TOWARDS A MORE REALISTIC TREATMENT OF POLARISATION IN LYMAN ALPHA RADIATIVE TRANSFER

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Abstract

Lyman α radiation can be used as an astronomical and cosmological observable, being the strongest line among the hydrogen transitions. Using modern radiative transfer routines, it is possible to create simulations of accurate physical conditions and create predictions on observable properties of Lyman α radiation. Until recently has most information been obtained from the intensity and the spectrum, but a few observations (Hayes et al. 2011; Oesch et al. 2015) have been made which indicate that the polarisation also is an observable property. These observations yielded results that were in accordance with the simulated predictions by Dijkstra & Loeb (2008). However, the simulations by Dijkstra & Loeb (2008) are unique among the increasingly physically complex radiative transfer routines of recent times, as these largely ignore polarisation. Despite being rather unique, the treatment of Dijkstra & Loeb (2008) was not accurate. An approach that is accurate quantum mechanically, based on the density matrix formalism as a description of quantum systems, was devised and applied by Lee & Ahn (2002).

In this thesis is this formalism incorporated into an existing radiative transfer routine developed by Gronke & Dijkstra (2014), called tlc. The method is applied to analytical scattering scenarios, single scattering events of polarised and unpolarised radiation and multiple scatterings in a plane-parallel, semi-infinite slab of line centre optical depths $\tau_0 = 2 \times 10^2, 2 \times 10^3, 2 \times 10^4, 2 \times 10^6$. We show that the density matrix formalism is coordinate dependent, and produce a polarisation signal specific to the scattering medium described by Lee & Ahn (2002). We reproduce some key results from Lee & Ahn (2002); Chandrasekhar (1960). We show that the intrinsic degree of polarisation associated with each photon increases as a function of number of wing scatterings, which again depends on the optical thickness of the scattering medium. This photon-intrinsic increase in polarisation does not necessarily correspond to a detectable polarisation signal, as the latter depends on (not exclusively) the scattering geometry, the viewing angle and the measurement method. We find that scattering of polarised light follows the same angular distribution as scattering of unpolarised light, as predicted by Dijkstra & Loeb (2008). However, the degree of polarisation obtained from scattering of polarised light differs from the degree obtained when unpolarised light scatters. Future applications of the modified tlc on physically realistic scattering media may provide observational predictions on the polarisation signal that future telescopes could detect.
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Chapter 1

Introduction

A monk, a clone and a Ferengi decided to go bowling together...

1.1 Motivation

The most abundant element in the Universe is hydrogen. It is filled with sources of Lyman α (abbreviated “Lyα”) radiation, which is created from the de-excitation from the first excited state of hydrogen, to its ground state. The characteristic wavelength of this transition is $\lambda = 1215.67 \, \text{Å}$, and it is the strongest of the hydrogen transitions.

Observations of cosmological sources both in Lyα emission and absorption have provided ways to both infer physical properties of the observable universe (eg. Burles & Tytler 1998) and to detect the most distant galaxies (eg. the six candidates at $z \sim 10$ or 500 million years after the Big Bang found by Bouwens et al. (2015), the record-breaking spectroscopic observations by Oesch et al. (2015) of a galaxy at $z = 7.7302 \pm 0.0006$ and Finkelstein et al. (2013) of a galaxy at $z = 7.51$, both approximately 700 million years after the Big Bang. This brief overview does not contain possibly lensed candidates).

However, detection of distant absorption/emission sources is one thing—another is to determine the physical properties of these. The

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1Various characters from Star Trek: the Next Generation are cited at the beginning of each chapter.
very nature of the emission and absorption systems are in some cases so uncertain that they are referred to as Lyα blobs or Lyα nebulae: cosmological Lyα-fluorescent fog that sometimes envelope luminous active galactic nuclei (Cantalupo et al. 2014).

The extended Lyα signal detected by Cantalupo et al. (2014) around bright quasars at $z \approx 2.3$ was far beyond the reach of a dark matter halo, making them conclude that the observed radiation in fact was scattered, and not produced in situ. Whereas high signal-to-noise spectroscopic measurements can provide insight into the kinematics of the Lyα system (eg. Dijkstra et al. 2006; Orsi et al. 2012), they do not reveal information on the emission and scattering process—where were the photons created, and how much were they scattered before being observed?

A polarisation signal has proven to shed light on the last questions. Hayes et al. (2011) and Humphrey et al. (2013) have detected radially increasing degrees of polarisation around AGNs, and conclude that (some of) the observed radiation is scattered. This conclusion was reached by comparing the obtained degrees of polarisation with results obtained from numerical simulations by Dijkstra & Loeb (2008). In the latter simulations were scattered photons given an unrealistic degree of polarisation, being 100 % after each scattering. However, to observationally obtain a measure on the degree of polarisation, one has to both observe many photons and assess whether these are correlated in some fashion—is there some preferred oscillation direction for the electric vector of all the photons?

These correlations may be stronger along some viewing directions (ie. looking at a sphere nadir versