations represented by Eq.(5.4) in terms of our new variables: this is done by summing and differencing the two equations for I_ν^+ and I_ν^- . If we subsequently divide through by χ_ν and rewrite the z -derivative in terms of the optical depth τ_ν along the ray, $d\tau_\nu(p, z) = -\chi_\nu(r)dz$, we find:

$$\frac{\partial u_\nu(z)}{\partial \tau_\nu} + \gamma_\nu(z) \frac{\partial v_\nu(z)}{\partial \nu} = v_\nu(z), \quad (5.7)$$

$$\frac{\partial v_\nu(z)}{\partial \tau_\nu} + \gamma_\nu(z) \frac{\partial u_\nu(z)}{\partial \nu} = u_\nu(z) - S_\nu(r), \quad (5.8)$$

where

$$\gamma_\nu(z) \equiv \frac{\alpha(r)}{\chi_\nu(r)} [1 - \mu^2 + \beta(r)\mu^2] \quad (5.9)$$

and $S_\nu(r) = \eta_\nu(r)/\chi_\nu(r)$ is a given estimate of the source function. We intend to solve Equations (5.7) and (5.8) for $u_\nu(z)$ and $v_\nu(z)$ along a particular ray with fixed impact parameter p . Our equations are part of a mixed initial-plus-boundary value problem, and require the specification of boundary conditions in z and an ‘initial condition’ in frequency.

5.1.1 Boundary Conditions

We specify a maximum and minimum radius of the spherical system under consideration, given respectively by R and R_C (the subscript ‘C’ here denotes the ‘core’, the central object/region of the spherical system). The boundary conditions are:

(a) $r = R, z = z_{\max}$: We assume that R has been chosen to be sufficiently large that there is no radiation scattered back into the system from this radius, i.e. $I_\nu(R, \mu) = 0$ for $\mu < 0$, and thus along our ray $I_\nu^-(p, z_{\max}) = 0$ where $z_{\max} = (R^2 - p^2)^{1/2}$. From the definitions given by Equations (5.5) and (5.6) we see that $v_\nu(z_{\max}) = u_\nu(z_{\max})$; we arrive at a suitable boundary condition by substituting this into Eq. (5.7):

$$\frac{\partial u_\nu(z_{\max})}{\partial \tau_\nu} + \gamma_\nu(z_{\max}) \frac{\partial u_\nu(z_{\max})}{\partial \nu} = u_\nu(z_{\max}). \quad (5.10)$$

(b) $r = R_C, z = z_{\min}$: For the inner boundary condition we need to consider 2 distinct cases applicable depending on the impact parameter of the ray chosen:

(i) $p \geq R_C$: We compute the radiative transfer along the ray which is considered to originate from $z_{\min} = 0$. Due to the symmetry of the problem we can say $I_\nu^+ = I_\nu^-$ at $z = 0$ and therefore $v_\nu(p, z_{\min}) = 0$. Thus Eq. (5.7) becomes:

$$\frac{\partial u_\nu(z = 0)}{\partial \tau_\nu} = 0. \quad (5.11)$$

(ii) $p < R_C$: The ray intersects the core and the minimum value of z denotes the distance along the ray at which the intersection occurs: $z_{\min} = (R_C^2 - p^2)^{1/2}$. The boundary condition is written as:

$$\frac{\partial u_\nu(z_{\min})}{\partial \tau_\nu} = v_\nu(z_{\min}) - \gamma_\nu(z_{\min}) \frac{\partial v_\nu(z_{\min})}{\partial \nu} \quad (5.12)$$

where we assume the function $v_\nu(R_C, \mu)$ is known.

If the optical depth at the core radius is sufficiently high then the intensity will display the angular behaviour found in the diffusion limit, $I_\nu(R_C, \mu) = J_{\nu,C} + 3\mu H_{\nu,C}$, where $J_{\nu,C}$ is the core mean intensity and $H_{\nu,C}$ is the core flux. From the definition of v_ν and the equation for $I_\nu(R_C, \mu)$ we find:

$$v_\nu(R_C, \mu) = 3|\mu|H_{\nu,C}. \quad (5.13)$$

In this limit we should take $H_{\nu,C}$ to be a solution valid in the diffusion limit, if such a solution is known. If the optical depth at the core radius is significantly less than unity then we can assume a free-streaming boundary condition of the form:

$$v_\nu(R_C, \mu) = H_{\nu,C}\delta_D(\mu - 1) \quad (5.14)$$

i.e. the radiation field is directed radially outward from the source. The flux and the mean intensity are equal in this limit and trivially related to the source spectrum L_ν by $H_{\nu,C} = J_{\nu,C} = L_\nu/(4\pi R_C)^2$.

5.1.2 Initial Condition

The medium is subject to a radial velocity $V(r)$ that satisfies $V(r) \geq 0$, $dV/dr \geq 0$ for all r ; this ensures that $\gamma_\nu \geq 0$ for all (p, z) . From subsequent analysis of the characteristics of the system given by Equations (5.7) and (5.8), we need to enforce an initial condition at high frequency (Mihalas et al. [1975]); we denote this frequency by $\nu_{\max}$. The properties of $V(r)$ tell us that every point moves away from every other point and all radiation intercepted at a specific point from elsewhere in the system is redshifted. From this argument we see that if $\nu_{\max}$ lies sufficiently blueward of the local line profile, such that no line photons ever reach $\nu_{\max}$, we can say:

$$I_\nu(r, \mu)|_{\nu_{\max}} = 0, \quad (5.15)$$

$$\left. \frac{\partial I_\nu(r, \mu)}{\partial \nu} \right|_{\nu_{\max}} = 0. \quad (5.16)$$

Note that Eq. (5.15) holds for a system interacting with resonance-line photons only, while the condition of zero frequency gradient given by Eq. (5.16) also applies in the more general case where we allow for continuum radiation as the continuum varies slowly with frequency.

5.1.3 Discretisation of Equations

At this stage it is necessary to discretise our system of equations. We choose a frequency grid given by the discrete set $\{\nu_k\}$, $k = 1, 2, 3, \dots, \text{NF}$, where $\nu_1 = \nu_{\text{max}}$ is the bluemost frequency and successive values of k denote redder frequencies:

$$\nu_1 = \nu_{\text{max}} > \nu_2 > \nu_3 > \dots > \nu_{\text{NF}}. \quad (5.17)$$

The radius grid is given by $\{r_d\}$, $d = 1, 2, 3, \dots, \text{ND}$, where $r_1 = R$ and $r_{\text{ND}} = R_C$; increasing values of the depth index d denote greater depths w.r.t. the ‘surface’ of the system at $r = R$:

$$r_1 = R > r_2 > r_3 > \dots > r_{\text{ND}} = R_C. \quad (5.18)$$

We also need a grid for the ray impact parameter p ; the values are chosen such that there are NC rays that intersect the core, starting with $p_1 = 0$, while another ND rays are chosen to be tangent to the spheres defined by the values of the radius grid (grid-spheres), i.e. $p_{\text{NC}+1} = r_{\text{ND}}$ (note that this ray is tangent to the core), $\dots$, $p_{\text{NC}+d} = r_{\text{ND}+1-d}$. The grid values in p are given by $\{p_j\}$, $j = 1, 2, 3, \dots, \text{NP}$ where $\text{NP} = \text{NC} + \text{ND}$:

$$p_1 = 0 < p_2 < \dots < p_{\text{NC}} < p_{\text{NC}+1} = R_C < \dots < p_{\text{NP}} = R. \quad (5.19)$$

Note that the grid in radius defines a grid in z , the distance along the ray, for a ray of given impact parameter. This grid is given by the intersections of the ray with the grid-spheres, in order of decreasing values of z :

$$z_1 = (R^2 - p^2)^{1/2} > z_2 > z_3 > \dots > z_{\text{NI}_j}, \quad (5.20)$$

$$\text{NI}_j = \begin{cases} \text{ND} + \text{NC} + 1 - j & ; \quad j > \text{NC} \\ \text{ND} & ; \quad j \leq \text{NC} \end{cases} \quad (5.21)$$

where NI_j is the number of grid-spheres intersected by ray p_j . The values of z along the ray are given by $z_d(p_j) = (r_d^2 - p_j^2)^{1/2}$ and for rays with $j \geq \text{NC} + 1$ that do not intersect the core, $z_{\text{NI}_j} = 0$. Note that it is also possible to work with a grid in the optical depth along the ray; as $d\tau_\nu = -\chi_\nu dz$, the grid in τ_ν starts at the largest value of z , $\tau_1 = \tau_\nu(p, z_1) \equiv 0$, and increases back along the ray deeper into the medium.

We seek finite-difference representations of Equations (5.7) and (5.8). Values of u_ν are evaluated on the grid in z , while values of v_ν are evaluated at intermediate grid-points denoted by a half-integer value of the depth index d . The derivatives of u_ν and v_ν with respect to frequency are represented by a fully implicit scheme. Such an implementation can be shown to be unconditionally stable (see Mihalas et al. [1975]). We obtain:

$$\frac{u_{k,d+1} - u_{k,d}}{\Delta\tau_{k,d+1/2}} = \frac{\gamma_{k,d+1/2}}{\Delta\nu_{k-1/2}}(v_{k,d+1/2} - v_{k-1,d+1/2}) + v_{k,d+1/2}, \quad (5.22)$$

$$\frac{v_{k,d+1/2} - v_{k,d-1/2}}{\Delta\tau_{k,d}} = \frac{\gamma_{k,d}}{\Delta\nu_{k-1/2}}(u_{k,d} - u_{k-1,d}) + u_{k,d} - S_{k,d} \quad (5.23)$$

which apply for $d = 2, 3, \dots, \text{NI} - 1$ and $k = 2, 3, \dots, \text{NF}$. We have utilised the definitions:

$$\Delta\tau_{k,d\pm 1/2} \equiv \chi_{k,d\pm 1/2}|z_{d\pm 1} - z_d|, \quad (5.24)$$

$$\Delta\nu_{k-1/2} \equiv \nu_{k-1} - \nu_k, \quad (5.25)$$

$$\chi_{k,d\pm 1/2} \equiv \frac{1}{2}[\chi_{k,d\pm 1} + \chi_{k,d}], \quad (5.26)$$

$$\Delta\tau_{k,d} \equiv \frac{1}{2}[\Delta\tau_{k,d+1/2} + \Delta\tau_{k,d-1/2}] \quad (5.27)$$

where the shorthand $y_{\nu_k}(z_d) = y_{k,d}$ is adopted and $z_{d\pm 1/2} \equiv (z_d + z_{d\pm 1})/2$. If we now rearrange Eq. (5.22) for $v_{k,d+1/2}$ we find:

$$v_{k,d+1/2} = \frac{u_{k,d+1} - u_{k,d}}{(1 + \delta_{k-1/2,d+1/2})\Delta\tau_{k,d+1/2}} + \frac{\delta_{k-1/2,d+1/2}}{1 + \delta_{k-1/2,d+1/2}}v_{k-1,d+1/2}, \quad (5.28)$$

where

$$\delta_{k-1/2,d+1/2} \equiv \frac{\gamma_{k,d+1/2}}{\Delta\nu_{k-1/2}} = \frac{\alpha_{d+1/2}}{\chi_{k,d+1/2}(\nu_{k-1} - \nu_k)} \left[1 - \mu_{d+1/2}^2 + \beta_{d+1/2}\mu_{d+1/2}^2 \right]. \quad (5.29)$$

We substitute Eq. (5.28) as given - as well as the same equation for $d \rightarrow (d-1)$ - into the LHS of Eq. (5.23) to obtain:

$$\begin{aligned} & \frac{1}{\Delta\tau_{k,d}} \left[\frac{u_{k,d+1}}{(1 + \delta_{k-1/2,d+1/2})\Delta\tau_{k,d+1/2}} - u_{k,d} \left(\frac{1}{(1 + \delta_{k-1/2,d+1/2})\Delta\tau_{k,d+1/2}} \right. \right. \\ & \quad \left. \left. + \frac{1}{(1 + \delta_{k-1/2,d-1/2})\Delta\tau_{k,d-1/2}} \right) + \frac{u_{k,d-1}}{(1 + \delta_{k-1/2,d-1/2})\Delta\tau_{k,d-1/2}} \right] \\ & = (1 + \delta_{k-1/2,d})u_{k,d} - \delta_{k-1/2,d}u_{k-1,d} - S_{k,d} \\ & + \frac{1}{\Delta\tau_{k,d}} \left[\frac{\delta_{k-1/2,d-1/2}}{1 + \delta_{k-1/2,d-1/2}}v_{k-1,d-1/2} - \frac{\delta_{k-1/2,d+1/2}}{1 + \delta_{k-1/2,d+1/2}}v_{k-1,d+1/2} \right]. \end{aligned} \quad (5.30)$$

It is also necessary to find similar difference representations for the boundary conditions. These are obtained as follows:

(a) $d = 1$: At the outer surface of the spherical system (beyond which no scattering occurs) the appropriate boundary condition is given by Eq. (5.7). We difference this equation as before to obtain:

$$\frac{u_{k,2} - u_{k,1}}{\Delta\tau_{k,3/2}} = (1 + \delta_{k-1/2,1})u_{k,1} - \delta_{k-1/2,1}u_{k-1,1}. \quad (5.31)$$

Note that this equation is only accurate to first order in $\Delta\tau$, unlike Eq. (5.30) which is accurate to second order.

(b)(i) $d = \text{NI}, j > \text{NC}$: The ray does not intersect the core and the inner boundary condition at $z = 0$ is given by Eq. (5.11). The resulting straightforward difference equation is once again only accurate to first order in $\Delta\tau$; this might be problematic if $\chi_\nu(r = p_j)$ is large, giving a large value for $\Delta\tau_{k,\text{NI}-1/2}$. The accuracy is improved by taking Eq. (5.30), and evaluating it at $d = \text{NI}$. Quantities defined at $z_{\text{NI}+1}$ are evaluated using the symmetry properties of the system about $z_{\text{NI}} = 0$; upon the reflection $z \rightarrow -z$ we see that $I_\nu^+ \rightarrow I_\nu^-$, $I_\nu^- \rightarrow I_\nu^+$ and thus $u_\nu \rightarrow u_\nu$ while $v_\nu \rightarrow -v_\nu$. The resulting boundary condition, accurate to second order in $\Delta\tau$, is:

$$\begin{aligned} \frac{u_{k,\text{NI}} - u_{k,\text{NI}-1}}{(1 + \delta_{k-1/2,\text{NI}-1/2})\Delta\tau_{k,\text{NI}-1/2}} &= -\frac{\delta_{k-1/2,\text{NI}-1/2}}{1 + \delta_{k-1/2,\text{NI}-1/2}}v_{k-1,\text{NI}-1/2} \\ &+ \frac{1}{2}\Delta\tau_{k,\text{NI}-1/2} [S_{k,\text{NI}} - (1 + \delta_{k-1/2,\text{NI}})u_{k,\text{NI}} + \delta_{k-1/2,\text{NI}}u_{k-1,\text{NI}}]. \end{aligned} \quad (5.32)$$

(b)(ii) $d = \text{NI}, j \leq \text{NC}$: The ray intersects the core and the appropriate boundary condition, applied at $z_{\min} = (R_C^2 - p_j^2)^{1/2}$, is given by discretising Eq. (5.12):

$$\frac{u_{k,\text{NI}} - u_{k,\text{NI}-1}}{\Delta\tau_{k,\text{NI}-1/2}} = v_{k,\text{C}} + \delta_{k-1/2,\text{NI}}(v_{k,\text{C}} - v_{k-1,\text{C}}). \quad (5.33)$$

In the diffusion limit, $v_{k,\text{C}} = 3\mu_{\text{C}}H_{\nu,\text{C}}$ for $\mu_{\text{C}} = z_{\min}/R_{\text{C}}$, while in the free-streaming limit $v_{k,\text{C}} = H_{k,\text{C}}$ for $j = 1$ (i.e. $p = 0$) and is zero otherwise. In both cases, $H_{k,\text{C}} = H_{\nu,\text{C}}|_{\nu_k}$.

Finally for this section we note that the initial condition in frequency, in the form of Eq. (5.15), tells us the solutions for u_ν and v_ν directly for $k = 1$ ($\nu = \nu_{\max}$):

$$u_{1,d} = v_{1,d} = 0, \quad d = 1, 2, 3, \dots, \text{NI}. \quad (5.34)$$

5.1.4 Rybicki Solution Method

We follow the scheme proposed by Rybicki [1971] in which it is necessary to utilise vector representations of the variables $u_\nu(z)$ and $v_\nu(z)$ defined at a particular frequency along a particular ray:

$$\mathbf{u}_k \equiv (u_{k,1}, u_{k,2}, \dots, u_{k,\text{NI}})^\top, \quad (5.35)$$

$$\mathbf{v}_k \equiv (v_{k,3/2}, v_{k,5/2}, \dots, v_{k,\text{NI}-1/2})^\top. \quad (5.36)$$

Note that $\mathbf{u}_k$ is a vector of dimension NI while $\mathbf{v}_k$ has dimension (NI - 1). Both vectors are ray-specific, both in terms of the value of their elements and the number of elements (in the case of rays that don't intersect the core) and should also technically be labelled with an additional j subscript, but such referencing is suppressed for notational simplicity. For a given impact parameter p_j , and at a given frequency ν_k , we represent Eq. (5.30) and the boundary conditions by the matrix equation:

$$\mathbf{T}_k \mathbf{u}_k + \mathbf{U}_k \mathbf{u}_{k-1} + \mathbf{V}_k \mathbf{v}_{k-1} = \mathbf{X}_k. \quad (5.37)$$

The matrices $\mathbf{T}_k$, $\mathbf{U}_k$ and $\mathbf{V}_k$, and the vector $\mathbf{X}_k$, are known; their elements are obtained by comparison with the appropriate equations in the previous section. Here we give only the non-zero elements.

(a) $d = 1$: Comparison of Eq. (5.37) with Eq. (5.31) gives non-zero elements:

$$\begin{aligned} (\mathbf{T}_k)_{1,1} &= \frac{1}{\Delta\tau_{k,3/2}} + 1 + \delta_{k-1/2,1}, \\ (\mathbf{T}_k)_{1,2} &= -\frac{1}{\Delta\tau_{k,3/2}}, \\ (\mathbf{U}_k)_{1,1} &= -\delta_{k-1/2,1}. \end{aligned} \quad (5.38)$$

(b) $d = 2, 3, \dots, \text{NI} - 1$: Comparison of Eq. (5.37) with the second order equation applicable across the ray (away from the boundaries), Eq. (5.30), yields:

$$(\mathbf{T}_k)_{d,d} = \frac{1}{\Delta\tau_{k,d}} \left[\frac{1}{(1 + \delta_{k-1/2,d+1/2})\Delta\tau_{k,d+1/2}} + \frac{1}{(1 + \delta_{k-1/2,d-1/2})\Delta\tau_{k,d-1/2}} \right] + 1 + \delta_{k-1/2,d},$$

$$\begin{aligned}
(\mathbf{T}_k)_{d,d+1} &= -\frac{1}{\Delta\tau_{k,d}} \times \frac{1}{(1 + \delta_{k-1/2,d+1/2})\Delta\tau_{k,d+1/2}}, \\
(\mathbf{T}_k)_{d,d-1} &= -\frac{1}{\Delta\tau_{k,d}} \times \frac{1}{(1 + \delta_{k-1/2,d-1/2})\Delta\tau_{k,d-1/2}}, \\
(\mathbf{U}_k)_{d,d} &= -\delta_{k-1/2,d}, \\
(\mathbf{V}_k)_{d,d} &= -\frac{1}{\Delta\tau_{k,d}} \times \frac{\delta_{k-1/2,d+1/2}}{1 + \delta_{k-1/2,d+1/2}}, \\
(\mathbf{V}_k)_{d,d+1} &= \frac{1}{\Delta\tau_{k,d}} \times \frac{\delta_{k-1/2,d-1/2}}{1 + \delta_{k-1/2,d-1/2}}, \\
(\mathbf{X}_k)_d &= S_{k,d}.
\end{aligned} \tag{5.39}$$

(c)(i) $d = \text{NI}$, $j > \text{NC}$: For rays that do not intersect the core, we compare Eq. (5.37) with the boundary condition Eq. (5.32) to find:

$$\begin{aligned}
(\mathbf{T}_k)_{\text{NI},\text{NI}} &= \frac{1}{(1 + \delta_{k-1/2,\text{NI}-1/2})\Delta\tau_{k,\text{NI}-1/2}} \\
&\quad + \frac{1}{2}(1 + \delta_{k-1/2,\text{NI}})\Delta\tau_{k,\text{NI}-1/2}, \\
(\mathbf{T}_k)_{\text{NI},\text{NI}-1} &= -\frac{1}{(1 + \delta_{k-1/2,\text{NI}-1/2})\Delta\tau_{k,\text{NI}-1/2}}, \\
(\mathbf{U}_k)_{\text{NI},\text{NI}} &= -\frac{1}{2}\delta_{k-1/2,\text{NI}}\Delta\tau_{k,\text{NI}-1/2}, \\
(\mathbf{V}_k)_{\text{NI},\text{NI}-1} &= \frac{\delta_{k-1/2,\text{NI}-1/2}}{1 + \delta_{k-1/2,\text{NI}-1/2}}, \\
(\mathbf{X}_k)_{\text{NI}} &= \frac{1}{2}\Delta\tau_{k,\text{NI}-1/2}S_{k,\text{NI}}.
\end{aligned} \tag{5.40}$$

(c)(ii) $d = \text{NI}$, $j \leq \text{NC}$: For rays intersecting the core, we need to compare Eq. (5.37) with the core boundary condition Eq. (5.33). The non-zero matrix elements are:

$$\begin{aligned}
(\mathbf{T}_k)_{\text{NI},\text{NI}} &= \frac{1}{\Delta\tau_{k,\text{NI}-1/2}}, \\
(\mathbf{T}_k)_{\text{NI},\text{NI}-1} &= -\frac{1}{\Delta\tau_{k,\text{NI}-1/2}}, \\
(\mathbf{X}_k)_{\text{NI}} &= v_{k,C} + \delta_{k-1/2,\text{NI}}(v_{k,C} - v_{k-1,C}).
\end{aligned} \tag{5.41}$$

The elements of the matrices given here are specific to the given ray and the frequency ν_k . The matrix $\mathbf{T}_k$ has dimensions $\text{NI} \times \text{NI}$ and is tridiagonal; $\mathbf{U}_k$ has dimensions $\text{NI} \times \text{NI}$ and is diagonal, while $\mathbf{V}_k$ has dimensions $\text{NI} \times (\text{NI} - 1)$ and has the form of an upper bidiagonal square matrix with an added first row consisting entirely of zeroes.

Another matrix equation that we will utilise results from adopting a matrix representation of Eq. (5.28) for different values of the depth index d ; we write this equation in the form:

$$\mathbf{v}_k = \mathbf{G}_k \mathbf{u}_k + \mathbf{H}_k \mathbf{v}_{k-1}. \quad (5.42)$$

Here we have introduced two new matrices; $\mathbf{G}_k$ has dimension $(\text{NI} - 1) \times \text{NI}$ while $\mathbf{H}_k$ has dimension $(\text{NI} - 1) \times (\text{NI} - 1)$. From comparison with Eq. (5.28) we see that the matrices have non-zero elements:

$$\begin{aligned} (\mathbf{G}_k)_{d,d} &= -\frac{1}{(1 + \delta_{k-1/2,d+1/2})\Delta\tau_{k,d+1/2}}, \\ (\mathbf{G}_k)_{d,d+1} &= \frac{1}{(1 + \delta_{k-1/2,d+1/2})\Delta\tau_{k,d+1/2}}, \\ (\mathbf{H}_k)_{d,d} &= \frac{\delta_{k-1/2,d+1/2}}{1 + \delta_{k-1/2,d+1/2}} \end{aligned} \quad (5.43)$$

for $d = 1, 2, \dots, \text{NI} - 1$. Clearly $\mathbf{H}_k$ is diagonal while $\mathbf{G}_k$ can be considered an upper bidiagonal square matrix with an added final column consisting of only one non-zero element in the last row.

We now describe the route to obtaining the radiation field solution from these matrix equations; note the steps here are less involved than in Mihalas et al. as we deal with a pure line scattering problem (no continuum contribution) and we assume a given form for the source function, as opposed to a form dependent on the frequency-averaged mean intensity. We start from the initial condition Eq.(5.34) which can be rewritten trivially in our vector formalism as:

$$\mathbf{u}_1 = \mathbf{v}_1 = 0. \quad (5.44)$$

We construct the solution vector $\mathbf{u}_k$ for the next value of the frequency index k by rearranging Eq. (5.37) to express $\mathbf{u}_k$ in terms of vectors evaluated at the previous frequency. The vector $\mathbf{u}_k$ can then be used together with the previously obtained vector $\mathbf{v}_{k-1}$ to obtain $\mathbf{v}_k$ according to Eq. (5.42). The formulae used are:

$$\mathbf{u}_k = \mathbf{T}_k^{-1} (\mathbf{X}_k - \mathbf{U}_k \mathbf{u}_{k-1} - \mathbf{V}_k \mathbf{v}_{k-1}), \quad (5.45)$$

$$\mathbf{v}_k = \mathbf{G}_k \mathbf{u}_k + \mathbf{H}_k \mathbf{v}_{k-1}. \quad (5.46)$$

The formulae are applied for successive frequencies ν_k , $k = 2, 3, \dots, \text{NF}$. The resulting set of NF vectors of dimension NI describe the variation of the radiation field with frequency and z along the particular ray p_j ; the process is then repeated for all NP rays. The resulting values for $u_\nu(p, z)$ and $v_\nu(p, z)$ comprise a complete description of the specific intensity: clearly $I_\nu(r, \mu) = u_\nu(p, z) + v_\nu(p, z)$ and $I_\nu(r, -\mu) = u_\nu(p, z) - v_\nu(p, z)$.

5.2 Solution of Moment Equations

We obtain angular moment equations of Eq. (5.1) by integrating over angle. The n th-order moment equation is obtained by acting on the equation with the operator $\frac{1}{2} \int_{-1}^1 d\mu \mu^n$, which yields the zeroth- and first-order moment equations:

$$\frac{1}{r^2} \frac{\partial(r^2 H_\nu)}{\partial r} - \alpha \left[\frac{\partial(J_\nu - K_\nu)}{\partial \nu} + \beta \frac{\partial K_\nu}{\partial \nu} \right] = \eta_\nu - \chi_\nu J_\nu, \quad (5.47)$$

$$\frac{\partial K_\nu}{\partial r} + \frac{3K_\nu - J_\nu}{r} - \alpha \left[\frac{\partial(H_\nu - N_\nu)}{\partial \nu} + \beta \frac{\partial N_\nu}{\partial \nu} \right] = -\chi_\nu H_\nu \quad (5.48)$$

where we have made use of the definitions of the first four moments of the specific intensity:

$$[J_\nu, H_\nu, K_\nu, N_\nu] = \frac{1}{2} \int_{-1}^1 d\mu I_\nu(\mu) [1, \mu, \mu^2, \mu^3]. \quad (5.49)$$

This section serves to outline the method of solution of this system as proposed by Mihalas et al. [1976].

It is necessary to utilise additional constraints relating the four angular moments of the radiation intensity to obtain closure of the system of moment equations. Following the Eddington approximation, in which the zeroth- and second-order moments of the intensity are assumed to be related by a constant independent of frequency and radius ($K_\nu = J_\nu/3$), we assume a relationship between the moments dictated by the ‘variable Eddington factor’ $f_\nu(r)$, defined as:

$$f_\nu(r) \equiv \frac{K_\nu(r)}{J_\nu(r)}. \quad (5.50)$$

The value of $f_\nu(r)$ depends on the degree of isotropy of the radiation field; in the case of the diffusion limit $I_\nu = J_\nu + 3\mu H_\nu$ or an entirely isotropic radiation field we find $f_\nu(r) \equiv 1/3$ as in the usual Eddington approximation, while for a highly anisotropic

radiation field such as the free-streaming limit $I_\nu = 2H_\nu\delta_D(\mu - 1)$ we find $f_\nu(r) \equiv 1$. Typically the value of $f_\nu(r)$ lies somewhere between these two extremes, see e.g. Mihalas [1978]. It is also possible to define a variable Eddington factor linking higher order angular moments. We define a further variable Eddington factor $g_\nu(r)$ linking the first- and third-order moments $H_\nu(r)$ and $N_\nu(r)$:

$$g_\nu(r) \equiv \frac{N_\nu(r)}{H_\nu(r)}. \quad (5.51)$$

The value of $g_\nu(r)$ is similarly dependent on the angular distribution of the radiation field at (r, ν) . For our immediate purposes we assume that both variable Eddington factors are given; in practice this might be the case if we can assume some limiting angular character of the radiation field but more likely we will have to construct them from a formal solution of the ray equations, as described in the next subsection.

We define the ‘sphericity factor’ $q_\nu(r)$, introduced by Auer [1971], by the relation:

$$\frac{\partial \ln(r^2 q_\nu)}{\partial r} = \frac{3f_\nu - 1}{f_\nu r}. \quad (5.52)$$

We calculate $q_\nu(r)$ given the variable Eddington factor $f_\nu(r)$ and the arbitrary normalisation $q_\nu(R_C) = 1$:

$$q_\nu(r) = \left(\frac{r}{R_C}\right)^{-2} \exp \left[\int_{R_C}^r \frac{3f_\nu(r') - 1}{r' f_\nu(r')} dr' \right]. \quad (5.53)$$

This quantity allows us to make a change of variable in the radial derivative to the dimensionless quantity $X_\nu(r)$, defined such that:

$$dX_\nu(r) = -\chi_\nu(r) q_\nu(r) dr. \quad (5.54)$$

This allows us to rewrite terms on the LHS of Equations (5.47) and (5.48) as:

$$\frac{\partial(r^2 H_\nu)}{\partial r} = -q_\nu \chi_\nu \frac{\partial(r^2 H_\nu)}{\partial X_\nu}, \quad (5.55)$$

$$\frac{\partial(f_\nu J_\nu)}{\partial r} + \frac{3f_\nu - 1}{r} J_\nu = -r^{-2} \chi_\nu \frac{\partial(r^2 q_\nu f_\nu J_\nu)}{\partial X_\nu}. \quad (5.56)$$

These relations and the definitions of f_ν and g_ν allow us to write the zeroth and first order moment equations as:

$$q_\nu \frac{\partial(r^2 H_\nu)}{\partial X_\nu} + \Gamma_\nu \left[\frac{\partial(1 - f_\nu)r^2 J_\nu}{\partial \nu} + \beta \frac{\partial(f_\nu r^2 J_\nu)}{\partial \nu} \right] = r^2 (J_\nu - S_\nu), \quad (5.57)$$

$$\frac{\partial(f_\nu q_\nu r^2 J_\nu)}{\partial X_\nu} + \Gamma_\nu \left[\frac{\partial(1 - g_\nu)r^2 H_\nu}{\partial \nu} + \beta \frac{\partial(g_\nu r^2 H_\nu)}{\partial \nu} \right] = r^2 H_\nu \quad (5.58)$$

where $\Gamma_\nu(r) = \alpha(r)/\chi_\nu(r)$ and once again $S_\nu(r) = \eta_\nu(r)/\chi_\nu(r)$ is the source function, although in solving the moment equations we will be able to account for the dependence of the source function on the radiation field and will not assume a given estimate as for the ray equations. Assuming the isotropic forms of the opacity and emissivity for resonance-line scattering, a good approximation in the comoving frame, the source function is given by:

$$S_\nu(r) \equiv \frac{\eta_\nu(r)}{\chi_\nu(r)} = \frac{1}{\varphi(\nu, r)} \int R(\nu', \nu, r) J_{\nu'}(r) d\nu' \quad (5.59)$$

where we have allowed for the redistribution function and absorption profile to vary with radius due to any variation in the temperature profile of the medium, $T(r)$.

5.2.1 Calculation of Eddington Factors

We describe the method used to obtain estimates of the variable Eddington factors $f_\nu(r)$ and $g_\nu(r)$ based on the ray-by-ray solution described in the previous section:

- (i) The ray-by-ray solution is constructed, starting from an estimate of the source function $S_\nu(r)$ and a boundary condition for the flux emerging from the core, $H_{\nu,C}$. This gives $u_\nu(p, z)$ and $v_\nu(p, z)$ for all gridpoints of the ray impact parameter p_j , distance along the ray $z_{d,j}$ and frequency ν_k .
- (ii) We need to estimate the n th-order angular moments of the intensity $I_\nu(r, \mu)$ for $n = 0, 1, 2, 3$; these quantities are defined according to Eq. (5.49), but we can rewrite the integrals as:

$$J_\nu(r) \equiv \frac{1}{2} \int_{-1}^1 I_\nu(r, \mu) d\mu = \int_0^1 u_\nu(r, \mu) d\mu, \quad (5.60)$$

$$H_\nu(r) \equiv \frac{1}{2} \int_{-1}^1 \mu I_\nu(r, \mu) d\mu = \int_0^1 \mu v_\nu(r, \mu) d\mu, \quad (5.61)$$

$$K_\nu(r) \equiv \frac{1}{2} \int_{-1}^1 \mu^2 I_\nu(r, \mu) d\mu = \int_0^1 \mu^2 u_\nu(r, \mu) d\mu, \quad (5.62)$$

$$N_\nu(r) \equiv \frac{1}{2} \int_{-1}^1 \mu^3 I_\nu(r, \mu) d\mu = \int_0^1 \mu^3 v_\nu(r, \mu) d\mu \quad (5.63)$$

where the second equality in each case is reached by utilising the definitions of $u_\nu(r, \mu)$ and $v_\nu(r, \mu)$ in terms of $I_\nu(r, \mu)$ and $I_\nu(r, -\mu)$. We can evaluate the integrals by a quadrature formula - we describe the case of $K_\nu(r)$, Eq. (5.62), as an example:

- From spherical symmetry, the radiation intensity along a ray of impact parameter p at the point of intersection with a sphere of radius $r > p$ is equal to the radiation intensity at r in the direction described by $\mu = z/r$, where z is the distance along the ray defined as in Figure 5.1. We know $u_\nu(p, z)$ at the gridpoint values of the arguments, p_j and $z_{d,j} \equiv (r_d^2 - p_j^2)^{1/2}$, and thus we know $u_\nu(r, \mu)$ for all values of r_d and $\mu_{d,j} = z_{d,j}/r_d$ for $j = 1, 2, \dots, \text{NR}_d$ where $\text{NR}_d = \text{ND} + \text{NC} + 1 - d$ is the number of rays intersected by the sphere of radius r_d . Discretisations are as described in section 5.1.3.
- We use a quadrature formula to write $K_\nu(r)$ as a sum of weighted values of the integrand in Eq. (5.62):

$$K_\nu(r) \rightarrow \sum_{j=1}^{\text{NR}_d} w_j(r_d) \mu_{d,j}^2 u_\nu(r_d, \mu_{d,j}) \quad (5.64)$$

where the $w_j(r_d)$ are angular/impact-parameter quadrature weights for the particular radial shell at r_d . In practice it is simpler to work with a Gauss-Legendre quadrature routine. We use linear interpolation between the appropriate values of $\mu_{d,j}$ to specify the function $u_\nu(r_d, \mu)$ at the Gauss-Legendre nodes.

This method is applied to Equations (5.60) to (5.63) to compute all four of the angular moments. Exceptions include a static medium or a medium subject to a linear velocity law with $\beta = 1$ for all r ; in these cases the moment equations are independent of g_ν and thus we need only compute J_ν and K_ν .

(iii) Now that we have estimated the four angular moments we find the variable Edington factors from $f_\nu(r) = K_\nu(r)/J_\nu(r)$ and $g_\nu(r) = N_\nu(r)/H_\nu(r)$. These estimates will be used in the process of solving the moment equations.

5.2.2 Discretised Moment Equations

In this section we obtain discrete versions of the moment equations applicable across our grids in frequency and radius, $\{\nu_k\}$ and $\{r_d\}$, described in section 5.1.3. Similarly to the ray equations for u_ν and v_ν , values of J_ν are evaluated on the grid in r , while values of H_ν are evaluated at intermediate gridpoints denoted by a half-integer value of the

radius index d . The derivatives of J_ν and H_ν with respect to frequency are represented by a fully implicit scheme.

Differencing the first-order moment equation, Eq. (5.58), we obtain:

$$\begin{aligned} & \frac{f_{k,d+1}q_{k,d+1}r_{d+1}^2J_{k,d+1} - f_{k,d}q_{k,d}r_d^2J_{k,d}}{\Delta X_{k,d+1/2}} + \frac{\Gamma_{k-1/2,d+1/2}}{\Delta \nu_{k-1/2}} \\ & \times r_{d+1/2}^2 \left[(1 - g_{k-1,d+1/2} + \beta_{d+1/2}g_{k-1,d+1/2})H_{k-1,d+1/2} \right. \\ & \left. - (1 - g_{k,d+1/2} + \beta_{d+1/2}g_{k,d+1/2})H_{k,d+1/2} \right] = r_{d+1/2}^2 H_{k,d+1/2}, \end{aligned} \quad (5.65)$$

where

$$\Delta X_{k,d+1/2} \equiv \frac{1}{2}(q_{k,d+1}\chi_{k,d+1} + q_{k,d}\chi_{k,d})(r_d - r_{d+1}), \quad (5.66)$$

$$\Gamma_{k-1/2,d+1/2} \equiv \alpha_{d+1/2}/\chi_{k-1/2,d+1/2}, \quad (5.67)$$

$$\chi_{k-1/2,d+1/2} \equiv \frac{1}{4}(\chi_{k,d+1} + \chi_{k,d} + \chi_{k-1,d+1} + \chi_{k-1,d}) \quad (5.68)$$

and $\Delta \nu_{k-1/2} = (\nu_{k-1} - \nu_k)$ as defined previously; functions $\alpha(r)$, $\beta(r)$ and $g_\nu(r)$ with subscript ‘ $d+1/2$ ’ are evaluated at $r_{d+1/2} = (r_d + r_{d+1})/2$. Eq. (5.65) can be rearranged to give:

$$\begin{aligned} r_{d+1/2}^2 H_{k,d+1/2} &= \frac{f_{k,d+1}q_{k,d+1}r_{d+1}^2J_{k,d+1} - f_{k,d}q_{k,d}r_d^2J_{k,d}}{(1 + \omega_{k,k,d+1/2})\Delta X_{k,d+1/2}} \\ &+ \frac{\omega_{k,k-1,d+1/2}}{1 + \omega_{k,k,d+1/2}} r_{d+1/2}^2 H_{k-1,d+1/2}, \end{aligned} \quad (5.69)$$

where we define new coefficients

$$\omega_{k,l,d+1/2} \equiv \frac{\Gamma_{k-1/2,d+1/2}}{\Delta \nu_{k-1/2}} (1 - g_{l,d+1/2} + \beta_{d+1/2}g_{l,d+1/2}). \quad (5.70)$$

At this point we need to make use of the initial condition in frequency (see section 5.1.2); for a medium with $V(r)$, $dV/dr \geq 0$ for all r , we stated previously that $\partial I_\nu / \partial \nu = 0$ at $\nu = \nu_{\max}$. Thus any terms in the moment equations arising from angle-averaging the last term on the LHS of Eq. (5.1) must vanish at $\nu = \nu_{\max}$. This condition forces us to set $\omega_{k,l,d+1/2} = 0$ at $k = 1$ for all values of l and d :

$$\omega_{1,l,d+1/2} \equiv 0. \quad (5.71)$$

The initial condition can be applied to Eq. (5.69) for $k = 1$ to find an expression for $r_{d+1/2}^2 H_{1,d+1/2}$ in terms of $J_{k,d}$ and $J_{k,d+1}$. If we continue to write the equation for

successive values of k we find that we can express $r_{d+1/2}^2 H_{k,d+1/2}$ in terms of the values of $J_{k',d}$ and $J_{k',d+1}$ for $k' \leq k$. The result is:

$$r_{d+1/2}^2 H_{k,d+1/2} = \sum_{k'=1}^k \psi_{k,k',d+1/2} \left[\frac{f_{k',d+1} q_{k',d+1} r_{d+1}^2 J_{k',d+1} - f_{k',d} q_{k',d} r_d^2 J_{k',d}}{\Delta X_{k',d+1/2}} \right], \quad (5.72)$$

where the coefficients $\psi_{k,k',d+1/2}$ are defined by (Mihalas et al. [1977]):

$$\psi_{k,k',d+1/2} \equiv \frac{1}{1 + \omega_{k,k,d+1/2}} \times \begin{cases} \prod_{l=k'+1}^k \frac{\omega_{l,l-1,d+1/2}}{1 + \omega_{l-1,l-1,d+1/2}} & ; k' < k \\ \delta_{k',k} & ; k' \geq k \end{cases}. \quad (5.73)$$

The zeroth-order moment equation Eq. (5.57) is differenced according to the same scheme to give:

$$\begin{aligned} \frac{q_{k,d}}{\Delta X_{k,d}} (r_{d+1/2}^2 H_{k,d+1/2} - r_{d-1/2}^2 H_{k,d-1/2}) + \frac{\Gamma_{k-1/2,d}}{\Delta \nu_{k-1/2}} \times r_d^2 [(1 - f_{k-1,d} + \beta_d f_{k-1,d}) J_{k-1,d} \\ - (1 - f_{k,d} + \beta_d f_{k,d}) J_{k,d}] = r_d^2 (J_{k,d} - S_{k,d}). \end{aligned} \quad (5.74)$$

We use Eq. (5.72) to replace the $H_{k,d\pm 1/2}$ values and obtain an equation containing only the $J_{k,d}$ values:

$$\begin{aligned} \frac{q_{k,d}}{\Delta X_{k,d}} \left[\sum_{k'=1}^k \frac{\psi_{k,k',d+1/2}}{\Delta X_{k',d+1/2}} (f_{k',d+1} q_{k',d+1} r_{d+1}^2 J_{k',d+1} - f_{k',d} q_{k',d} r_d^2 J_{k',d}) \right. \\ \left. - \sum_{k'=1}^k \frac{\psi_{k,k',d-1/2}}{\Delta X_{k',d-1/2}} (f_{k',d} q_{k',d} r_d^2 J_{k',d} - f_{k',d-1} q_{k',d-1} r_{d-1}^2 J_{k',d-1}) \right] \\ = r_d^2 [(1 + \pi_{k,k,d}) J_{k,d} - \pi_{k,k-1,d} J_{k-1,d} - S_{k,d}] \end{aligned} \quad (5.75)$$

where we define coefficients

$$\pi_{k,l,d} \equiv \frac{\Gamma_{k-1/2,d}}{\Delta \nu_{k-1/2}} (1 - f_{l,d} + \beta_d f_{l,d}). \quad (5.76)$$

Eq. (5.75) is applicable for $d = 2, 3, \dots, \text{ND} - 1$ and $k = 1, 2, \dots, \text{NF}$ and we note that the initial condition in frequency indicates that:

$$\pi_{1,l,d} = 0. \quad (5.77)$$

In terms of our discrete grids in ν and r we write the source function $S_{k,d}$ as a quadrature sum:

$$S_{k,d} = \sum_{k'=1}^{\text{NF}} \mathcal{R}_{k',k,d} J_{k',d}. \quad (5.78)$$

We need to use suitable coefficients $\mathcal{R}_{k',k,d}$ for $k, k' = 1, 2, \dots, \text{NF}$ and $d = 1, 2, \dots, \text{ND}$. A particularly useful representation of the source function results from assuming the diffusion approximation described in section 2.4.5, in which a Taylor expansion of $J_\nu(r)$ under the integral in Eq. (5.59) gives:

$$S_\nu(r) = J_\nu(r) + \frac{(\Delta\nu_D)^2}{2\varphi(\nu)} \frac{\partial}{\partial\nu} \left[\varphi(\nu) \frac{\partial J_\nu(r)}{\partial\nu} \right]. \quad (5.79)$$

Representing this form using a centred finite-difference scheme we arrive at an expression for $S_{k,d}$ of the form of Eq. (5.78) with coefficients $\mathcal{R}_{k',k,d}$ given by:

$$\begin{aligned} \mathcal{R}_{k',k,d} &= \frac{1}{8} \left(\frac{\Delta\nu_D}{\Delta\nu_k} \right) \left[\frac{\Delta\nu_k \varphi_{k+1,d}}{\Delta\nu_{k+1} \varphi_{k,d}} \right] \delta_{k',k+2} \\ &+ \left\{ 1 - \frac{1}{8} \left(\frac{\Delta\nu_D}{\Delta\nu_k} \right) \left[\frac{\Delta\nu_k \varphi_{k+1,d}}{\Delta\nu_{k+1} \varphi_{k,d}} + \frac{\Delta\nu_k \varphi_{k-1,d}}{\Delta\nu_{k-1} \varphi_{k,d}} \right] \right\} \delta_{k',k} \\ &+ \frac{1}{8} \left(\frac{\Delta\nu_D}{\Delta\nu_k} \right) \left[\frac{\Delta\nu_k \varphi_{k-1,d}}{\Delta\nu_{k-1} \varphi_{k,d}} \right] \delta_{k',k-2} \end{aligned} \quad (5.80)$$

where $\Delta\nu_k \equiv (\nu_{k-1} - \nu_{k+1})/2$ and we have made use of the Kronecker Delta symbol $\delta_{i,j}$. Throughout the remainder of this section we will retain the generalised specification of $S_{k,d}$ given by Eq. (5.78).

Boundary Conditions

The boundary conditions required to complement Eq. (5.75) are given by consideration of Eq. (5.65) at the minimum and maximum values of the grid in radius.

(i) $d = 1, r = R$ (surface boundary): We define the frequency-dependent ‘boundary Edington factors’ which relate the moments of the radiation field at the outer boundary:

$$h_k \equiv H_{k,1}/J_{k,1}, \quad (5.81)$$

$$n_k \equiv N_{k,1}/J_{k,1}. \quad (5.82)$$

The factors h_k and n_k can be estimated from the results of the ray-by-ray solution - no additional effort is required as we already estimate the moments via the Equations

(5.60) to (5.63) in order to find f_ν and g_ν , we just use the values for J_ν , H_ν and N_ν found at $d = 1$. We can rewrite the discretised first-order moment equation for $d = 1$ as:

$$\frac{f_{k,2}q_{k,2}r_2^2J_{k,2} - f_{k,1}q_{k,1}r_1^2J_{k,1}}{\Delta X_{k,3/2}} = r_1^2[(h_k + \theta_{k,k,1})J_{k,1} - \theta_{k,k-1,1}J_{k-1,1}] \quad (5.83)$$

where we have defined

$$\theta_{k,l,1} \equiv \frac{\Gamma_{k-1/2,1}}{\Delta \nu_{k-1/2}}(h_l - n_l + \beta_1 n_l), \quad (5.84)$$

$$\Gamma_{k-1/2,1} = \alpha_1/\chi_{k-1/2,1}, \quad (5.85)$$

$$\chi_{k-1/2,1} \equiv \frac{1}{2}(\chi_{k-1,1} + \chi_{k,1}). \quad (5.86)$$

The initial condition in frequency indicates that:

$$\theta_{1,l,1} = 0. \quad (5.87)$$

(ii) $d = \text{ND}$, $r = R_C$ (core boundary): We use a boundary condition amounting to a discretised form of the Eq. (5.58) with the given form for the flux from the core, $H_{\nu,C}$; this condition is:

$$\begin{aligned} \frac{f_{k,\text{ND}}q_{k,\text{ND}}r_{\text{ND}}^2J_{k,\text{ND}} - f_{k,\text{ND}-1}q_{k,\text{ND}-1}r_{\text{ND}-1}^2J_{k,\text{ND}-1}}{\Delta X_{k,\text{ND}-1/2}} &= r_{\text{ND}-1/2}^2 [H_{k,C} \\ &+ \omega_{k,k,\text{ND}-1/2}H_{k,C} - \omega_{k,k-1,\text{ND}-1/2}H_{k-1,C}] \end{aligned} \quad (5.88)$$

where $H_{k,C} \equiv H_{\nu_k,C}$ as for the core boundary condition for the ray equations.

5.2.3 Feautrier Solution Method

Following Feautrier [1964], we utilise a vector representation of the frequency variation of the mean intensity at a fixed radius, $J_\nu(r_d)$:

$$\mathbf{J}_d \equiv (J_{1,d}, J_{2,d}, \dots, J_{\text{NF},d})^\text{T}. \quad (5.89)$$

Referring to Equations (5.75), (5.83) and (5.88), we see that all equations for a given radius index d can be condensed into the matrix equation:

$$-\mathbf{A}_d\mathbf{J}_{d-1} + \mathbf{B}_d\mathbf{J}_d - \mathbf{C}_d\mathbf{J}_{d+1} = \mathbf{L}_d \quad (5.90)$$

where the matrices A_d , B_d and C_d have dimensions $NF \times NF$ and $\mathbf{L}_d$ is a vector of dimension NF ; examination of the boundary conditions tells us that $A_1 \equiv 0$ and $C_{ND} \equiv 0$. The elements of each matrix and the vector $\mathbf{L}_d$ follow from examination of the appropriate equation at each radius:

(a) $d = 1$: referring to Eq. (5.83), we find the matrices B_1 and C_1 have:

$$\begin{aligned} (B_1)_{k,k} &= r_1^2 \left[\frac{f_{k,1} q_{k,1}}{\Delta X_{k,3/2}} + h_k + \theta_{k,k,1} \right], \\ (B_1)_{k,k-1} &= -r_1^2 \theta_{k,k-1,1}, \\ (C_1)_{k,k} &= r_2^2 \frac{f_{k,2} q_{k,2}}{\Delta X_{k,3/2}} \end{aligned} \quad (5.91)$$

while the vector $\mathbf{L}_d$ is identically zero, as are all unspecified matrix elements.

(b) $d = 2, 3, \dots, ND - 1$: We seek to write Eq. (5.75), with the source function term given by Eq. (5.78), in the matrix form of Eq. (5.90). The matrix elements are:

$$\begin{aligned} (A_d)_{k,k'} &= r_{d-1}^2 \frac{q_{k,d} f_{k',d-1} q_{k',d-1} \psi_{k,k',d-1/2}}{\Delta X_{k,d} \Delta X_{k',d-1/2}}, \\ (B_d)_{k,k'} &= r_d^2 \left[\frac{q_{k,d} f_{k',d} q_{k',d}}{\Delta X_{k,d}} \left\{ \frac{\psi_{k,k',d+1/2}}{\Delta X_{k',d+1/2}} + \frac{\psi_{k,k',d-1/2}}{\Delta X_{k',d-1/2}} \right\} \right. \\ &\quad \left. + (1 + \pi_{k,k,d}) \delta_{k',k} - \pi_{k,k-1,d} \delta_{k',k-1} - \mathcal{R}_{k',k,d} \right], \\ (C_d)_{k,k'} &= r_{d+1}^2 \frac{q_{k,d} f_{k',d+1} q_{k',d+1} \psi_{k,k',d+1/2}}{\Delta X_{k,d} \Delta X_{k',d+1/2}}. \end{aligned} \quad (5.92)$$

Again the vector $\mathbf{L}_d$ is identically zero.

(c) $d = ND$: We write the core boundary condition Eq. (5.88) in the required matrix form as follows:

$$\begin{aligned} (A_{ND})_{k,k} &= r_{ND-1}^2 \frac{f_{k,ND-1} q_{k,ND-1}}{\Delta X_{k,ND-1/2}}, \\ (B_{ND})_{k,k} &= r_{ND}^2 \frac{f_{k,ND} q_{k,ND}}{\Delta X_{k,ND-1/2}} \end{aligned} \quad (5.93)$$

and the vector $\mathbf{L}_d$ has elements

$$(\mathbf{L}_{ND})_k = r_{ND-1/2}^2 [H_{k,C} + \omega_{k,k,ND-1/2} H_{k,C} - \omega_{k,k-1,ND-1/2} H_{k-1,C}]. \quad (5.94)$$

Once again all unspecified matrix elements are zero.

The matrix equations of the form Eq. (5.90) for $d = 1, 2, \dots, \text{ND}$ are solved by the method devised by Feautrier. At the outer boundary, Eq. (5.90) reduces to:

$$\mathbf{B}_1 \mathbf{J}_1 - \mathbf{C}_1 \mathbf{J}_2 = \mathbf{L}_1. \quad (5.95)$$

Thus we can write

$$\mathbf{J}_1 = \mathbf{D}_1 \mathbf{J}_2 + \mathbf{v}_1 \quad (5.96)$$

where $\mathbf{D}_1 \equiv \mathbf{B}_1^{-1} \mathbf{C}_1$ and $\mathbf{v}_1 \equiv \mathbf{B}_1^{-1} \mathbf{L}_1$. If we make the substitution

$$\mathbf{J}_d = \mathbf{D}_d \mathbf{J}_{d+1} + \mathbf{v}_d \quad (5.97)$$

into Eq. (5.90) we find

$$\mathbf{D}_d \equiv (\mathbf{B}_d - \mathbf{A}_d \mathbf{D}_{d-1})^{-1} \mathbf{C}_d, \quad (5.98)$$

$$\mathbf{v}_d \equiv (\mathbf{B}_d - \mathbf{A}_d \mathbf{D}_{d-1})^{-1} (\mathbf{L}_d + \mathbf{A}_d \mathbf{v}_{d-1}). \quad (5.99)$$

Thus, as we know $\mathbf{A}_d$, $\mathbf{B}_d$, $\mathbf{C}_d$ and $\mathbf{L}_d$ for all d we can calculate $\mathbf{D}_d$ and $\mathbf{v}_d$, starting from $d = 1$ up to $d = \text{ND} - 1$. At the core boundary, $d = \text{ND}$, Eq. (5.90) reads:

$$-\mathbf{A}_{\text{ND}} \mathbf{J}_{\text{ND}-1} + \mathbf{B}_{\text{ND}} \mathbf{J}_{\text{ND}} = \mathbf{L}_{\text{ND}}. \quad (5.100)$$

Clearly $\mathbf{C}_{\text{ND}} \equiv 0$ and thus $\mathbf{D}_{\text{ND}} \equiv 0$. Substituting Eq. (5.97) for $d = \text{ND} - 1$, we see that

$$\mathbf{J}_{\text{ND}} = (\mathbf{B}_{\text{ND}} - \mathbf{A}_{\text{ND}} \mathbf{D}_{\text{ND}-1})^{-1} (\mathbf{L}_{\text{ND}} + \mathbf{A}_{\text{ND}} \mathbf{v}_{\text{ND}-1}) \quad (5.101)$$

as also follows from noting $\mathbf{J}_{\text{ND}} \equiv \mathbf{v}_{\text{ND}}$. Finally, we can obtain $\mathbf{J}_d$ for $d = \text{ND} - 1$ to $d = 1$ by using Eq. (5.97). Thus we obtain $J_{k,d}$ for all k, d and our solution for $J_\nu(r)$ is complete. We can then construct $H_\nu(r)$ from Eq. (5.72) while the higher-order moments follow from the Eddington factors, completing our solution of the Equations (5.47) and (5.48).

In some cases it might be necessary to attempt to improve on our estimate of the Eddington factors by repeating the ray solution steps with an improved source function estimate taken from Eq. (5.78) applied to our moment solution $J_{k,d}$, a process that can be iterated until convergence. We will give details of this strategy as applied to particular test problems in the remaining sections of this chapter.

5.3 Test Problem: Static Sphere (II)

We return to the problem of Ly α scattering in a finite, static, spherically symmetric scattering medium of radius R with uniform temperature T and line-centre opacity κ_0 . We introduced this problem in section 2.8.2 and described the analytic solution valid in the Eddington approximation as derived by Dijkstra et al. [2006]. We also considered this problem using Monte Carlo methods to determine the exact solution in section 4.5. In this section we will reconsider this problem using the methods described in sections 5.1 and 5.2; this will serve as a test of our implementation of the methods as well as a general example of their use.

The source is assumed to be a thin shell of radius $r_S \ll R$. The inner boundary condition is applied at a ‘core radius’ R_C . As the moment equations that we solve do not account for a source term, it is important that the source is contained within the core, $r_S < R_C$, such that the properties of the source are described by the core boundary condition. This boundary condition is given by Eq. (5.88) for solving the moment equations and Eq. (5.33) with $v_{k,C} = 3\mu_C H_{\nu,C}$ for solving the ray equations. In all cases we take the analytic solution Eq. (4.33) for $H_{\nu,C}$ with the Q_n coefficients given by Eq. (4.35). We take a linear grid in radius spanning $[R_C, R]$ and a linear grid of frequency values $\{x_k\}$ spanning the range over which the analytic solution is non-negligible.

When solving the moment equations it is necessary to specify the coefficients $\mathcal{R}_{k',k,d}$ used in the quadrature sum representing the source function. We attempt this using the form given by the diffusion approximation applied to the source function integral, Eq. (5.80), and specifying the result for a medium of uniform temperature resulting in no dependence on radius i.e. $\mathcal{R}_{k',k,d} \rightarrow \mathcal{R}_{k',k}$:

$$\begin{aligned} \mathcal{R}_{k',k} &= \left[1 - \frac{\phi_{k-1} + \phi_{k+1}}{8\phi_k(\Delta x)^2} \right] \delta_{k',k} \\ &+ \left[\frac{\phi_{k-1}}{8\phi_k(\Delta x)^2} \right] \delta_{k',k-2} + \left[\frac{\phi_{k+1}}{8\phi_k(\Delta x)^2} \right] \delta_{k',k+2} \\ &+ \epsilon \left[\frac{\phi_{k-1}}{2\phi_k\Delta x} \right] \delta_{k',k-1} - \epsilon \left[\frac{\phi_{k+1}}{2\phi_k\Delta x} \right] \delta_{k',k+1}, \end{aligned} \quad (5.102)$$

where we have also included extra terms accounting for the recoil correction of Eq. (2.50).

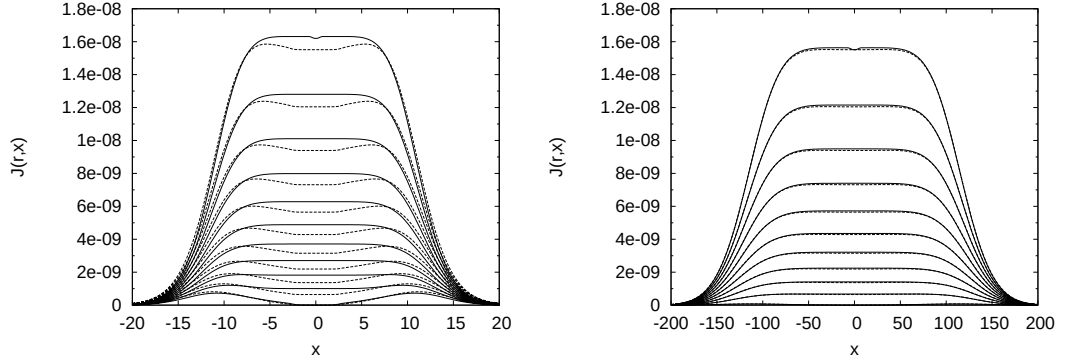


Figure 5.2: Plots of the solution $J(r, x)$ for $\text{Ly}\alpha$ scattering in a static, uniform sphere in the Eddington approximation. Solutions assume a source of the form Eq.(4.34) at a radius $r_S = 5$, temperature $T = 10$ K, and a line-centre opacity $\kappa_0 = 100$ (left panel) and $\kappa_0 = 1.2 \times 10^5$ (right panel). Frequency profiles are given from $R_C = 500$ (highest values of J) to $R = 1000$ (lowest values of J) in steps of 50. In each panel we display our solutions of the moment equations in the Eddington approximation (solid line) together with the corresponding analytic solution of Dijkstra et al. (dashed line).

By contrast the source function in the ray equations is only required to be estimated; for the current problem it is sufficient to evaluate the integral Eq. (5.59) using the analytic solution Eq. (2.82) as an estimate of the mean intensity.

5.3.1 Reproduction of Analytic Solution

As a first step we attempt to solve the problem in the Eddington approximation by solving the moment equations alone. In this limit we can assume $f_\nu(r) \equiv 1/3$ and therefore from Eq. (5.53) we can write for the sphericity factor $q_\nu(r) = (r/R_C)^{-2}$. At the outer boundary we specify the ratio $h_k \equiv H(x_k, R)/J(x_k, R)$ by assuming the usual boundary condition in the Eddington approximation, see Eq. (2.81), with the result $h_k \equiv 1/2$. As the medium is static, $V(r) \equiv 0$ and we can set the ‘ ω ’, ‘ π ’ and ‘ θ ’ coefficients to zero while $\psi_{k,k',d+1/2} \rightarrow \delta_{k,k'}$.

Examples of the resulting moment equation solution are given in Figure 5.2. We find our results agree with the analytic solution of Dijkstra et al. [2006] apart from differences across the line centre in the case with $\kappa_0 = 100$; presumably the moment

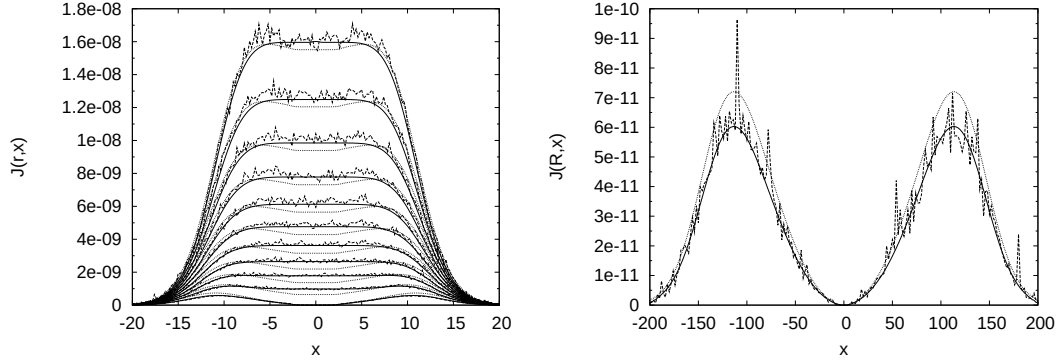


Figure 5.3: Plots of the solution $J(r, x)$ for $\text{Ly}\alpha$ scattering in a static, uniform sphere. Solutions assume a source of the form Eq.(4.34) at a radius $r_S = 5$, temperature $T = 10$ K, and a line-centre opacity $\kappa_0 = 100$ (left panel) and $\kappa_0 = 1.2 \times 10^5$ (right panel). In the left panel, frequency profiles are given from $R_C = 500$ (highest values of J) to $R = 1000$ (lowest values of J) in steps of 50 while we display only $J(R, x)$ in the right panel. We compare our moment/ray equation solutions (solid line) with the corresponding Monte Carlo solution (dashed line) and the analytic solution in the Eddington approximation (dotted line).

equation solution is the more accurate of the two as the analytic solution is an exact solution within the Eddington approximation only in the limit $(a\tau_0)^{1/3} \gg 1$.

5.3.2 Reproduction of Monte Carlo Solution

A numerical solution can be constructed by solving the moment equations, using Eddington factors determined from solving the ray equations, as described in section 5.2.1. We note that when solving the ray equations in a static medium, the ‘ δ ’ coefficients reduce to zero and consequently the U , V and H matrices are identically zero. As a result, Equations (5.45) and (5.46) reduce to $\mathbf{u}_k = \mathbf{T}_k^{-1} \mathbf{X}_k$ and $\mathbf{v}_k = \mathbf{G}_k \mathbf{u}_k$, respectively, and no initial condition in frequency is necessary.

The Monte Carlo solutions obtained in section 4.5 do not assume the Eddington approximation as in the analytic solution of Dijkstra et al. [2006], and thus we compare them with our moment/ray equation solutions in Figure 5.3. While the analytic solution only agrees closely with the Monte Carlo solution in the high optical depth case, we find that our ray/moment equation solutions agree for both optical depths. As the

ray/moment solution in the optically thick case looks largely identical at interior radii to the analytic and Monte Carlo solutions seen in Figure 4.6, we have only plotted the radiation field at the outer boundary $J(R, x)$; clearly the ray/moment solution is more accurate than the analytic solution here. We incurred no significant alterations to our ray/moment solutions upon re-solving the ray and moment equations with an estimated source function obtained from the moment solution, suggesting that for this problem the combined method converges in a single iteration.

5.3.3 Source Function Coefficients using R_{II}

We examine the validity of the representation of the source function for type II redistribution using the diffusion approximation in the form of Eq. (5.102). The mean intensity at a given radius $J(x, r_d)$ is expanded in a basis of cubic splines $\{\psi_k\}$, as described by Adams et al. [1971]:

$$J(x, r_d) \rightarrow \sum_{k=1}^{NF} J(x_k, r_d) \psi_k(x), \quad \psi_k(x_{k'}) = \delta_{k,k'} \quad (5.103)$$

where we have repeated the strategy used to obtain solutions for a homogeneous system described in section 3.5. We use a direct representation of the scattering integral, as opposed to the expansion used in the diffusion approximation, to write:

$$\begin{aligned} S(x_k, r_d) &= \frac{1}{\phi(x_k)} \int J(x', r_d) R(x', x_k) dx' \\ &= \frac{1}{\phi(x_k)} \sum_{k'=1}^{NF} J(x_{k'}, r_d) \left[\int R(x', x_k) \psi_{k'}(x') dx' \right]. \end{aligned} \quad (5.104)$$

Thus from comparison with the representation of the source function used in solving the moment equations, $S_{k,d} = \sum_{k'} \mathcal{R}_{k',k} J(x_{k'}, r_d)$, we obtain:

$$\mathcal{R}_{k',k} = \frac{1}{\phi(x_k)} \int R(x', x_k) \psi_{k'}(x') dx'. \quad (5.105)$$

We can construct the splines $\psi_{k'}$ by standard methods and then calculate the coefficients $\mathcal{R}_{k',k}$ by integration. We have followed this treatment in the lower optical depth example problems presented in this section and found the results to match those obtained using the diffusion approximation almost exactly. As such we recommend the use of the easily computed form given by Eq. (5.102) or its variable-temperature generalisation.

5.4 Test Problem: Homogeneous Expanding Universe (II)

In this section we apply the methods for solving the ray and moment equations to the problem looked at by Loeb and Rybicki [1999] and described previously in section 2.8.3, the case of coherent scattering of photons from a monochromatic Ly α point source in the homogeneous expanding universe. Loeb and Rybicki obtained an approximate analytic solution and an exact Monte Carlo solution for the mean intensity, and in section 4.6 we extended their analysis to determine the corresponding flux.

We work in Loeb and Rybicki's dimensionless units of frequency, radius and intensity, given by $\tilde{\nu} = \nu/\nu_*$, $\tilde{r} = r/r_*$ and $\tilde{J} = J_\nu/I_*$ where ν_* , r_* and I_* are as defined in section 2.8.3. We take our grid in radius to be spaced logarithmically from $\tilde{R}_C$ to $\tilde{R}$; anticipating output of the form displayed in Figure 2.8, we take $\tilde{R}_C = 10^{-3}$ and $\tilde{R} = 100$. The outer boundary condition results from assuming no photons are scattered back into the system from $\tilde{r} \geq \tilde{R}$ - this is technically not guaranteed to apply in an infinite scattering medium, but we expect no significant effect on the solution at interior radii.

Our frequency grid is subject to the restriction that the highest frequency (and therefore smallest value of $\tilde{\nu}$) lies bluewards of any frequency at which there are photons, in order to ensure compatibility with the frequency initial condition (see section 5.1.2). As the source in this problem generates photons at $\tilde{r} = 0$ with frequency $\tilde{\nu} = 0$, we can see that any photons observed at the radius $\tilde{r}$ will have redshifted to $\tilde{\nu} \geq \tilde{r}$. Thus we need only ensure $\tilde{\nu}_1 < \tilde{R}_C$. We take a logarithmically spaced grid spanning the range from $\tilde{\nu}_1 = 10^{-3.5}$ to $\tilde{\nu}_{\text{NF}} = 10^{1.5}$.

The problem assumes a zero-temperature medium that provides no Doppler broadening of the Ly α line, giving a Lorentz profile for the opacity which is written in the wing form $\tilde{\chi} = r_*\chi_\nu = 1/\tilde{\nu}^2$. The frequency redistribution results in coherent scattering and the source function is simply $S_\nu(r) = J_\nu(r)$. Referring to Eq. (5.78) we see that we can write the redistribution coefficients for coherent scattering as follows:

$$S_{k,d} = \sum_{k'} \mathcal{R}_{k',k} J_{k',d} = J_{k,d} \implies \mathcal{R}_{k',k} = \delta_{k',k}. \quad (5.106)$$

When estimating the source function in order to solve the ray equations it is sufficient to take $S_{k,d} = J_{k,d}$ and assume the analytic solution Eq. (2.86).

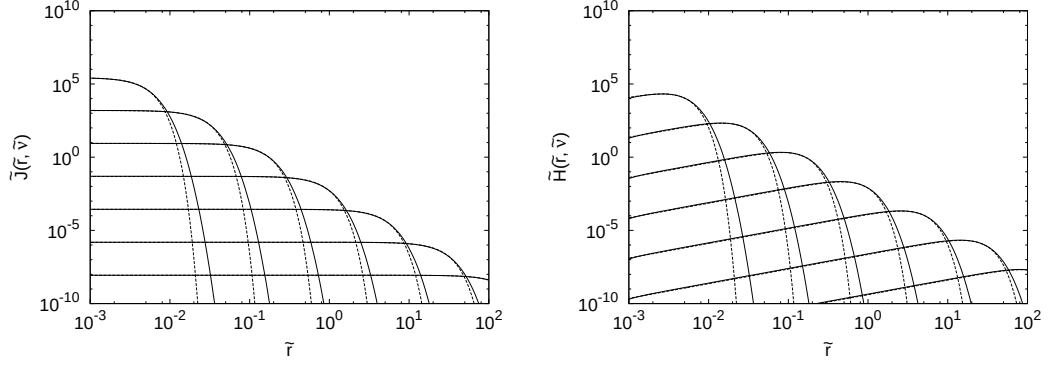


Figure 5.4: Plots of our solutions for $\tilde{J}(\tilde{r}, \tilde{\nu})$ (left panel) and $\tilde{H}(\tilde{r}, \tilde{\nu})$ (right panel) from the moment equations in the diffusion regime (solid lines) together with the analytic diffusion solutions (dashed lines). Profiles are given for $\log \tilde{\nu} = -1.5, -1.0, -0.5, 0.0, 0.5, 1.0, 1.5$ in order of decreasing values of $\tilde{J}/\tilde{H}$.

5.4.1 Reproduction of Analytic Solution

A useful test of the moment equation solution method developed in section 5.2 is provided by the Loeb and Rybicki's analytic solution for $\tilde{J}$, Eq. (2.86), together with the corresponding flux Eq. (4.39). These analytic expressions apply in the diffusion regime where the Eddington approximation is used, and the frequency derivative of the flux in Eq. (5.48) is assumed to be negligible. The former point requires that we write $f_\nu(r) \equiv 1/3^1$, while the latter is enforced in the moment equations by setting all ‘ ω ’ and ‘ θ ’ coefficients to zero with the further consequence that $\psi_{k',k,d+1/2} \rightarrow \delta_{k',k}$ from Eq. (5.73). In addition, we adopt Eq. (4.39) for the flux at the core boundary and at the outer boundary we specify $h(\tilde{\nu}) \equiv H(\tilde{R}, \tilde{\nu})/J(\tilde{R}, \tilde{\nu}) = 3\tilde{R}/(2\tilde{\nu})$ using the analytic solutions. We have obtained solutions of the moment equations for $\tilde{J}$ and $\tilde{H}$; these are given in Figure 5.4 and are seen to agree very well with the analytic solutions.

5.4.2 Reproduction of Monte Carlo Solution

A more comprehensive example of the utility of the combined ray and moment equation solution method is provided by seeking an exact solution of the homogeneous expanding

¹We note that as the velocity law is linear, clearly $\beta \equiv 1$ and the moment equations are independent of $g_\nu(r)$.

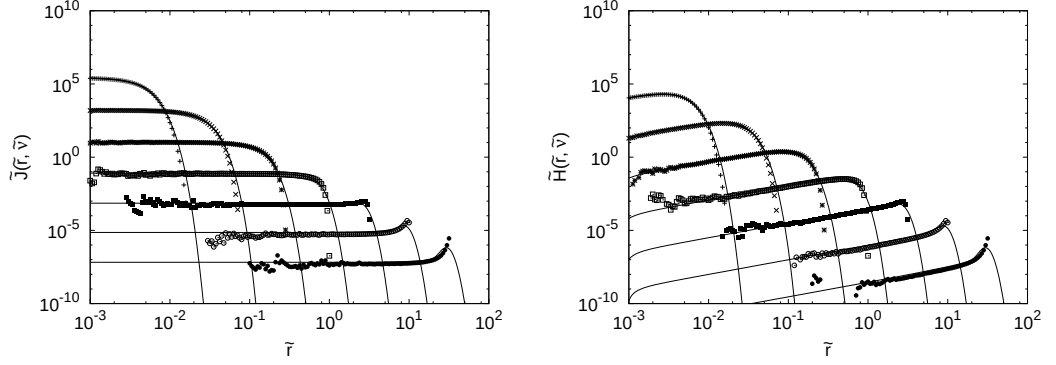


Figure 5.5: Plots of $\tilde{J}(\tilde{r}, \tilde{\nu})$ (left panel) and $\tilde{H}(\tilde{r}, \tilde{\nu})$ (right panel) obtained from 2 iterations of the combined moment/ray method with a diffusion solution inner boundary condition (solid lines), compared with the respective Monte Carlo solutions (various points). Profiles are given for $\log \tilde{\nu} = -1.5, -1.0, -0.5, 0.0, 0.5, 1.0, 1.5$ in order of decreasing values of $\tilde{J}/\tilde{H}$.

medium problem and comparing our results with the Monte Carlo solutions obtained in section 4.6. We take as an inner boundary condition the analytic solution Eq. (4.39); this is physically reasonable as the moment equations are expected to adhere to the diffusion limit at great depth. No coefficients are artificially altered as was required to reproduce the analytic solutions. In Figure 5.5 we show the results of the combined moment/ray equation solution strategy. Both the mean intensity and the flux are shown to closely match the corresponding solutions determined from the Monte Carlo method.

The solutions were obtained from 2 iterations: the moment solution, determined using Eddington factors from the ray solution, determines the source function estimate for a second ray solution, which determines the Eddington factors for a second moment solution. Upon further iterations we found that both methods had converged upon the same solution, independent of the initial estimate of the source function used in the first ray solution, as we tested by using a free streaming source function estimate of the form $\tilde{J} = \delta_D(\tilde{\nu} - \tilde{r})/(4\pi\tilde{r})^2$. We also solved the problem using this mechanism with a free streaming boundary condition of the form $\tilde{H} = \delta_D(\tilde{\nu} - \tilde{R}_C)/(4\pi\tilde{R}_C)^2$. Our results are displayed in Figure 5.6: we found solutions identical to those produced by the diffusion boundary condition with the exception of the flux at the boundary which is specified directly by the boundary condition.

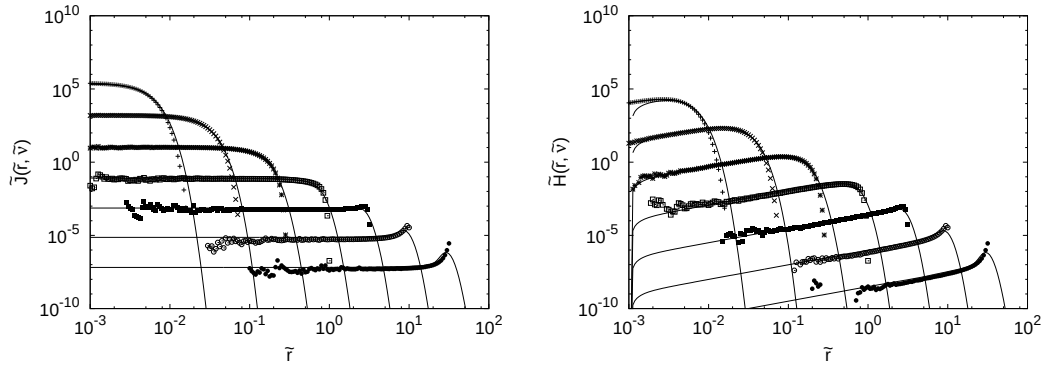


Figure 5.6: Plots of $\tilde{J}(\tilde{r}, \tilde{\nu})$ (left panel) and $\tilde{H}(\tilde{r}, \tilde{\nu})$ (right panel) obtained from 2 iterations of the combined moment/ray method with a free streaming solution inner boundary condition (solid lines), compared with the respective Monte Carlo solutions (various points). Profiles are given for $\log \tilde{\nu} = -1.5, -1.0, -0.5, 0.0, 0.5, 1.0, 1.5$ in order of decreasing values of $\tilde{J}/\tilde{H}$.

5.5 Discussion

We have described in detail methods developed to solve the radiative transfer problem using systems of ray/angular moment equations derived from the transfer equation in a spherically symmetric medium. Our implementation of these methods has borrowed heavily from previous authors (Mihalas et al. [1975], Mihalas et al. [1976]), but as previous applications have been concerned with the more specific problem of a stellar atmosphere we have had to generalise some aspects such as the particular form of the boundary conditions. We used an iterative implementation of these methods to obtain test problem solutions that agreed with our Monte Carlo solutions described in the last chapter. We also obtained an efficient prescription for the representation of the source function in Ly α scattering based on the diffusion approximation.

The use of the moment and ray equations to solve spherically symmetric problems was found to have many advantages over Monte Carlo methods. In cases where many photon scatterings must be tracked to obtain a Monte Carlo solution, we found the ray and moment solution methods significantly more efficient. These methods also produce solutions that are free of statistical noise, and they can examine idealised regimes such as the Eddington approximation that cannot be physically enforced using Monte Carlo

methods. While it is necessary to assume an inner boundary condition for the medium, we expect the final solution will be largely independent of the exact form of the boundary condition as long as it is physically representative of the same source.

A possible problem with the use of the ray and moment equation methods is the restriction on the properties of the velocity profile of the medium, namely that it is positive and monotonically increasing. The methods can be adapted to treat a negative velocity that is monotonically decreasing by working with a frequency grid extending bluewards from an initial condition at some minimum frequency redward of line centre, but a more general velocity profile would require a more complicated treatment. Additionally the inner boundary must be taken to enclose the source and thus problems with e.g. spatially uniform Ly α photon creation are excluded from solution by this approach. The greatest constraint on the applicability of this approach, however, is the restriction to spherical symmetry; while we have not described an extension of the Monte Carlo methods to more general geometries, such an extension is possible unlike in the moment/ray solution method.

In the next chapter we will apply the moment/ray and Monte Carlo methods to an idealised spherically symmetric model of an isolated continuum source in a homogeneous expanding IGM prior to reionisation, where we will find that the moment/ray method is a powerful tool with which to investigate the effect on the Ly α scattering rate of various redistribution types and different velocity and density profiles.

CHAPTER 6

Continuum Source in the Spherically Symmetric IGM

In this chapter we apply the methods described and tested in Chapters 4 and 5 to a model of the Ly α scattering in the IGM induced by the first sources. We examine the case of a continuum source with a spectrum that is flat across the frequency range that interacts with the Ly α line, and focus on a homogeneous expanding scattering medium.

- We derive an analytic solution for the problem based on the solution of Loeb and Rybicki [1999] for a monochromatic Ly α point source, valid for coherent scattering in the wings of the line in the diffusion regime, which predicts an $r^{-7/3}$ dependence in the scattering rate profile as found numerically by other authors.
- We compare our analytic solution with numerical solutions obtained using the moment/ray and Monte Carlo methods. We find effects on the Ly α scattering rate profile arising from the maximum source frequency and the form of redistribution assumed. Finally, we extend our analysis to examine test cases with different density and velocity profiles.

6.1 Radiative Transfer Equation

We consider the problem of Ly α scattering induced by a point source of UV photons in the neutral hydrogen intergalactic medium at high redshift, prior to the large-scale onset of reionisation. It is assumed that the scattering medium can be treated as spherically symmetric. For a scattering medium with a radial velocity $V(r)$, the equation of radiative transfer is written:

$$\begin{aligned} \mu \frac{\partial I_\nu(r, \mu)}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial I_\nu(r, \mu)}{\partial \mu} - (\nu_0/c) \frac{V}{r} \left[1 - \mu^2 + \mu^2 \left(\frac{d \ln V}{d \ln r} \right) \right] \frac{\partial I_\nu(r, \mu)}{\partial \nu} \\ = -\chi_\nu(r) I_\nu(r, \mu) + \eta_\nu(r) + S(\nu, r). \end{aligned} \quad (6.1)$$

The opacity $\chi_\nu(r)$ and emissivity $\eta_\nu(r)$ for resonance-line scattering are given by Equations (2.25) and (2.26) respectively; both quantities are proportional to the scattering medium density $n_I(r)$. The source is assumed to have a continuum emission spectrum that is approximately flat in frequency around the Ly α line. Mathematically we represent the source's Ly α emissivity as:

$$S(\nu, r) = \dot{N}_\nu \frac{\delta(r)}{(4\pi r)^2} \quad (6.2)$$

where the constant $\dot{N}_\nu$ is the rate of emission of photons per unit frequency. The source term is analogous to that given in Eq. (2.85) for a monochromatic point source emitting $\dot{N}_\alpha$ photons per second at the Ly α frequency, assumed in the problem studied by Loeb and Rybicki [1999].

Loeb and Rybicki considered the problem in the case of the homogeneous expanding medium at redshift z , where the scattering medium density is just the uniform neutral hydrogen density, $n_I = n_{\text{HI}}(z)$, and the radial velocity is given by the Hubble-flow $V(r) = H(z)r = (c/\nu_0)\alpha r$, where $\alpha \equiv (\nu_0/c)H(z)$. They made approximations corresponding to a zero temperature medium, namely that photons are (a) absorbed in the Lorentz wing with opacity $\chi_\nu = \beta(\nu - \nu_0)^{-2}$, where $\beta \equiv n_{\text{HI}}(z)\sigma\Gamma_\alpha/(4\pi^2)$, and (b) scattered coherently with emissivity $\eta_\nu = \chi_\nu J_\nu$. They defined the characteristic frequency ν_* such that the optical depth from the source to infinity for a photon of initial frequency ν_* redwards of line centre is unity:

$$\tau = \int_0^\infty \frac{\beta}{(\nu_* + \alpha r)^2} dr = \int_{\nu_*}^\infty \frac{\beta}{\alpha t^2} dt = \frac{\beta}{\alpha \nu_*} = 1 \quad (6.3)$$

and thus

$$\begin{aligned}\nu_* &\equiv \frac{\beta}{\alpha} = \frac{\sigma\Gamma_\alpha\lambda_\alpha n_{\text{HI}}(z)}{4\pi^2 H(z)} \simeq \frac{\sigma\Gamma_\alpha\lambda_\alpha n_{\text{HI}}(0)}{4\pi^2 \Omega_{\text{m}}^{1/2} H_0} (1+z)^{3/2} \\ &\simeq 5.52 \times 10^{12} \left[\frac{\Omega_{\text{b}} h}{\Omega_{\text{m}}^{1/2}} \right] (1+z)^{3/2} \text{ Hz}\end{aligned}\quad (6.4)$$

where we have used $n_{\text{HI}}(z) \simeq n_{\text{H}}(z) = n_{\text{H}}(0)(1+z)^3$ for a neutral IGM and $H(z) = H_0 \Omega_{\text{m}}^{1/2} (1+z)^{3/2}$ as the universe is matter-dominated at the redshifts of interest. Loeb and Rybicki defined the characteristic radius r_* as the radius at which a photon free streaming from the source redshifts from ν_0 to $(\nu_0 - \nu_*)$, i.e. $\alpha r_* = \nu_*$:

$$\begin{aligned}r_* &\equiv \frac{\nu_*}{\alpha} = \frac{\sigma\Gamma_\alpha\lambda_\alpha^2 n_{\text{HI}}(z)}{4\pi^2 H^2(z)} \simeq \frac{\sigma\Gamma_\alpha\lambda_\alpha^2 n_{\text{HI}}(0)}{4\pi^2 \Omega_{\text{m}} H_0^2} \\ &\simeq 6.72 \left[\frac{\Omega_{\text{b}}}{\Omega_{\text{m}}} \right] \text{ Mpc}.\end{aligned}\quad (6.5)$$

We seek to rewrite Eq. (6.1) in a dimensionless form using the frequency and radius variables of Loeb and Rybicki given by $\tilde{\nu} = (\nu_0 - \nu)/\nu_*$ and $\tilde{r} = r/r_*$. We define a dimensionless radiation intensity $\tilde{I} = I_\nu/I_*$ or $\tilde{J} = J_\nu/I_*$, where I_* is chosen to ensure the magnitude of the source is factored out of the equation. This is achieved by taking $I_* = \dot{N}_\nu/r_*^2$ and consequently the transfer equation can be written in the dimensionless form:

$$\begin{aligned}\mu \frac{\partial \tilde{I}}{\partial \tilde{r}} + \frac{1-\mu^2}{\tilde{r}} \frac{\partial \tilde{I}}{\partial \mu} + \tilde{\alpha} \left[1 - \mu^2 + \mu^2 \left(\frac{d \ln V}{d \ln r} \right) \right] \frac{\partial \tilde{I}}{\partial \tilde{\nu}} \\ = -\tilde{\chi} \tilde{I} + \tilde{\eta} + \frac{\delta(\tilde{r})}{(4\pi \tilde{r})^2}\end{aligned}\quad (6.6)$$

where $\tilde{\alpha} \equiv V/[H(z)r]$, $\tilde{\chi} \equiv r_*\chi_\nu$ and $\tilde{\eta} \equiv (r_*/I_*)\eta_\nu$. The angular moment equations obtained from Eq. (6.6) are:

$$\frac{1}{\tilde{r}^2} \frac{\partial(\tilde{r}^2 \tilde{H})}{\partial \tilde{r}} + \tilde{\alpha} \left[\frac{\partial(\tilde{J} - \tilde{K})}{\partial \tilde{\nu}} + \left(\frac{d \ln V}{d \ln r} \right) \frac{\partial \tilde{K}}{\partial \tilde{\nu}} \right] = -\tilde{\chi} \tilde{J} + \tilde{\eta} + \frac{\delta(\tilde{r})}{(4\pi \tilde{r})^2}, \quad (6.7)$$

$$\frac{\partial \tilde{K}}{\partial \tilde{r}} + \frac{3\tilde{K} - \tilde{J}}{\tilde{r}} + \tilde{\alpha} \left[\frac{\partial(\tilde{H} - \tilde{N})}{\partial \tilde{\nu}} + \left(\frac{d \ln V}{d \ln r} \right) \frac{\partial \tilde{N}}{\partial \tilde{\nu}} \right] = -\tilde{\chi} \tilde{H}, \quad (6.8)$$

where $\tilde{H}$, $\tilde{K}$ and $\tilde{N}$ are the higher order angular moments defined in section 5.2 and divided by I_* . A normalisation condition for solving the problem by Monte Carlo

methods is obtained by an appropriate integral constraint form of the zeroth-order moment equation. If we multiply Eq. (6.7) by $\tilde{r}^2$, integrate in radius from $\tilde{r} = 0$ to $\tilde{R}$, and integrate in frequency from $\tilde{\nu} = -\tilde{\nu}_{\max}$ to $+\tilde{\nu}_{\max}$, we obtain:

$$\tilde{R}^2 \int_{-\tilde{\nu}_{\max}}^{\tilde{\nu}_{\max}} \tilde{H} \Big|_{\tilde{R}} d\tilde{\nu} + \int_0^{\tilde{R}} \tilde{\alpha} \tilde{r}^2 \left[\tilde{J} + \left(\frac{d \ln V}{d \ln r} - 1 \right) \tilde{K} \right]_{-\tilde{\nu}_{\max}}^{\tilde{\nu}_{\max}} d\tilde{r} = \frac{2\tilde{\nu}_{\max}}{(4\pi)^2}, \quad (6.9)$$

where upon integrating the equation in frequency across the line centre the sum of terms $-\tilde{\chi}\tilde{J}$ and $\tilde{\eta}$ reduces to zero.

For realistic problems the properties of the local scattering medium should approach those of the homogeneous expanding medium at large r , i.e. $\tilde{\alpha} \rightarrow 1$ and $n_{\text{I}}(r) \rightarrow n_{\text{HI}}(z)$. Note that for a zero-temperature homogeneous expanding medium the dimensionless equations given reduce to the equations examined by Loeb and Rybicki, with the exception of the source for which they have the same point source term multiplied by $\delta(\tilde{\nu})$ which results from scaling intensities by $I'_* = \dot{N}_\alpha/(r_*^2\nu_*)$ in their problem.

6.2 Homogeneous Expanding Medium

In this section we focus on the Ly α scattering induced by a spectrally flat point source in the high- z homogeneous expanding medium with uniform density $n_{\text{I}} = n_{\text{HI}}(z)$ and linear velocity profile $V(r) = H(z)r$. We will first attempt to solve an idealised version of the problem analytically using an analogous treatment to that of Loeb and Rybicki [1999] for a monochromatic point source, before solving the problem numerically with the various simplifying assumptions removed using the Monte Carlo and moment/ray equation methods.

6.2.1 Analytic Treatment

We seek a solution in the same zero-temperature limit examined by Loeb and Rybicki i.e. coherent scattering using the Lorentz wing form of the opacity, $\tilde{\chi} = 1/\tilde{\nu}^2$ and $\tilde{\eta} = \tilde{\chi}\tilde{J}$. For ease of reference in comparing our problem to that solved by Loeb and Rybicki we will write the source term in the transfer equation with a general frequency dependence given by the function $f(\tilde{\nu})$, i.e. $\delta(\tilde{r})/(4\pi\tilde{r})^2 \rightarrow f(\tilde{\nu})\delta(\tilde{r})/(4\pi\tilde{r})^2$, where it is

clear that the problem of a source with a flat spectrum is recovered by taking $f(\tilde{\nu}) \equiv 1$. Equations (6.7) and (6.8) then give:

$$\frac{1}{\tilde{r}^2} \frac{\partial(\tilde{r}^2 \tilde{H})}{\partial \tilde{r}} + \frac{\partial \tilde{J}}{\partial \tilde{\nu}} = f(\tilde{\nu}) \frac{\delta(\tilde{r})}{(4\pi \tilde{r})^2}, \quad (6.10)$$

$$\frac{\partial \tilde{K}}{\partial \tilde{r}} + \frac{3\tilde{K} - \tilde{J}}{\tilde{r}} + \frac{\partial \tilde{H}}{\partial \tilde{\nu}} = -\frac{\tilde{H}}{\tilde{\nu}^2}. \quad (6.11)$$

The moment equations can be simplified further by assuming the diffusion limit, for which we neglect the $\partial \tilde{H} / \partial \tilde{\nu}$ term and assume the Eddington approximation $\tilde{K} = \tilde{J}/3$ with the result that Eq. (6.11) reduces to $\tilde{H} = -(\tilde{\nu}^2/3) \partial \tilde{J} / \partial \tilde{r}$. The main advantage of assuming the diffusion regime is in the reduction of the system of moment equations to a single equation for $\tilde{J}$, obtained by substituting the diffusion relation between $\tilde{H}$ and $\tilde{J}$ to eliminate $\tilde{H}$ from Eq. (6.10); if we do this and change frequency variable to $\sigma = \tilde{\nu}^3/9$ we obtain:

$$\frac{\partial \tilde{J}}{\partial \sigma} - \frac{1}{\tilde{r}^2} \frac{\partial}{\partial \tilde{r}} \left(\tilde{r}^2 \frac{\partial \tilde{J}}{\partial \tilde{r}} \right) = \frac{\delta(\tilde{r})}{(4\pi \tilde{r})^2} \times \frac{f(\sigma)}{(3\sigma^2)^{1/3}}, \quad (6.12)$$

where we have multiplied by the factor $d\tilde{\nu}/d\sigma = (3\sigma^2)^{-1/3}$.

We use a Green's function approach to solve Eq. (6.12) by first considering a monochromatic source emitting at a single frequency $\tilde{\nu}_s$ with $f(\tilde{\nu}) = \delta(\tilde{\nu} - \tilde{\nu}_s) = (3\sigma^2)^{1/3} \delta(\sigma - \sigma_s)$ where $\sigma_s = \tilde{\nu}_s^3/9$. We label the solution as $\tilde{G}(\tilde{r}, \sigma, \sigma_s)$. The Green's function satisfies:

$$\frac{\partial \tilde{G}}{\partial \sigma} - \frac{1}{\tilde{r}^2} \frac{\partial}{\partial \tilde{r}} \left(\tilde{r}^2 \frac{\partial \tilde{G}}{\partial \tilde{r}} \right) = \frac{\delta(\tilde{r})}{(4\pi \tilde{r})^2} \times \delta(\sigma - \sigma_s), \quad (6.13)$$

and if we solve for $\tilde{G}$, the solution to the problem for a source of general frequency dependence satisfying Eq. (6.12) is given by:

$$\tilde{J}(\tilde{r}, \sigma) = \int_{-\infty}^{\infty} \tilde{G}(\tilde{r}, \sigma, \sigma_s) \frac{f(\sigma_s)}{(3\sigma_s^2)^{1/3}} d\sigma_s. \quad (6.14)$$

Loeb and Rybicki examined the case of a point source emitting only at the Lyman-alpha frequency itself ($\sigma_s = 0$) for which Eq. (6.13) reduces to the diffusion equation in 3 dimensions with σ acting as the time variable, given a point source impulse at $\sigma = 0$, with a solution given by their equation (21). The solution satisfies Eq. (6.13) with the

substitution $\sigma \rightarrow \sigma - \sigma_s$. Thus the Green's function is given by the 3D diffusion solution for a point source impulse at $\sigma = \sigma_s$:

$$\tilde{G}(\tilde{r}, \sigma - \sigma_s) = \frac{1}{4\pi} \left\{ \frac{1}{4\pi(\sigma - \sigma_s)} \right\}^{3/2} \exp \left[-\frac{\tilde{r}^2}{4(\sigma - \sigma_s)} \right], \quad (\sigma > \sigma_s) \quad (6.15)$$

where the factor $1/(4\pi)$ ensures normalisation. Clearly $\tilde{G}(\tilde{r}, \sigma - \sigma_s) = 0$ for $\sigma < \sigma_s$ as photons can only move in frequency space by redshifting.

We now return to the case of a flat source spectrum as an approximation to the spectrum of a continuum source in the IGM. We specify a blue cutoff frequency $\tilde{\nu}_m < 0$, the maximum frequency (or minimum value of $\tilde{\nu}$) at which the source emits photons capable of interacting with the Ly α line, giving a step-function form for the source frequency distribution:

$$f(\sigma) = \Theta(\sigma - \sigma_m) \equiv \begin{cases} 1 & ; \sigma > \sigma_m \\ 0 & ; \sigma \leq \sigma_m \end{cases}, \quad (6.16)$$

where $\sigma_m = \tilde{\nu}_m^3/9$. We use the Green's function and the source frequency distribution to obtain the solution according to Eq. (6.14), valid for $\sigma > \sigma_m$:

$$\begin{aligned} \tilde{J}(\tilde{r}, \sigma) &= \frac{1}{3^{1/3}} \int_{\sigma_m}^{\sigma} \sigma_s^{-2/3} \tilde{G}(\tilde{r}, \sigma - \sigma_s) d\sigma_s \\ &= \frac{1}{3^{1/3}(4\pi)^{5/2}} \int_{\sigma_m}^{\sigma} \frac{1}{\sigma_s^{2/3}(\sigma - \sigma_s)^{3/2}} \exp \left[-\frac{\tilde{r}^2}{4(\sigma - \sigma_s)} \right] d\sigma_s, \end{aligned} \quad (6.17)$$

$$\begin{aligned} \tilde{H}(\tilde{r}, \sigma) &= -\frac{\tilde{\nu}^2}{3^{4/3}} \frac{\partial}{\partial \tilde{r}} \int_{\sigma_m}^{\sigma} \sigma_s^{-2/3} \tilde{G}(\tilde{r}, \sigma - \sigma_s) d\sigma_s \\ &= \frac{\sigma^{2/3} \tilde{r}}{2(4\pi)^{5/2}} \int_{\sigma_m}^{\sigma} \frac{1}{\sigma_s^{2/3}(\sigma - \sigma_s)^{5/2}} \exp \left[-\frac{\tilde{r}^2}{4(\sigma - \sigma_s)} \right] d\sigma_s. \end{aligned} \quad (6.18)$$

We rewrite these analytic solutions with the change of variable $t = 9\tilde{r}^2/[4(\tilde{\nu}^3 - \tilde{\nu}_s^3)]$:

$$\tilde{J}(\tilde{r}, \tilde{\nu}) = \frac{2}{3^{1/3}(4\pi)^{5/2} \tilde{r}} \int_{\frac{9\tilde{r}^2}{4(\tilde{\nu}^3 - \tilde{\nu}_m^3)}}^{\infty} \left[\frac{\tilde{\nu}^3}{9} - \frac{\tilde{r}^2}{4t} \right]^{-2/3} t^{-1/2} e^{-t} dt, \quad (6.19)$$

$$\tilde{H}(\tilde{r}, \tilde{\nu}) = \frac{4\tilde{\nu}^2}{3^{4/3}(4\pi)^{5/2} \tilde{r}^2} \int_{\frac{9\tilde{r}^2}{4(\tilde{\nu}^3 - \tilde{\nu}_m^3)}}^{\infty} \left[\frac{\tilde{\nu}^3}{9} - \frac{\tilde{r}^2}{4t} \right]^{-2/3} t^{1/2} e^{-t} dt. \quad (6.20)$$

Note that in the case of a spectrally flat source with no blue cutoff frequency, we can take $\tilde{\nu}_m \rightarrow -\infty$ and the lower limit in each integral reduces to zero.

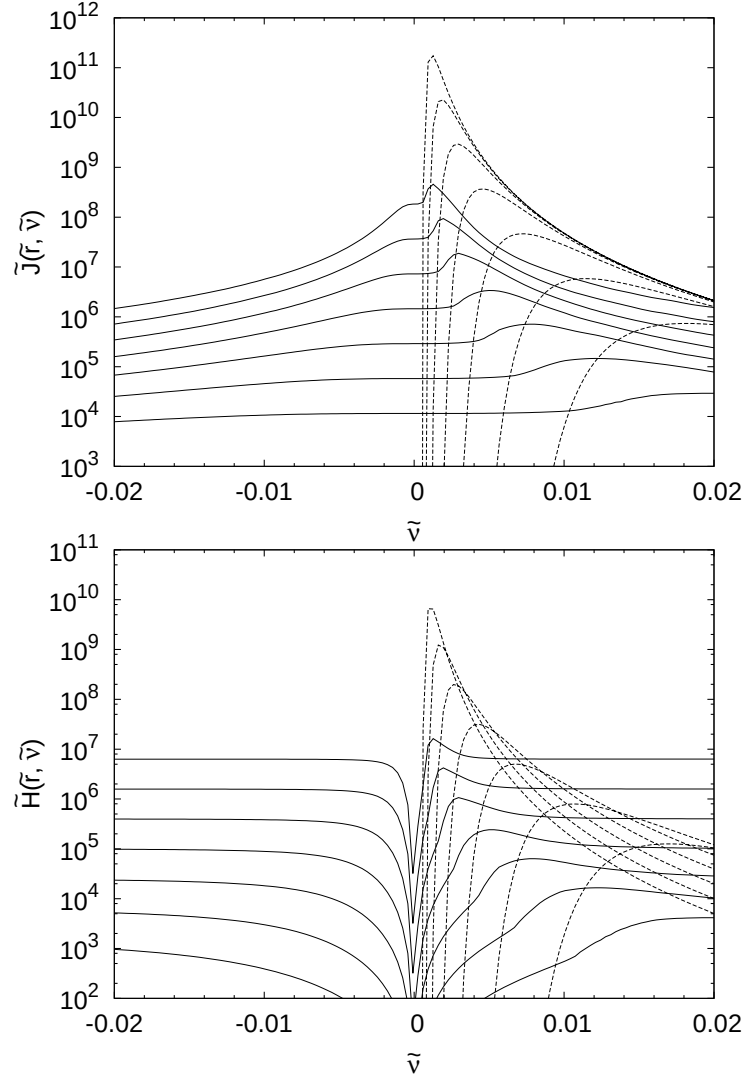


Figure 6.1: Analytic solution for $\tilde{J}$ (upper panel) and $\tilde{H}$ (lower panel) for a spectrally flat source in a homogeneous expanding medium in the zero-temperature diffusion regime (solid lines), together with the corresponding analytic solution of Loeb and Rybicki for a monochromatic Ly α source (dashed lines). Values of $\tilde{r}$ are given by $10^{-4.5}$, $10^{-4.2}$, $10^{-3.9}$, $10^{-3.6}$, $10^{-3.3}$, $10^{-3.0}$, $10^{-2.7}$ in order of decreasing $\tilde{J}$ or $\tilde{H}$.

We have evaluated our analytic solutions for $\tilde{J}$ and $\tilde{H}$ by numerical integration and plotted them as a series of frequency profiles in Figure 6.1; we found some numerical artefacts resulting from the integration which we have interpolated over for the purpose of presentation. We find a peak in both the mean intensity and the flux that

drifts redwards further from the source, corresponding to the contribution from photons emitted by the source at the line centre. This is seen from a comparison of the peak frequency with that found from the analytic solutions for $\tilde{J}$ and $\tilde{H}$ for a monochromatic Ly α source, given by Equations (2.86) and (4.39). By solving $\partial\tilde{J}/\partial\tilde{\nu} = 0$ for the analytic solution of Loeb and Rybicki, we find the frequency of the peak satisfies $\tilde{\nu} = (3/2)^{1/3}\tilde{r}^{2/3}$. For $\tilde{\nu} \neq 0$, it is possible to extract a factor $[\tilde{\nu}^3]^{-2/3} = \tilde{\nu}^{-2}$ from the square brackets in each of the Equations (6.19) and (6.20), and we see that the solutions have the approximate scalings away from line centre $\tilde{J} \sim (\tilde{\nu})^{-2}(\tilde{r})^{-1}$ and $\tilde{H} \sim (\tilde{r})^{-2}$. The scalings with frequency are apparent far from the line centre in Figure 6.1.

The most physically relevant aspect of the solution for the Ly α photon spectrum is the scattering rate. We can see from the upper panel of Figure 6.1 that for radii exceeding some minimum distance from the source, $\tilde{J}(\tilde{\nu})$ is approximately flat across the line centre. In this case the scattering rate varies as the average intensity at line centre, i.e.

$$P_\alpha \equiv 4\pi\sigma \int J_\nu(r)\varphi(\nu) d\nu \simeq 4\pi\sigma I_* \tilde{J}(\tilde{r}, 0) \quad (6.21)$$

where

$$\tilde{J}(\tilde{r}, 0) = \frac{2^{7/3}}{3^{1/3}(4\pi)^{5/2}\tilde{r}^{7/3}} \int_{\frac{9\tilde{r}^2}{4|\tilde{\nu}_m|^3}}^{\infty} t^{1/6} e^{-t} dt \quad (6.22)$$

$$= \frac{2^{7/3}}{3^{1/3}(4\pi)^{5/2}\tilde{r}^{7/3}} \times \Gamma\left(\frac{7}{6}, \frac{9\tilde{r}^2}{4|\tilde{\nu}_m|^3}\right), \quad (6.23)$$

and we have used the definition of the upper incomplete Gamma function $\Gamma(q, y) \equiv \int_y^\infty t^{q-1} e^{-t} dt$. This function saturates at the limiting value $\Gamma(7/6) \simeq 0.92$ for values of the argument $y \lesssim 10^{-2}$ or, for our problem, $\tilde{r} \lesssim 0.1 \times (2/3)|\tilde{\nu}_m|^{3/2}$. In this case we can describe the scattering rate $\tilde{P}_\alpha \equiv P_\alpha/P_*$, where $P_* \equiv 4\pi\sigma I_*$, by $\tilde{P}_\alpha^{\text{diff}}$:

$$\tilde{P}_\alpha^{\text{diff}} \equiv \frac{2^{7/3}\Gamma(7/6)}{3^{1/3}(4\pi)^{5/2}\tilde{r}^{7/3}}. \quad (6.24)$$

This form for the scattering rate applies for all $\tilde{r}$ if $|\sigma_m| \rightarrow \infty$ i.e. it applies in the absence of any cutoff in the source spectrum. For a finite $|\sigma_m|$ the effect of the cutoff is to suppress $\tilde{J}(\tilde{r}, 0)$ for sufficiently large $\tilde{r}$ - physically this corresponds to the redshifting past line centre of all photons at these radii.

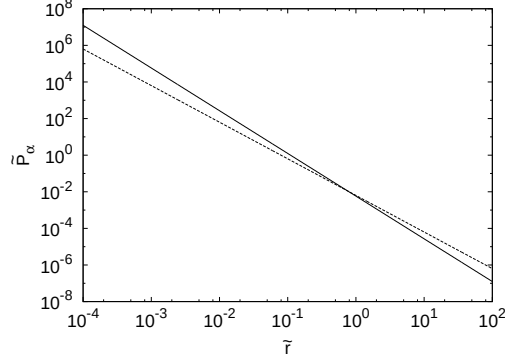


Figure 6.2: Scaled scattering rate from the diffusion solution for a flat source spectrum extending infinitely bluewards, $\tilde{P}_\alpha^{\text{diff}}$ (solid line) and the expected result in the corresponding free-streaming limit, $\tilde{P}_\alpha^{\text{free}}$ (dashed line).

A useful comparison can be made with the expected scattering rate in the free streaming limit. This is represented by the Equations (6.10) and (6.11) in the limit of zero opacity, $1/\tilde{\nu}^2 \rightarrow 0$, and a radially directed specific intensity, $\tilde{J} = \tilde{H} = \tilde{K}$, with the source term $f(\tilde{\nu}) = \Theta(\tilde{\nu} - \tilde{\nu}_m)$. The solution is $\tilde{J} = \Theta(\tilde{\nu} - \tilde{\nu}_m - \tilde{r})/(4\pi\tilde{r})^2$ and the corresponding scattering rate for sufficiently negative $\tilde{\nu}_m$ is simply:

$$\tilde{P}_\alpha^{\text{free}} \equiv \frac{1}{(4\pi\tilde{r})^2}. \quad (6.25)$$

We examine the radial dependence of the Ly α scattering rate induced around the source in Figure 6.2. The diffusion limit scattering rate exceeds the corresponding result in the free streaming limit close to the source; we expect the diffusion scattering rate to drop below the free streaming rate for $\tilde{r} \geq 2^7(\Gamma(7/6))^3/(3(4\pi)^{3/2}) \simeq 0.75$.

We can describe the size of the Ly α scattering region around the source by determining the maximum radius at which the scattering rate is non-zero. This radius will depend upon $\tilde{\nu}_m$, which we take to be the bluemoest frequency at which the source emits photons that are capable of redshifting into the Ly α line. Typically this cutoff will be the Lyman-beta frequency, $\nu_\beta = (32/27)\nu_\alpha$, as photons emitted bluewards of Lyman-beta redshift into the Lyman-beta or higher-energy resonance lines and do not produce Ly α photons (except for products of cascades which we do not consider here). Assuming a Ly α source term of the form of Eq. (6.16), we can say that the scattering

rate found in the diffusion limit given by Eq. (6.23) drops below one-tenth of its value in the absence of a cutoff when the second argument y of the upper incomplete Gamma function satisfies $y \geq f \simeq 2.5$, or:

$$\tilde{r} \geq (2/3)f^{1/2}|\tilde{\nu}_\beta|^{3/2} \simeq 1.05|\tilde{\nu}_\beta|^{3/2}. \quad (6.26)$$

Outside of the diffusion regime, an upper limit for the size of the Ly α scattering region is given by free streaming: all photons will have redshift past the line centre at radii $\tilde{r} > |\tilde{\nu}_\beta|$.

Our analytic solution in the zero-temperature diffusion regime for the Ly α spectrum around a continuum source gives a radial dependence for the scattering rate of the form $P_\alpha \propto r^{-7/3} \simeq r^{-2.3}$. This is the same result as that found by Chuzhoy and Zheng [2007], who determined the scattering rate produced by a source of UV photons subject to natural broadening and coherent scattering by a Monte Carlo method for both the continuum photons we consider and ‘injected photons’ from higher energy transitions. This result was also found to apply more generally by Semelin et al. [2007], who performed Monte Carlo radiative transfer simulations using the full Voigt function form of the absorption profile and type II frequency redistribution.

6.2.2 Numerical Treatment

In this section we examine the same problem of a source of continuum Ly α photons in the H I homogeneous expanding medium, although this time we use the Monte Carlo and moment/ray equation solution methods to remove the need to simplify the problem further. Note that outside of the zero-temperature regime looked at by Loeb and Rybicki for a monochromatic source, it becomes necessary to specify the temperature and density etc. of the scattering medium in formulating the problem. As such, we assume a redshift $z = 10$; using this value and the accepted values of the cosmological parameters given in Ch. 1, we find $\nu_* = 1.22 \times 10^{13}$ Hz, $r_* = 1.12$ Mpc, $n_{\text{H}}(z) = 246 \text{ m}^{-3}$ and $H(z) = 1330 \text{ km s}^{-1} \text{ Mpc}^{-1}$. The Sobolev parameter is $\gamma = \nu_\alpha H / (\sigma c n_{\text{H}}) \simeq 1.30 \times 10^{-6}$. If we also assume a temperature $T = 10$ K, we obtain $\Delta\nu_{\text{D}} = 3.35 \times 10^9$ Hz and a line-centre opacity $\kappa_0 = n_{\text{H}}\sigma / (\pi^{1/2}\Delta\nu_{\text{D}}) = 1.41 \times 10^9 \text{ Mpc}^{-1}$.

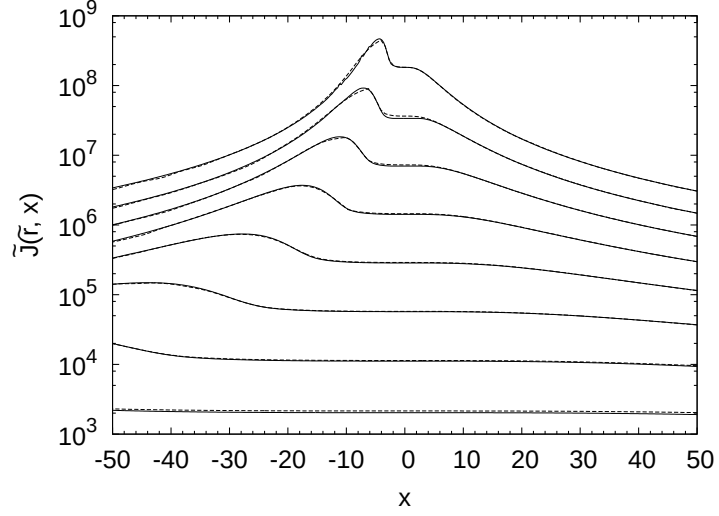


Figure 6.3: Diffusion regime moment solution for $\tilde{J}$ in a homogeneous expanding medium assuming coherent scattering and a Voigt line profile (solid line), together with the corresponding analytic solution in the wing approximation (dashed line). The frequency dependence is shown as a function of x assuming a temperature $T = 10$ K for values of $\tilde{r}$ given by $10^{-4.5}$, $10^{-4.2}$, $10^{-3.9}$, $10^{-3.6}$, $10^{-3.3}$, $10^{-3.0}$, $10^{-2.7}$, $10^{-2.4}$.

We expect that we would reproduce our analytic solutions by using them to define inner and outer boundary conditions for the moment equations in the diffusion regime, and solving the equations as described in section 5.2. The initial condition in frequency is enforced by taking $\tilde{\nu}_1 < \tilde{\nu}_m < 0$ i.e. the frequency grid must extend bluewards of the source emission cutoff frequency. Unless otherwise stated, we have taken $x_m = -(\nu_*/\Delta\nu_D)\tilde{\nu}_m = 1000$ for all solutions. In cases with large x_m , we take a frequency grid with small grid spacing across the line centre for x lying in the range $[-x_{\max}, x_{\max}]$ where e.g. $x_{\max} = 100$, and larger grid spacing across $[x_{\max}, x_1]$ where $x_1 > x_m$. We solve the moment equations with the addition of the full Voigt profile form for χ_ν with an opacity given by $\tilde{\chi} = \sqrt{\pi}r_*\kappa_0\phi_V(x)$. The diffusion limit is enforced by setting $f_\nu(r) = 1/3$ and all ‘ ω ’ and ‘ θ ’ coefficients equal to zero as in section 5.4.1. Our moment solution for $\tilde{J}$ is given in Figure 6.3; it is seen to be coincident with the analytic solution, indicating that the assumption of the wing form of the opacity does not affect the solution in this regime. A similarly identical solution was found for the flux.

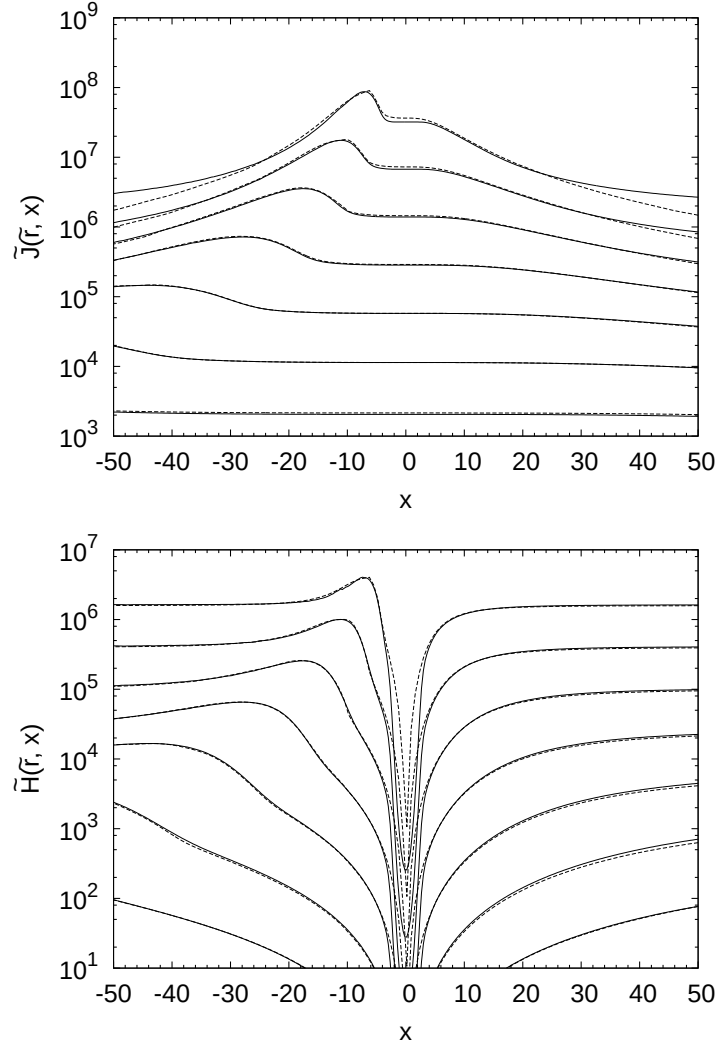


Figure 6.4: Coherent scattering solution for $\tilde{J}$ (upper panel) and $\tilde{H}$ (lower panel) obtained from ray and moment equations outside of the diffusion regime (solid lines), compared with the analytic solutions for the zero-temperature diffusion regime (dashed lines). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

We solved the problem outside of the diffusion regime using the moment/ray method applied to the exact forms of the ray and moment equations for the homogeneous expanding medium problem, given by Equations (6.6) to (6.8) with $\tilde{\alpha} = 1$ and $d(\ln V)/d(\ln r) = 1$. Again, we used the Voigt profile form for $\tilde{\chi}$ and assumed coherent scattering, $\tilde{\eta} = \tilde{\chi}\tilde{J}$. We assumed the diffusion limit solutions given by Equations (6.19)

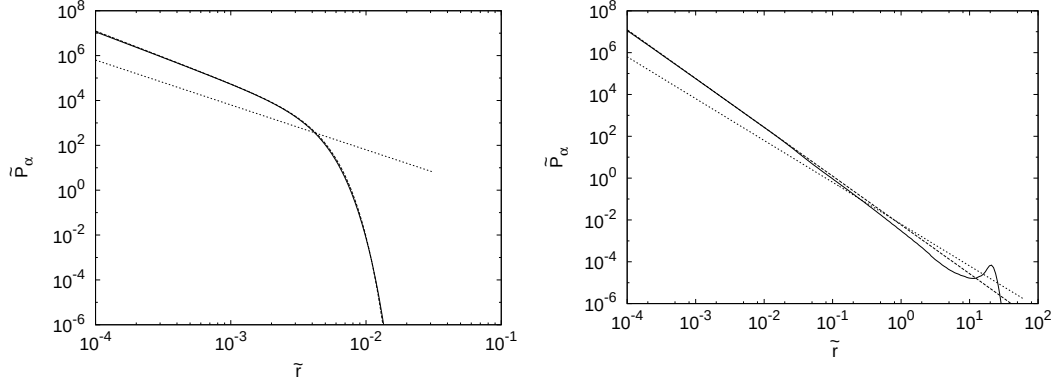


Figure 6.5: Scaled scattering rate derived from numerical integration of coherent scattering solution obtained from moment/ray equations (solid line) and analytic diffusion solution (long-dashed line) for $T = 10$ K and source cutoff frequencies $x_m = 100$ (left panel) and $x_m = 1.4 \times 10^5$ (right panel). For comparison we also show $\tilde{P}_\alpha^{\text{free}}$ (short-dashed line).

and (6.20) in specifying the inner boundary condition and the initial estimate of the source function used in solving the ray equations. Note that for this and subsequent problems where the conditions do not match those that determine the solution used for the boundary condition, the ray/moment solution at the boundary is subject to an unphysical constraint and we should not assume it is accurate there.

Our solutions are displayed in Figure 6.4. For distances sufficiently far from the source we find the moment/ray solution is a close match to the diffusion solution. Closer to the source we find both solutions match across the line centre, while away from line centre there is some deviation and the moment/ray solution approaches a flat profile closer to the free streaming solution. This is presumably a result of the negligible optical depth out to these radii away from line centre. The flux is altered from the analytic solution to a limited extent. We have also plotted the corresponding scattering rate in Figure 6.5 for two examples with different values of the source frequency cutoff ν_m . The left panel has $x_m = 100$ and thus $|\tilde{\nu}_m| \simeq 10^{-1.6}$ and the ‘diffusion-limited’ effective radius of the Ly α scattering region as given by Eq. (6.26) for general $\tilde{\nu}_m$ is $\tilde{r} = 1.05|\tilde{\nu}_m|^{3/2} \simeq 10^{-2.3}$, in approximate agreement with the figure. The right panel has $x_m = x_\beta$, where $x_\beta = 5\nu_\alpha/(27\Delta\nu_D) \simeq 1.4 \times 10^5$ denotes the source cutoff corresponding to the Lyman-beta frequency. For $\tilde{r} \gtrsim 10^{-1.5}$ there is a noticeable decrease in the

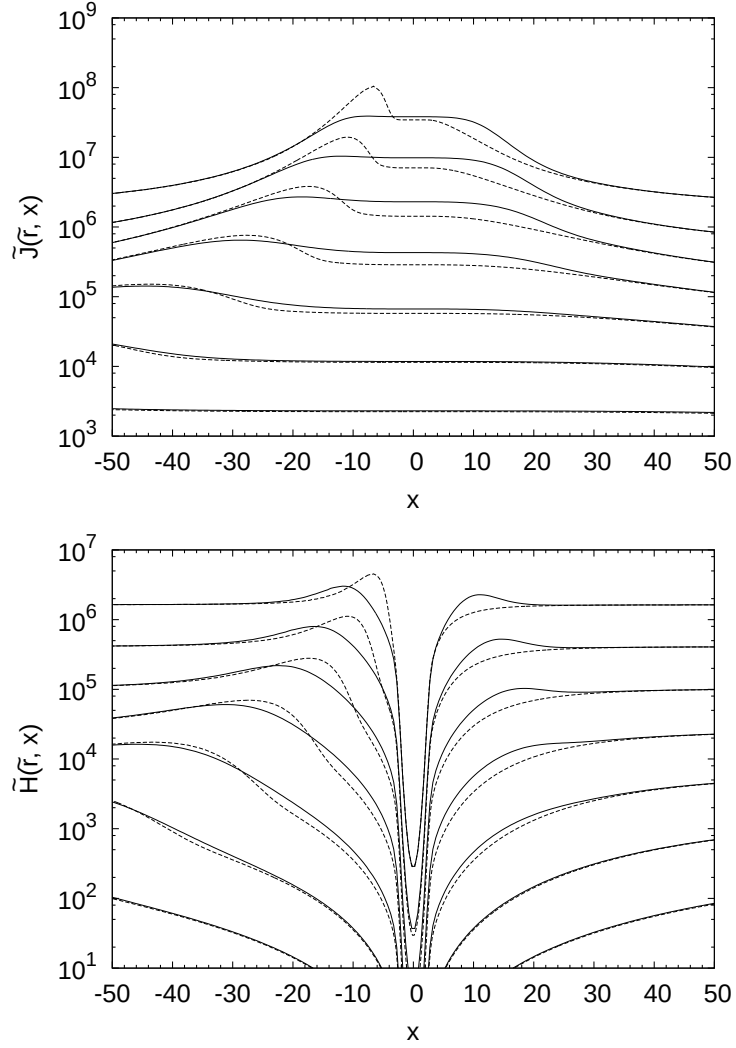


Figure 6.6: Type II redistribution solution for $\tilde{J}$ (upper panel) and $\tilde{H}$ (lower panel) obtained from ray and moment equations outside of the diffusion regime (solid lines), compared with the corresponding solution for coherent scattering (dashed lines). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

scattering rate relative to the diffusion regime case, however an approximate $\tilde{r}^{-7/3}$ scaling is maintained. The scattering region does not display the gradual Γ -function drop-off of the diffusion regime solution given by Eq. (6.23), but shows a peak followed by a sharp drop-off at $\tilde{r} \simeq 10^{1.5}$. This is consistent with the free streaming limit of $|\tilde{\nu}_m| \simeq 10^{1.6}$ which in this case is less than the diffusion limit of $1.05|\tilde{\nu}_m|^{3/2} \simeq 10^{2.4}$.

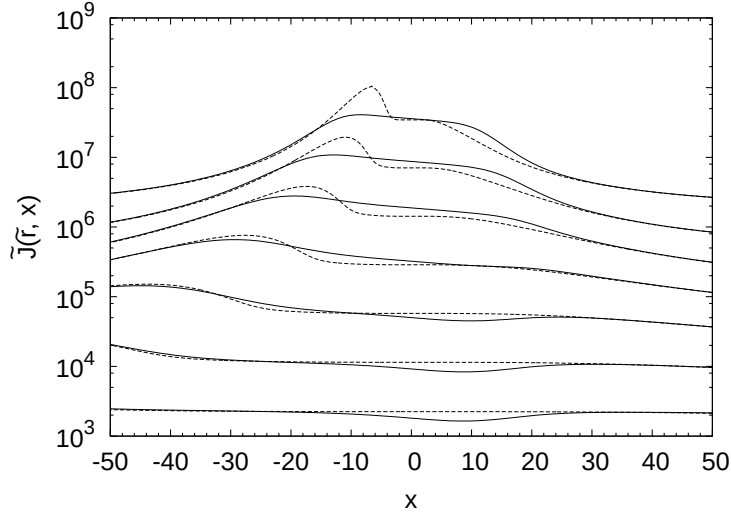


Figure 6.7: Type II redistribution solution with recoil obtained from ray and moment equations outside of the diffusion regime (solid lines), compared with the corresponding solution for coherent scattering (dashed lines). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

The assumption of coherent scattering is valid for photons scattering at frequencies far from line centre, but as we examine photons redshifting across the line centre such an assumption is not physically motivated. We now treat the added effect of Doppler shifts due to the thermal- and recoil-induced atomic velocities. The thermal velocities of the atoms are responsible for the type II frequency redistribution picture assumed in Ly α scattering. We consider the addition of this effect to the problem in isolation by ignoring the effect of recoil. Moment/ray equation solutions are obtained similarly to the coherent solution with the type II form for the coefficients $\mathcal{R}_{k',k,d}$ with $\epsilon = 0$ as given in Eq. (5.102). We display our solution for $\tilde{J}$ in Figure 6.6. There is some redistribution of photons across the line centre relative to the red peak seen in the coherent scattering case, resulting in a small boost to the scattering rate over a limited range in radius as seen in the left panel of Figure 6.8. The difference in the spectrum from the coherent scattering case is not particularly significant at large radii, an effect also seen in the scattering rate. In the lower panel of Figure 6.6 we show how the flux is affected by frequency redistribution.

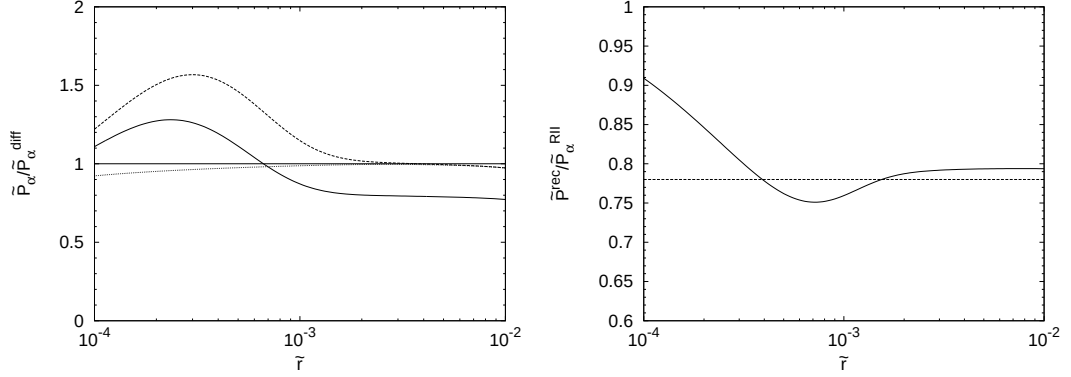


Figure 6.8: Left panel: Ratio of scattering rate derived from numerical integration of the appropriate moment/ray solution, to the analytic diffusion limit result $\tilde{P}_\alpha^{\text{diff}}$, for type II redistribution with recoil (solid line), type II redistribution without recoil (dashed line) and coherent scattering (dotted line).

Right panel: Ratio of scattering rate assuming redistribution and recoil to that with redistribution alone (solid line), compared with an estimate of the suppression factor of Furlanetto and Pritchard in a uniformly expanding homogeneous medium, $S_\alpha = 0.78$ (dashed line).

We include the effect of atomic recoil by seeking moment/ray solutions without setting the recoil parameter ϵ to zero. Our solution is displayed in Figure 6.7. We see that the expected Boltzmann distribution gradient is recovered across the line centre. We find a suppression of the scattering rate relative to the type II case without recoil as shown in Figure 6.8. The suppression factor S_α defined by Furlanetto and Pritchard [2006] for the inclusion of the recoil effect in a uniformly expanding homogeneous system is given by Equations (2.69) and (2.70); for our system the values of γ and T give $\delta_J(0) \simeq 0.22$ and thus $S_\alpha \simeq 1 - \delta_J(0) \simeq 0.78$. This is close to the average value of the radius-dependent suppression factor determined from our solutions.

We seek a Monte Carlo solution to the problem using the method described in section 4.4. The normalisation condition Eq. (6.9) can be written for $V = Hr$ as:

$$\tilde{R}^2 \int_{-\tilde{\nu}_{\text{max}}}^{\tilde{\nu}_{\text{max}}} \tilde{H}(\tilde{R}, \tilde{\nu}) d\tilde{\nu} + \int_0^{\tilde{R}} \tilde{r}^2 \left\{ \tilde{J}(\tilde{r}, \tilde{\nu}_{\text{max}}) - \tilde{J}(\tilde{r}, -\tilde{\nu}_{\text{max}}) \right\} d\tilde{r} = \frac{2\tilde{\nu}_{\text{max}}}{(4\pi)^2}. \quad (6.27)$$

The integrals are computed from the Monte Carlo output and the intensity $\tilde{I}$ is multiplied by an appropriate factor to match the value of the RHS. Our solution for coherent

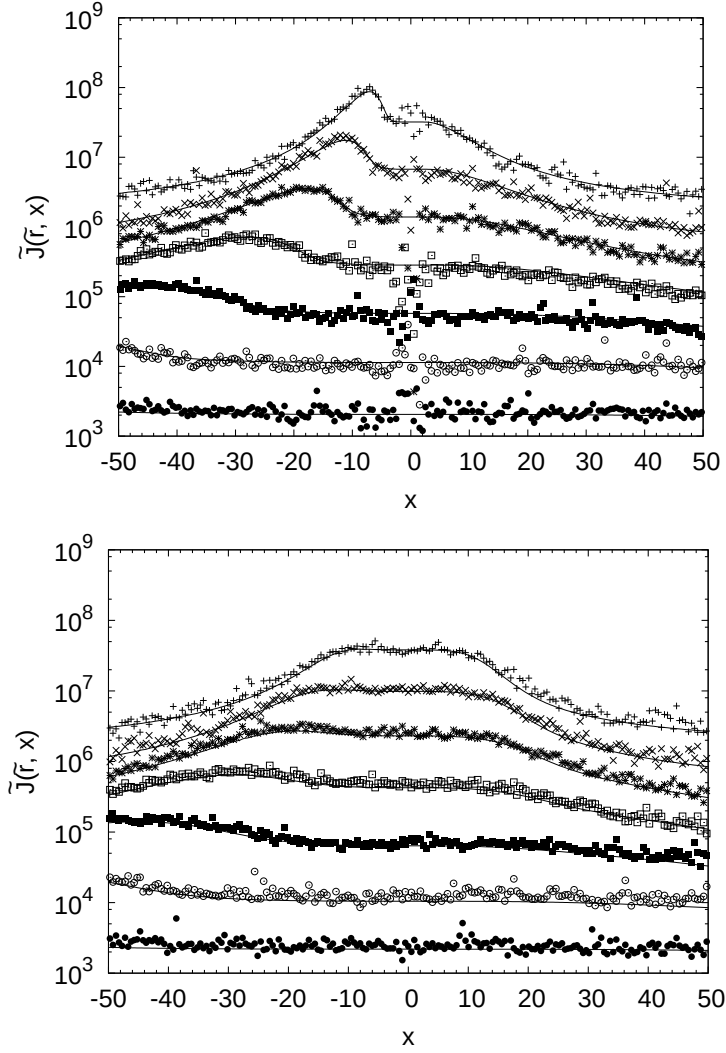


Figure 6.9: Upper panel: Monte Carlo solution (various points) for coherent scattering, together with the corresponding ray/moment equation solution (solid line).

Lower panel: Monte Carlo solution (various points) for type II redistribution, together with the corresponding ray/moment equation solution (solid line).

scattering is displayed in the upper panel of Figure 6.9; it is seen to match the moment/ray solution closely, although it appears distorted and very noisy at line centre. This is presumably a result of the assumptions used to calculate the optical depth between scattering events in the Monte Carlo method as described in section 4.4.3; the assumption of constant properties between the radial grid-spheres allows accurate de-

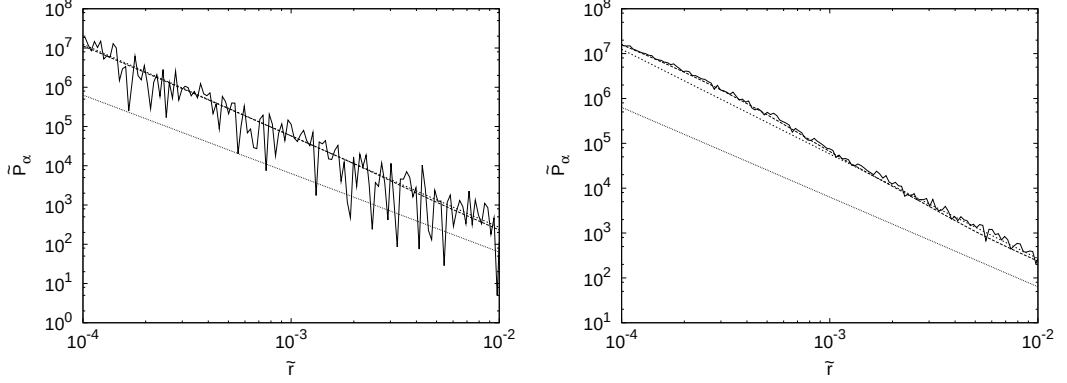


Figure 6.10: Scaled scattering rate derived from numerical integration of Monte Carlo solution (solid lines) for both coherent scattering (left panel) and type II redistribution (right panel), compared with the scattering rate obtained from the moment/ray equation method in each case (long-dashed line). For comparison we also show $\tilde{P}_\alpha^{\text{diff}}$ (short-dashed line) and $\tilde{P}_\alpha^{\text{free}}$ (dotted line).

termination of the optical depth for long path lengths, but this accuracy is significantly reduced for short path lengths such as those of photons near the line centre. The distortion at line centre produces significant noise in the scattering rate calculated from the Monte Carlo solution as seen in the left panel of Figure 6.10. We also obtained a solution including type II redistribution using the Monte Carlo method with the redistribution treatment of Zheng and Miralda-Escudé [2002] discussed in section 4.2 using $\epsilon = 0$. This solution is displayed in the lower panel of Figure 6.9 and is seen to match the corresponding ray/moment solution closely. There is no significant distortion at the line centre and the noise in the scattering rate is reduced with respect to that in the coherent scattering Monte Carlo solution, as seen in the right panel of Figure 6.10.

We found the time required to obtain the Monte Carlo solutions far exceeded that required to obtain our moment/ray equation solutions. Our Monte Carlo solutions were obtained from following 100,000 photons in ~ 10 hours and ~ 30 hours for coherent scattering and redistribution respectively. In contrast, the moment equations are solved in a time that scales approximately with the number of grid-zones in frequency and radius as $\tau \sim (\text{NF})^3 \text{ND}$ and required from 20 to 60 minutes in the examples presented.

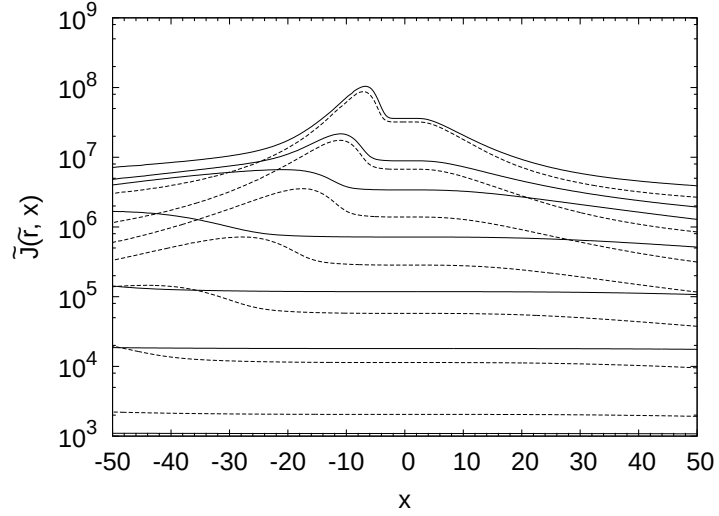


Figure 6.11: Coherent scattering solution obtained from ray and moment equations with the density profile specified in Eq. (6.28) (solid lines), compared with the corresponding solution for a uniform density $n_1 = n_H(z)$ (dashed lines). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

6.3 Non-Uniform Density Profile

As an example application for a non-uniform density profile, we examine the continuum source Ly α scattering problem for a scattering medium undergoing Hubble expansion with the following density profile:

$$n_1(r) = \begin{cases} 10n_H(z) & ; \quad 10^{-3.5} \leq \tilde{r} \leq 10^{-2.5} \\ n_H(z) & ; \quad \tilde{r} < 10^{-3.5}, \tilde{r} > 10^{-2.5} \end{cases} \quad (6.28)$$

i.e. the neutral hydrogen around the source is distributed as an overdense shell between $10^{-3.5} < \tilde{r} < 10^{-2.5}$. In the case of the moment/ray solution method, this affects the spatial dependence of the opacity coefficients $\chi_{k,d}$. We plot our ray/moment solution to the problem for coherent scattering in Figure 6.11, while the corresponding scattering rate is denoted by the solid line in Figure 6.13. Compared with the spectrum for a uniform density scattering medium the frequency peaks at the overdense radii are displaced further redward, while the scattering rate across this range is boosted. At the outer edge of the shell the scattering rate dips below the uniform density value.

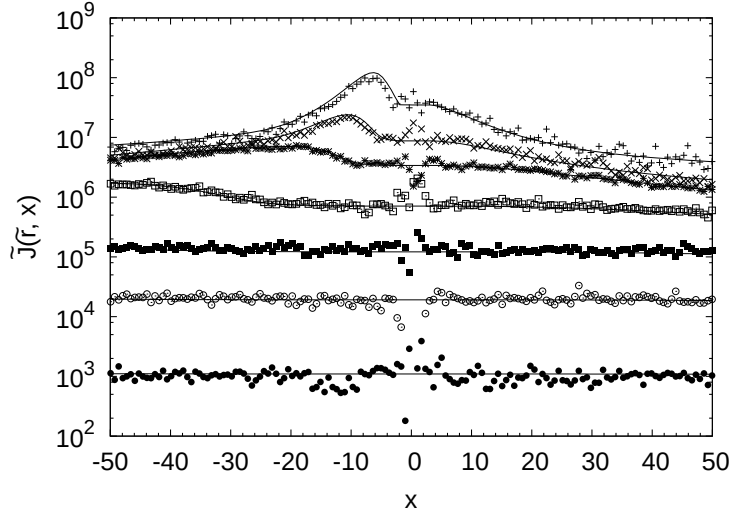


Figure 6.12: Monte Carlo solution (various points) for coherent scattering with the density profile specified in Eq. (6.28), compared with the corresponding ray/moment equation solution (solid line). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

We also attempted to determine a Monte Carlo solution for the problem, plotted in Figure 6.12, which required significantly more time to follow the photons through the overdensity. The corresponding scattering rate is displayed as the dashed line in

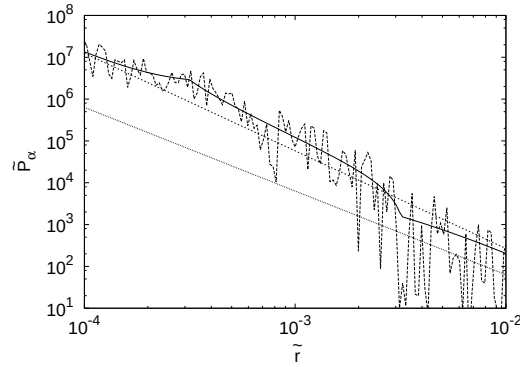


Figure 6.13: Scaled scattering rate derived from numerical integration of moment/ray equation solution (solid lines) and Monte Carlo solution (long-dashed line) for coherent scattering in a medium with an overdense shell as described in the text. For comparison we also show $\tilde{P}_\alpha^{\text{diff}}$ (short-dashed line) and $\tilde{P}_\alpha^{\text{free}}$ (dotted line).

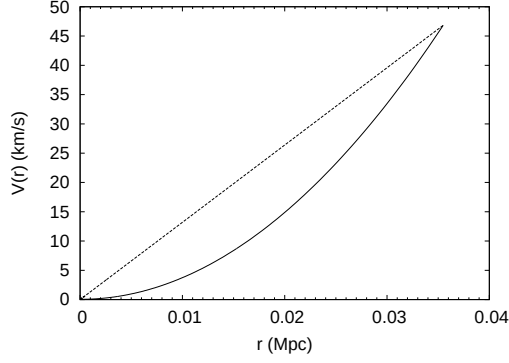


Figure 6.14: Velocity profile given by the quadratic relation of Eq. (6.29) with $\tilde{R}_{\min} = 10^{-4.5}$, $\tilde{R}_{\max} = 10^{-1.5}$ and $V_{\max/\min} = HR_{\max/\min}$ (solid line), compared with the Hubble law $V(r) = Hr$ (dashed line).

Figure 6.13. The excessive noise in the Monte Carlo scattering rate is reduced if we adopt a more suitable estimator for the mean intensity (see Appendix A), however the ray/moment method is clearly more suited to solving this problem.

6.4 Non-Hubble Velocity Profile

In this section we consider a continuum source in a medium of uniform density, however we move beyond the assumption of a simple Hubble velocity profile $V = Hr$. As we are primarily interested in examining general effects of the radial velocity profile and not any particular realistic case, we consider a quadratic velocity law. We parameterise the radial velocity profile $V(r)$ for $R_{\min} < r < R_{\max}$ as:

$$V(r) = (V_{\max} - V_{\min}) \left[\frac{r - R_{\min}}{R_{\max} - R_{\min}} \right]^2 + V_{\min}. \quad (6.29)$$

We have plotted both the quadratic velocity profile given by Eq. (6.29) and the corresponding Hubble profile in Figure 6.14, where we have taken $V_{\max} \equiv V(R_{\max}) = HR_{\max}$ and $V_{\min} \equiv V(R_{\min}) = HR_{\min}$. Using this velocity profile we can obtain Ly α radiative transfer solutions from the ray/moment method applied to the ray and moment equations in their general form as given by Equations (6.6)-(6.8). We obtained a moment/ray equation solution for coherent scattering which is displayed in Figure 6.15. In order to

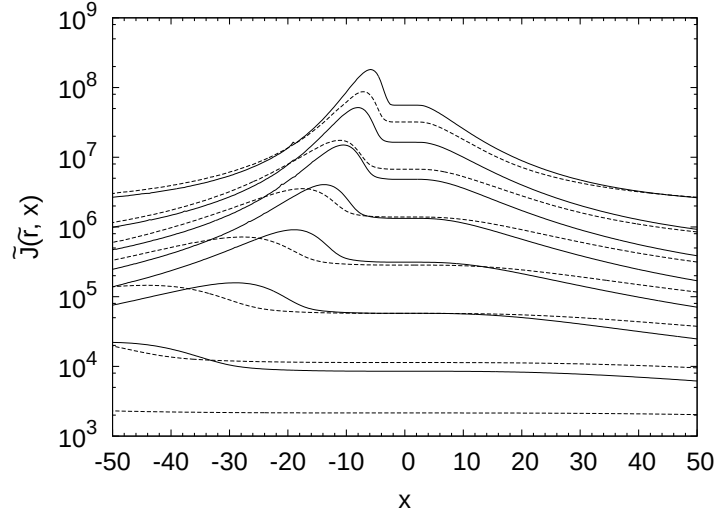


Figure 6.15: Coherent scattering solution obtained from ray and moment equations with the quadratic velocity profile displayed in Figure 6.14 (solid lines), compared with the corresponding solution for a Hubble velocity profile (dashed lines). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

isolate the effect of the velocity profile, the solution is compared with the equivalent ray/moment solution for the Hubble profile previously displayed in the upper panel of Figure 6.4. The solution presents the same qualitative features as the coherent scattering solution for the Hubble velocity profile, in particular the peak in intensity that drifts redwards from line centre further from the source, although significant quantitative differences are apparent. The frequency displacement of the peak increases more slowly with radius than in the Hubble velocity case, presumably a result of a reduced velocity across the range in radius which is less efficient in redshifting photons. Also apparent is an increase in the average intensity at line centre compared with the Hubble velocity solution, which approaches an order of magnitude at the largest radii considered.

It is also possible to determine a Monte Carlo solution using the general form for the photon comoving frequency between scattering events, Eq. (4.27), and the general normalisation constraint Eq. (6.9). We obtained a Monte Carlo solution for the coherent scattering problem which is compared with our ray/moment solution in the upper panel of Figure 6.16. Similarly to the coherent scattering case with a Hubble velocity profile,

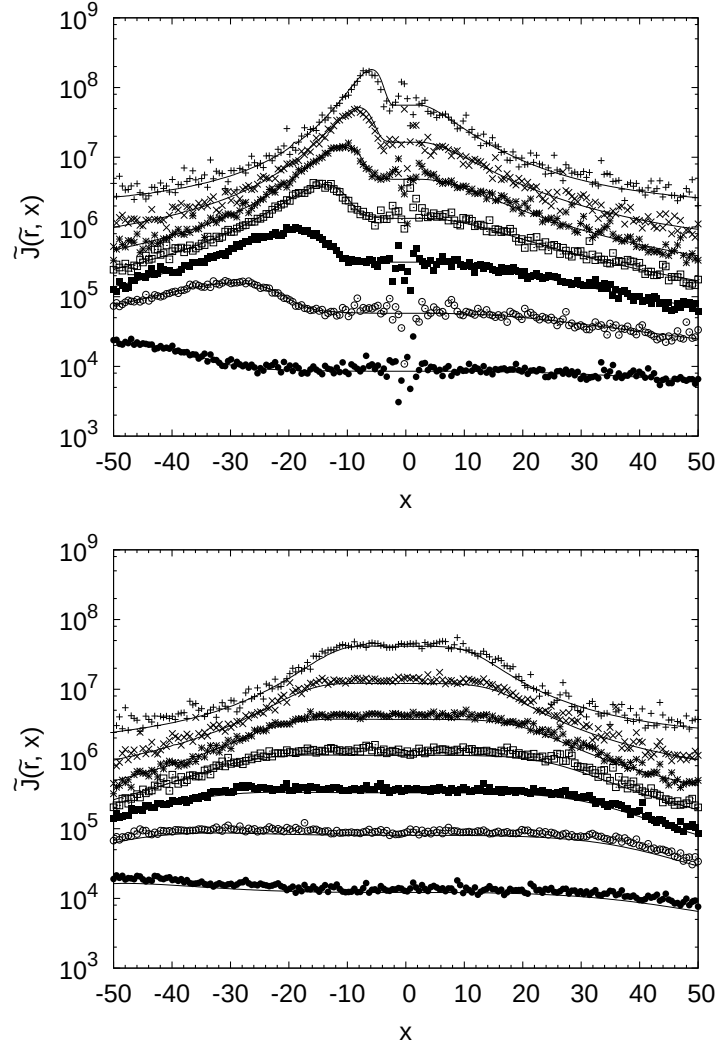


Figure 6.16: Monte Carlo solution (various points) for coherent scattering (upper panel) and type II redistribution (lower panel) with the quadratic velocity profile of Eq. (6.29), compared with the corresponding ray/moment equation solution (solid line). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

we find significant distortion of the profile across the line centre. This distortion is reduced if we allow for redistribution, as seen in the lower panel of Figure 6.16. The Monte Carlo scattering rate is compared with that determined from the equivalent ray/moment solution for both coherent scattering and redistribution in Figure 6.17. In all cases the scattering rate is seen to be boosted by up to an order of magnitude

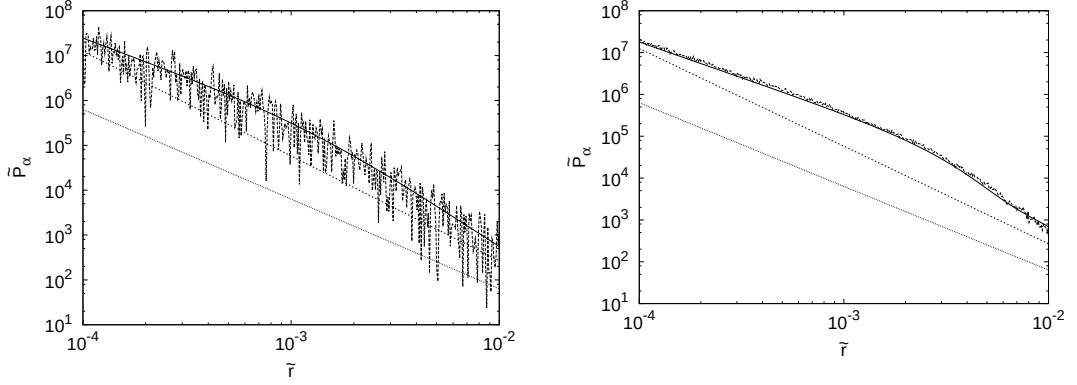


Figure 6.17: Scaled scattering rate for a uniform medium with a velocity profile given by Eq. (6.29), derived from numerical integration of the moment/ray equation method (solid lines) for both coherent scattering (left panel) and type II redistribution (right panel), together with the scattering rate obtained from the Monte Carlo method in each case (long-dashed line). For comparison we also show $\tilde{P}_\alpha^{\text{diff}}$ (short-dashed line) and $\tilde{P}_\alpha^{\text{free}}$ (dotted line).

compared with the expected rate for a Hubble velocity profile, given approximately by $\tilde{P}_\alpha^{\text{diff}}$. The Monte Carlo scattering rate in the coherent case is extremely noisy but upon introducing redistribution the level of noise is reduced significantly. Again, the moment/ray method was significantly faster in solving the problem.

6.5 Discussion

We formulated the comoving-frame radiative transfer equation for the Ly α scattering induced by a continuum source in a spherically symmetric medium with a general velocity profile $V(r)$. In the case of a homogeneous expanding medium with $V = Hr$, we were able to utilise the analytic solution derived by Loeb and Rybicki [1999] - for the Ly α intensity induced by a monochromatic point source emitting at the Ly α frequency - as a Green's function to derive an analogous solution for our continuum source valid in the diffusion regime and assuming coherent scattering. The scattering rate predicted by the analytic solution displays a $P_\alpha \propto r^{-7/3}$ radial profile which is enhanced relative to the free-streaming scattering rate close to the source. This same scaling was found numerically in Monte Carlo treatments by Semelin et al. [2007] and Chuzhoy and Zheng [2007].

The scattering rate profile outside of the diffusion regime, determined using the ray/moment and Monte Carlo methods, was found to closely match the analytically predicted scaling with minor differences close to the source found upon the inclusion of redistribution and recoil. Another difference was the effect of a finite frequency cutoff in the source spectrum, which can induce a significant deviation from the analytic scattering profile and a free-streaming limit to the size of the Ly α scattering region as seen in Figure 6.5. We also looked at problems with a non-uniform density profile and a non-Hubble velocity profile, for which we found significant differences in the scattering rate. Overall we found the moment/ray method to be more accurate and efficient in the problems we studied, particularly in the case of an overdense H I shell for which the required Monte Carlo runtime increased significantly.

In this chapter, we obtained results for the scattering rate in the form of the dimensionless quantity $\tilde{P}_\alpha = P_\alpha/P_*$. If we are to determine the physical scattering rate P_α to allow a comparison with the 21 cm thermalisation rate P_{th} defined by Eq. (1.35), it is necessary to specify the characteristic scattering rate $P_* = 4\pi\sigma\dot{N}_\nu/r_*^2$ and thus $\dot{N}_\nu$, the number of photons emitted by the source per second per unit frequency. We assume a star-forming galaxy source with properties determined by the Starburst 99 simulations of Leitherer et al. [1999]; specifically, we assume a continuous star formation rate of $1\text{ M}_{\text{solar}}\text{ yr}^{-1}$, a low metallicity $Z = 0.001$ and a Salpeter Initial Mass Function between 1 and 100 solar masses. The Starburst 99 online archive provides a table¹ of the time-dependent specific luminosity L_λ ; after 30 Myr this luminosity is given by $L_\lambda = 10^{40.43}\text{ erg s}^{-1}\text{ \AA}^{-1}$ at the Ly α wavelength. This corresponds to a rate of photon emission at the Ly α frequency of $\dot{N}_\nu = \lambda_\alpha^3 L_\lambda / (h_P c^2) \simeq 8.11 \times 10^{38}\text{ s}^{-1}\text{ Hz}^{-1}$. The spectrum is approximately flat around the Ly α frequency ($\lambda = 1216\text{ \AA}$) and in fact the luminosity at Lyman beta ($\lambda = 1026\text{ \AA}$) is only a factor of $\simeq 1.5$ greater, and thus we might model such a galaxy as a source of Ly α photons with constant $\dot{N}_\nu = 8.11 \times 10^{38}\text{ s}^{-1}\text{ Hz}^{-1}$ between the Ly α and Lyman-beta frequencies.

This model galaxy allows us to relate our previously derived results for $\tilde{P}_\alpha = P_\alpha/P_*$ to the physical scattering rate. As an example of the physical utility of results that we

¹<http://www.stsci.edu/science/starburst99/data/fig2e.dat>

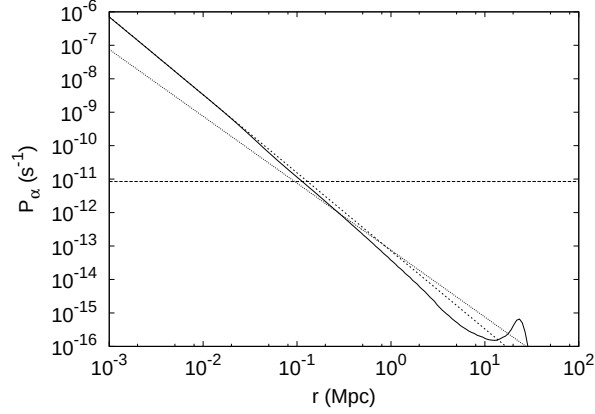


Figure 6.18: Physical scattering rate derived from numerical integration of coherent scattering solution with $x_m = 1.4 \times 10^5$ (solid line) and adopting the value $\dot{N}_\nu \simeq 8.11 \times 10^{38} \text{ s}^{-1} \text{ Hz}^{-1}$ derived in the text, compared with the ‘thermalisation’ scattering rate $P_{\text{th}} \simeq 8.47 \times 10^{-12} \text{ s}^{-1}$ (dashed line). For comparison we also show P_α^{diff} (short-dashed line) and P_α^{free} (dotted line).

have derived in this chapter we compare the scattering rate profile around an isolated continuum source in a homogeneous expanding medium with the thermalisation rate needed to decouple the H I spin temperature from the CMB temperature and allow the hydrogen to be detected in 21 cm observations, $P_{\text{th}} = 27 A_{\text{ul}} T_{\text{CMB}} / (4 T_*) \simeq 8.47 \times 10^{-12} \text{ s}^{-1}$ at $z = 10$. Using the value $P_* \equiv 4\pi\sigma\dot{N}_\nu/r_*^2 \simeq 9.49 \times 10^{-12} \text{ s}^{-1}$ for our model galaxy source to normalise our scaled results and comparing with the value of P_{th} , we can find the radius at which P_α drops below P_{th} . We have attempted a comparison of this type in Figure 6.18 in which we have plotted the physical scattering rate corresponding to the solution displayed in the right panel of Figure 6.5, describing the scattering rate resulting from coherent scattering with a source cutoff frequency corresponding to Lyman beta. The upper-left panel of Figure 6.19 is a zoomed-in display of the same solution with linear scales, focused on the ‘crossover radii’ at which the full radiative transfer solution obtained using the moment/ray method, and the analytic results in the free streaming and diffusion regimes, drop below the 21 cm thermalisation rate. We have also provided similar displays in the other panels for a source luminosity stronger by 1, 2 and 3 orders of magnitude; as the source luminosity increases, the scattering rate profiles in Figure 6.18 slide upwards and the crossover radii are shifted to larger

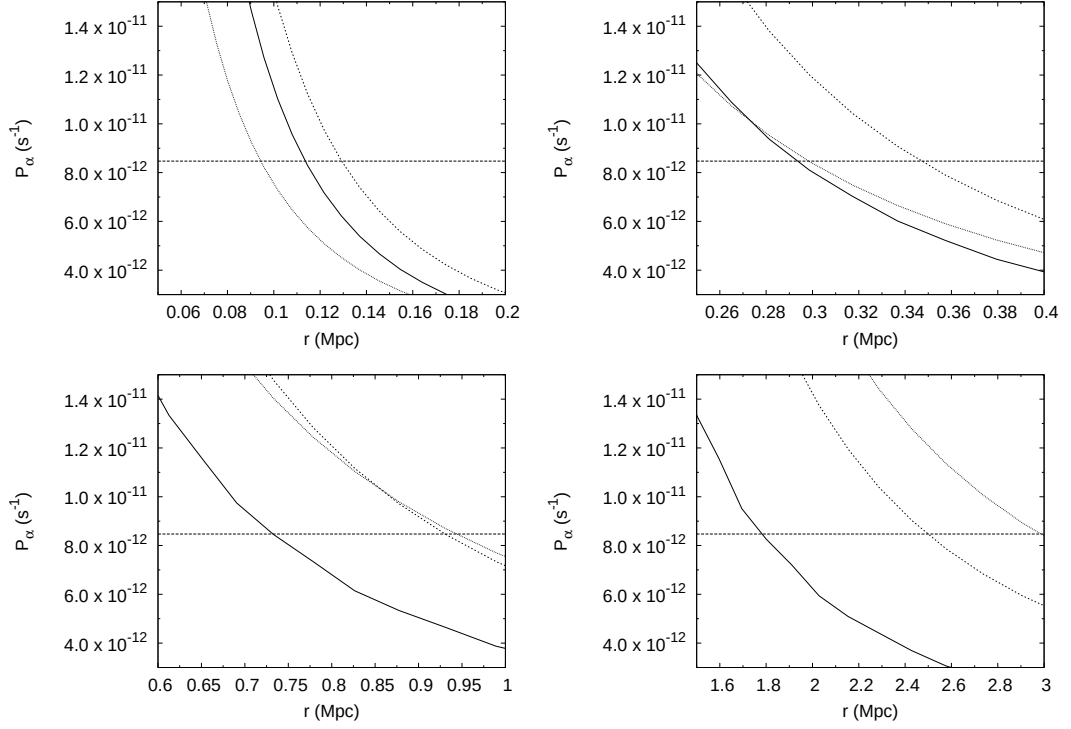


Figure 6.19: Linear scale plots of the physical scattering rates compared with the thermalisation rate as displayed in Figure 6.18, with radius values chosen to allow identification of the ‘crossover radii’; we take a continuum source luminosity corresponding to $\dot{N}_\nu \simeq 8.11 \times 10^{38} \text{ s}^{-1} \text{ Hz}^{-1}$ in the upper-left panel, while the other panels correspond to stronger sources with $\dot{N}_\nu$ multiplied by a factor of 10 (upper-right panel), 100 (lower-left panel) and 1000 (lower-right panel). The labelling of the lines is as for Figure 6.18.

r . Clearly the radius of the spherical region about the source detectable via 21 cm tomography, given by the range in r for which $P_\alpha(r) \gtrsim P_{\text{th}}$, is heavily dependent upon the radiative transfer of the Ly α photons; in particular, for high source luminosities this region is significantly more compact than would be expected from the analytic solutions in the free streaming or diffusion regimes.

There are some caveats to the application of our results in this way. Firstly, we have assumed that our time-independent solutions are applicable, which is incorrect in the case that the time-independent solution is not achieved within the lifetime of the source. In Chapter 3 we used a time-dependent solution method for Ly α scattering in

a homogeneous medium to estimate the relaxation time t_r for the solution to approach the time-independent solution; such a time-dependent approach is not possible for the current spherically symmetric problem using the ray/moment equation solution method, although time-dependent Monte Carlo solutions as implemented by e.g. Xu et al. [2011] are possible². In the absence of a quantitative estimate of the relaxation time capable of treating the spatial transfer important to the current problem, we adopt the uniformly expanding homogeneous medium estimate of Rybicki and dell’Antonio [1994]: $t_r \sim [a/\gamma^4]^{1/3} t_s$, where $a = 0.015$ for $T = 10\text{ K}$, $\gamma = 1.30 \times 10^{-6}$ for $z = 10$ and the scattering time at line centre $t_s \simeq 4.1 \times 10^4\text{ s}$, giving $t_r \simeq 0.02\text{ Myr}$. This is much less than the characteristic lifetime of our source, however the true relaxation time for our problem is clearly a function of radius and it might be significantly longer than this homogeneous medium estimate at large distances from the source. If we determine that the time-independent scattering rate exceeds the thermalisation rate up to some radius r , an obvious lower limit to the time required to achieve that steady state is the free-streaming time $t_{\text{free}} = r/c = 3.27[r/\text{Mpc}]\text{ Myr}$, which does not rule out the estimates of the 21 cm-detectable regions suggested by Figure 6.19.

We have described the scattering rate profiles determined from our radiative transfer solutions as defining some maximum radius out to which the H I gas 21 cm spin temperature is decoupled from the CMB background against which we observe it. Important to note is that the detectable 21 cm signal is proportional to $(1 - T_s/T_{\text{CMB}})$ where the value of the spin temperature T_s lies in the range bracketed by T_{CMB} and T_K at a value determined by the scattering rate P_α [see Eq. (1.32)], and thus the H I gas kinetic temperature T_K will have a significant effect on the signal and whether it is seen as absorption or emission. The temperature of the medium will generally be a function of radius due to the heating effects of the source and the temperature profile will have an effect on the scattering rate profile, similarly to the density and velocity profiles. Finally, additional effects upon the 21 cm observational properties will arise from deviations from spherical symmetry, and contributions from multiple sources.

²Xu et al. [2011] examined an IGM model with a continuum source similar to our model, however our results are not comparable as they examined observable properties arising from photons escaping to infinity as opposed to the Ly α spectrum as a function of radius.

CHAPTER 7

Conclusions

We examined the radiative transfer of resonance line photons in both homogeneous and spherically symmetric systems using various methods. We applied these methods to the $\text{Ly}\alpha$ scattering of continuum photons in a neutral IGM, relevant to the 21cm signal of the first sources during the EoR via the Wouthuysen-Field effect.

We initially examined the problem of the radiative transfer of $\text{Ly}\alpha$ scattering in the H I IGM using a simple locally homogeneous model, allowing analytic calculations of the local $\text{Ly}\alpha$ spectrum and scattering rate arising from trapped photons intercepted from a distant source in a homogeneous expanding medium. The $\text{Ly}\alpha$ optical depth of a homogeneous expanding IGM for photons emitted at frequencies bluewards of $\text{Ly}\alpha$ implies that an observer far from the source sees a complete suppression of the free streaming flux due to scattering out of the line of sight for received frequencies (i) redwards of $\text{Ly}\alpha$, due to the Gunn-Peterson optical depth, and (ii) bluewards of $\text{Ly}\alpha$ by up to hundreds or thousands of Doppler widths, due to the accumulated optical depth in the wings of the $\text{Ly}\alpha$ absorption profile. We assumed that the incident free streaming flux blueward of line centre could act as a source of photons repeatedly scattered within a clump in the IGM, creating a locally homogeneous $\text{Ly}\alpha$ spectrum that achieves a steady state when the rate of photons intercepted from the source balances the rate of photons

escaping the system by diffusing to frequencies at which the clump is optically thin. The approximations and assumptions involved reduced the problem to a 1D radiative transfer equation in frequency, allowing analytic solutions to be calculated for various properties of the absorbing clump.

We determined steady-state analytic solutions for the locally homogeneous Ly α spectrum and scattering rate using the diffusion approximation to reduce the integro-differential radiative transfer equation to an ordinary differential equation. Additionally we adopted a numerical grid-based method to treat the full integro-differential problem which we found to confirm our analytic results. We found that, depending on absorber temperature and density etc., scattering rates orders of magnitude greater than the free streaming limit of an optically thin homogeneous IGM could be produced. The effects of atomic recoil at low temperatures or high column densities could reduce this scattering rate substantially, as could the red-/blue-shifting effect for a clump undergoing expansion/contraction with a significant uniform velocity gradient, while the right peculiar velocity of the clump is capable of redshifting the intercepted source photons towards line centre and increasing the steady-state scattering rate. We also considered the corresponding time-dependent radiative transfer problem for which we determined numerical solutions for the Ly α spectrum as a function of frequency and time, and approximate scaling relations for the time required to reach a steady state in both static and uniformly expanding clumps. We applied our results for the steady state scattering rate and the time required to achieve such a steady state to various example systems and compared these quantities with the scattering rate required to decouple the 21cm spin temperature from the CMB via the Wouthuysen-Field Effect, and the estimated lifetimes of the first sources, respectively.

In order to enable a less limited treatment of the problem of Ly α scattering in the IGM we looked at a Monte Carlo formulation of the resonance line radiative transfer problem in which the properties of many Ly α photons are tracked in a simulation from emission at the source, through many scattering events until some escape criterion is satisfied. We developed a lookup table method based on the angle-averaged frequency redistribution function to determine the scattered frequency of a photon resulting from

the atomic thermal velocity, which we found to be approximately three times faster than the widely adopted method of Chen and Miralda-Escudé [2004] based on the distributions of the atomic thermal velocity components. We described in detail implementations to determine the $\text{Ly}\alpha$ spectrum from (i) frequency histograms of scattering events in a homogeneous medium, and (ii) histograms in frequency and crossing angle for photons crossing spherical reference surfaces in a spherically symmetric medium. In the homogeneous medium case we applied our method using our locally homogeneous IGM clump model as a test problem, for which we obtained results in agreement with our analytic results. For the spherically symmetric case we looked at two test problems: (a) $\text{Ly}\alpha$ scattering in an optically thick static sphere as studied by Dijkstra et al. [2006] and (b) the $\text{Ly}\alpha$ scattering halo of a monochromatic $\text{Ly}\alpha$ point source in a homogeneous expanding medium studied by Loeb and Rybicki [1999]. We found our Monte Carlo results agreed with analytic solutions found by these authors, at least in the optically thick regime where the analytic solutions are valid, while in case (b) our solution agreed exactly with the Monte Carlo solution found by Loeb and Rybicki based on the binning of scattering events in frequency and radius.

Motivated by limitations of the Monte Carlo method such as the noise in the output and the large numbers of scattering events undergone by photons in the line core, we sought a grid-based approach to solving the radiative transfer equation in spherical symmetry. We adopted methods described by Mihalas et al. [1975], [1976] to solve the ray and angular moment forms of the comoving frame transfer equation in a spherically symmetric medium subject to a velocity profile $V(r)$, where $V, V' > 0$ for all r . We described in detail the implementation of these methods for treating the radiative transfer of $\text{Ly}\alpha$ scattering, and obtained an efficient prescription for the finite difference representation of the source function for partial frequency redistribution, Eq. (5.80), based on the diffusion approximation. We applied the ray and moment equation solution methods to the test problems that we previously examined with Monte Carlo methods, (a) and (b) above. We found that we were able to successfully reproduce the Monte Carlo solutions using an iterative procedure based on solving the moment equations with variable Eddington factors obtained by solving the ray equations.

In Chapter 6, we studied Ly α scattering induced by a continuum point source in a spherically symmetric homogeneous expanding medium. This problem is analogous to the monochromatic Ly α point source problem studied by Loeb and Rybicki [1999], and we utilised their analytic solution valid in the zero-temperature diffusion regime as a Green’s function to obtain the equivalent solution for a flat source spectrum. This solution suggests a radial profile for the Ly α scattering rate that varies as $r^{-7/3}$, steeper than the free-streaming expectation of r^{-2} and the same dependence found by other authors in Monte Carlo studies of this problem. This result could serve as the basis for a useful test problem for more advanced radiative transfer solution methods intended to simulate the Ly α scattering rate from the first sources during the EoR.

We attempted to solve our test problem of a continuum source in a homogeneous expanding IGM numerically, outside of the diffusion regime, using our Monte Carlo and ray/moment equation solution methods for spherical symmetry. This was necessary as the diffusion regime omits terms in the moment equations responsible for accurate treatment of redshifting and is not reproducible via physically consistent Monte Carlo methods. In applying both methods to the problem, we found the ray/moment method to be significantly more efficient while our Monte Carlo method displayed difficulties in treating the redshifting of photons through the line centre, a critical requirement necessary to allow accurate determination of the scattering rate for this problem. An alternative Monte Carlo approach, discussed in Appendix A, utilises more information in estimating the mean intensity of Ly α radiation and was found to be more successful in solving the problem and reducing the noise in the scattering rate profile. We believe that such a method would be necessary to treat the Ly α radiative transfer in cosmological simulations, as it can be easily extended to Cartesian grids with general configurations of sources and density / peculiar velocity of the scattering medium; however, in suitable spherically symmetric problems such as this test problem we would recommend the combined moment/ray equation solution method which gives noise-free results.

Our model of a continuum source in a homogeneous expanding IGM serves a similar purpose to that described in Chapter 3, in that it allows for an analysis of various effects on the Ly α scattering rate induced by the first sources during the EoR, although

it is clearly more robust due to its treatment of scattering in both frequency and space. For coherent scattering outside of the diffusion regime, we found that the spectrum deviated from the analytic solution at large distances from the source for a finite cutoff in the source spectrum. This cutoff necessitates a limiting radius beyond which the scattering rate drops to zero as all source photons have redshift past the line centre, and for a sufficiently blue source cutoff frequency outside of the diffusion regime we find that the limiting radius is determined by free streaming which is not allowed in the diffusion regime modelled by the analytic solution. We found frequency redistribution and atomic recoil to produce solutions with different features across the line centre near the source with minor effects on the scattering rate, variations of order unity about the coherent scattering result. Outside of these effects the solutions for a homogeneous expanding IGM were found to maintain the analytically predicted $r^{-7/3}$ dependence. We also examined the continuum source Ly α scattering problem using some alternative profiles for the density and velocity; we found that changing either can have a significant effect on the profile of the Ly α scattering rate.

Our test problem results obtained from solution of the ray and moment equations could be applicable locally around an isolated source during the early stages of the EoR. Some of the possible consequences for the 21 cm signature of such objects have been considered, based on the radius around the source for which the scattering rate exceeds the thermalisation rate necessary to decouple the H I spin temperature from the CMB temperature and render the hydrogen detectable in 21 cm observations. Clearly, realistic studies of Ly α scattering caused by the first sources during the EoR will need to make use of three-dimensional density and velocity fields derived from cosmological simulations, and treat the time-dependent radiative transfer of photons contributed from multiple sources of finite lifetime, the detailed properties and spatial distributions of which are largely uncertain and will have to be extrapolated from lower-redshift observations. There is much work involved but, together with the extensive work currently underway in removing radio foregrounds and isolating the signal from the EoR, these detailed analyses will be critical in predicting and interpreting future 21 cm tomographic observations made by SKA-type radio interferometric arrays.

APPENDIX A

Improved Monte Carlo: Path Length Method

The method for computing the specific intensity I_ν of radiation in a spherically symmetric Monte Carlo simulation described in Chapter 4 is based on the definition i.e. photons crossing a reference surface. This method has been applied by many authors e.g. Och et al. [1998] and allows for a complete description of the radiation field. By comparison the method described in Chapter 2 based on the number of scattering events can only recover the angle-averaged (mean) intensity J_ν . There are some disadvantages to the reference surface method, however; we have found that the resulting solutions for the mean intensity near line centre are typically quite noisy, which induces noise in the corresponding $\text{Ly}\alpha$ scattering rate. The noise in J_ν at line centre found using the definition of I_ν is most likely a result of the short path lengths travelled by photons at line centre, reducing the likelihood of such photons crossing the radial boundaries and questioning the assumption of constant properties between the boundaries.

A method more suited to our purposes is that applied by Lucy [1999] which adopts a Monte Carlo estimator for the mean intensity based on the time-averaged number density of photons in a cell of a given volume. We tailor the method to solve problems

in spherical symmetry. We denote the volume of the shell between two radial grid-spheres of radius r and $r + \Delta r$ by $V \simeq 4\pi r^2 \Delta r$. If a Monte Carlo photon travels a distance $\delta\lambda$ in the shell between two scattering events, the photon occupies the shell for a time $\delta t = \delta\lambda/c$ and contributes to the specific number density within the shell, at the frequency of the photon, the increment $V^{-1}\delta t/\Delta t$ where the quantity Δt is the physical time represented by the entire Monte Carlo run. The total number density $n_\nu(r) \Delta\nu$ comes from the sum of all $\delta\lambda$'s between any two general ‘events’ (scattering events, boundary crossings or redshifting between adjacent frequency bins) arising from photons travelling within the shell while having frequency within the range $[\nu, \nu + \Delta\nu]$. The mean intensity is then computed from $J_\nu = [c/(4\pi)]n_\nu$ as follows:

$$J_\nu = \frac{1}{4\pi V(\Delta\nu)(\Delta t)} \sum_{\text{events}} \delta\lambda. \quad (\text{A.1})$$

Outside of this calculation the Monte Carlo method is implemented nearly identically to that described in section 4.4. The distances $\delta\lambda$ between scattering events and/or boundary crossings are already necessary to compute in order to determine optical depths. Some additional calculation is needed for non-static media in order to record redshifting/blueshifting between adjacent frequency bins while photons are ‘in transit’ i.e. in between scattering events and/or boundary crossings, and we will discuss this later when looking at particular examples.

The major advantage of this method is that it makes use of all information output from the Monte Carlo simulation, unlike the other methods which discard all information on a given photon between scattering events or boundary crossings. The resulting estimate for J_ν suffers minimal noise for a given number of photons followed in the Monte Carlo run. Most affected is the estimate of the mean intensity at line centre; while line-centre photons rarely cross radial boundaries compared to photons in the line wings due to their short mean-free path, they do build up a significant summed path length between their many scatters. The path length method offers no information on the angular dependence of the radiation field as would be recovered by the method based on the definition of I_ν , however any noise or error arising from the choice of angular binning and angular integration to obtain J_ν is removed.

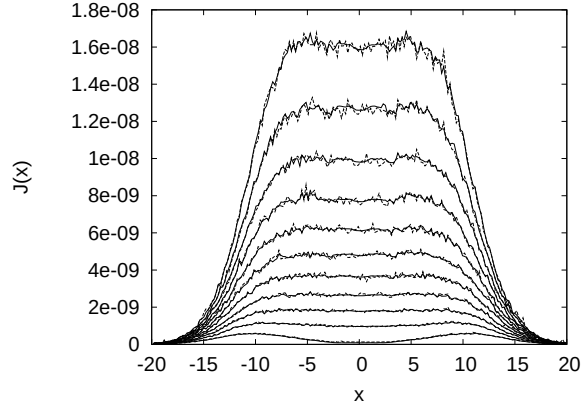


Figure A.1: Path length Monte Carlo solution for $J(r, x)$ in a static, uniform sphere obtained using the path length method (solid line) and the reference surface method described in section 4.4 (dashed line). We assume a temperature $T = 10$ K, line-centre opacity $\kappa_0 = 100$ and a thin shell source at radius $r_S = 5$. Frequency profiles are given from $r = 500$ (highest values of J) to $r = 1000$ (lowest values of J) in steps of 50.

In the problems that we have previously solved by Monte Carlo, we discarded the dependence of the normalised result on the physical time represented by the Monte Carlo run Δt as shown by Eq. (4.22). In these cases we instead normalised our result using some integral constraint on the moments of the radiation field such as Eq. (4.32) or Eq. (6.9), however as this path length method only computes the mean intensity J_ν and not I_ν we typically cannot adopt this approach. Instead, we use a method that is arguably more direct and efficient: we simply relate the time interval Δt to the number of photons N followed during the Monte Carlo run. How this is done depends upon the particular source being modelled; we consider both a $\text{Ly}\alpha$ point source and a continuum point source. In the case of a $\text{Ly}\alpha$ point source that is either monochromatic or only emits photons tightly distributed in frequency about ν_α , we represent by $\dot{N}_\alpha$ the number of photons emitted per second by the source which satisfies:

$$\dot{N}_\alpha = \frac{N}{\Delta t} \quad (\text{A.2})$$

i.e. the correctly normalised result is obtained from Eq. (A.1) with $1/\Delta t = \dot{N}_\alpha/N$. This can be used to solve the static sphere problem of Dijkstra et al. [2006] which was

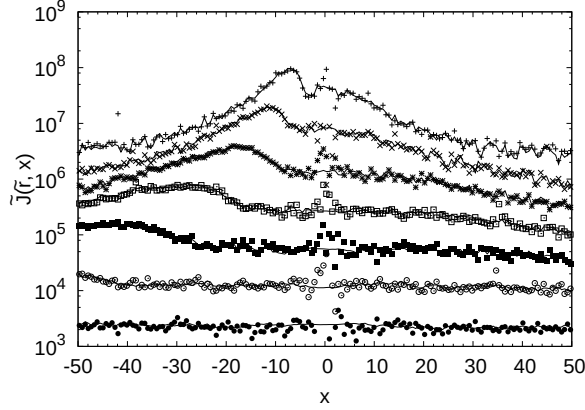


Figure A.2: Path length Monte Carlo solution (solid line) for coherent scattering arising from a continuum source in a homogeneous expanding medium, compared with the corresponding reference surface Monte Carlo solution (various points). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

previously presented with $\dot{N}_\alpha = 1$, or the homogeneous expanding medium problem of Loeb and Rybicki [1999] in which $\dot{N}_\alpha$ is scaled out of the solution. We have attempted a solution of the Dijkstra et al. [2006] test problem using the path length Monte Carlo method and a comparison of the solutions obtained using the path length and shell crossing methods, both normalised using Eq. (A.2), is displayed in Figure A.1. The differences in the results are modest, however the path length Monte Carlo solution is noticeably less noisy at the line centre.

In the case of a continuum source that emits $\dot{N}_\nu$ photons per second per Hertz across the range $[x_{\min}, x_{\max}]$ where $\dot{N}_\nu$ is independent of ν , we can write:

$$\dot{N}_\nu \Delta\nu = \frac{N}{\Delta t} \times \left[\frac{\Delta x}{x_{\max} - x_{\min}} \right] \quad (\text{A.3})$$

where $\Delta\nu$ is the frequency bin width and the factor in square brackets is the fraction of the N photons emitted within a single frequency bin. We examined the problem of a continuum source in a homogeneous expanding IGM in Chapter 6 where $\dot{N}_\nu$ was again scaled out of the solution. In the case of a source cutoff at x_m , we take $x_{\max} = x_m$. In Figure A.2 we present a comparison of results obtained from the two different Monte Carlo methods for the problem of a continuum source in a homogeneous expanding

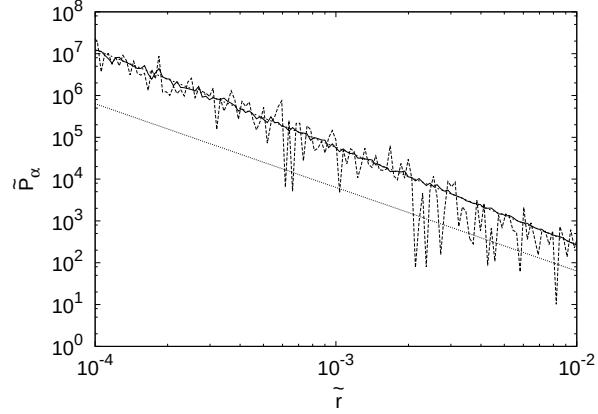


Figure A.3: Scaled scattering rate derived from numerical integration of Monte Carlo solution obtained using path length method (solid line), compared with that derived from the corresponding reference surface Monte Carlo solution (long-dashed line). For comparison we also show $\tilde{P}_\alpha^{\text{diff}}$ (short-dashed line) and $\tilde{P}_\alpha^{\text{free}}$ (dotted line).

medium, described in section 6.2. In this example the excessive noise across the line centre seen in the reference surface results is significantly reduced, and consequently the scattering rate is visibly less noisy as seen in Figure A.3. A similar comparison is provided for the non-uniform density profile described in section 6.3; the Monte Carlo solutions are displayed in Figure A.4 while the corresponding scattering rate is displayed in Figure A.5. The path-length Monte Carlo scattering rate is significantly less noisy than the reference surface result.

A disadvantage of the path length Monte Carlo estimator is the need to treat the continuous variation of the comoving photon frequencies along the path length, especially in a non-Hubble velocity field. The effort expended in the Monte Carlo code is significantly reduced if we can assume the photon occupies only a single frequency bin between scattering or boundary crossing events, which we take to be that corresponding to the ‘final’ frequency prior to scattering. In a Hubble velocity field the comoving frequency changes with path length λ as $x = x_{\text{em}} - (H/b)\lambda$, and the approximate treatment is accurate in the limit that the path length between scattering or boundary crossing events satisfies $\delta\lambda \ll b\Delta x/H$, where Δx is the frequency bin size, a condition which is certainly satisfied in our examples for distances between scattering events at

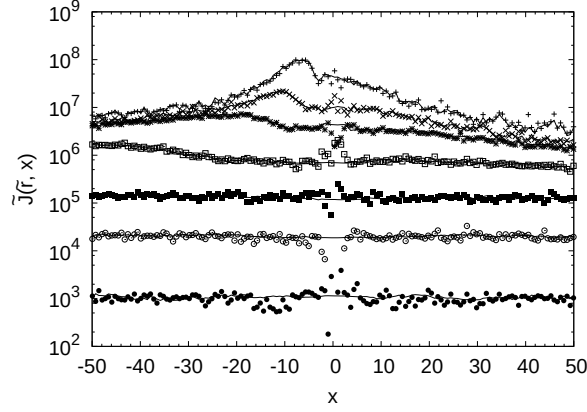


Figure A.4: Path length Monte Carlo solution (solid line) for coherent scattering arising from a continuum source with a Hubble expansion profile and the density profile specified in Eq. (6.28), compared with the corresponding reference surface Monte Carlo solution (various points). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

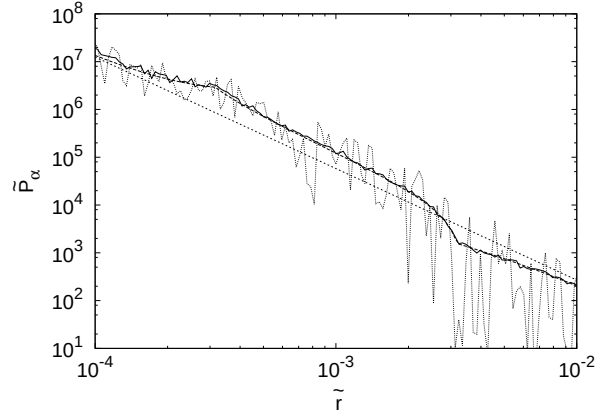


Figure A.5: Scaled scattering rate for the density profile given by Eq. (6.28), derived from the Monte Carlo solution obtained using the path length method (solid line), compared with that derived from the corresponding reference surface Monte Carlo solution (dotted line). For comparison we also show the corresponding moment/ray solution (dashed line) and $\tilde{P}_\alpha^{\text{diff}}$ (short-dashed line).

line centre important in determining the scattering rate. For a general velocity profile this condition is essentially replaced with $\delta\lambda \ll b\Delta x/|dV/dr|$, and so this approximate treatment is valid as long as $V(r)$ does not change too rapidly. As an example of a

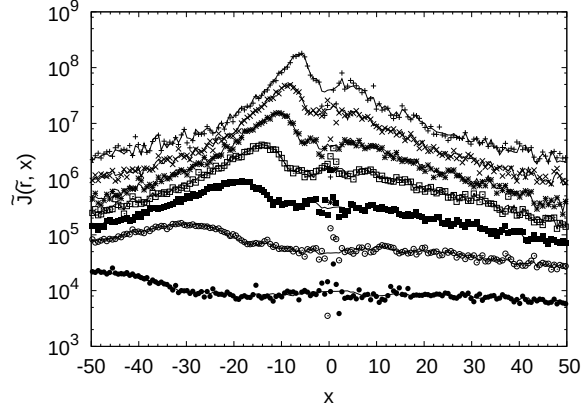


Figure A.6: Path length Monte Carlo solution (solid line) for coherent scattering arising from a continuum source with a uniform density profile and the velocity profile specified in Eq. (6.29), compared with the corresponding reference surface Monte Carlo solution (various points). Frequency profiles correspond to radii $\tilde{r} = 10^{-4.2}, 10^{-3.9}, 10^{-3.6}, 10^{-3.3}, 10^{-3.0}, 10^{-2.7}, 10^{-2.4}$.

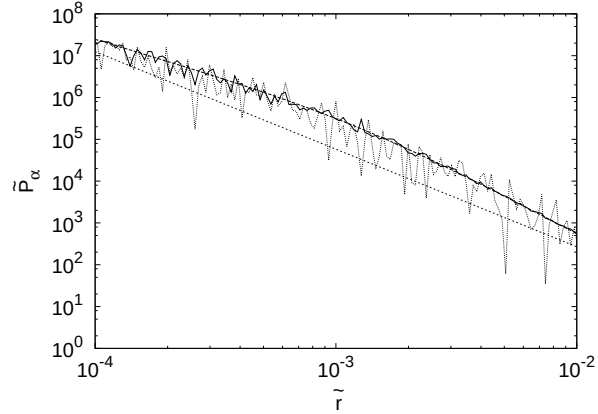


Figure A.7: Scaled scattering rate for the velocity profile given by Eq. (6.29), derived from the Monte Carlo solution obtained using the path length method (solid line), compared with that derived from the corresponding reference surface Monte Carlo solution (dotted line). For comparison we also show the corresponding moment/ray solution (dashed line) and $\tilde{P}_\alpha^{\text{diff}}$ (short-dashed line).

problem with a non-Hubble velocity profile, we have compared the path-length Monte Carlo solution with the previous Monte Carlo solution for coherent scattering from a continuum source in a uniform medium with the quadratic velocity profile of Eq. (6.29).

Our results are displayed in Figures A.6 and A.7 which show that, once again, the noise at line centre is significantly reduced, although there is still some non-negligible noise in the scattering rate close to the source.

From the various example problems examined in this appendix it is clear that the path length Monte Carlo method is superior to the reference surface method in determining the Ly α scattering rate. While we have only examined spherically symmetric problems, the path length method is easily generalisable via replacement of the volume V used in Eq. (A.1) with an appropriate cell volume. This method was brought to our attention after the rest of the work for the thesis was completed, hence the placement within an appendix, however it would be our preferred method for accurate computations of the Ly α scattering rate moving beyond spherical symmetry.

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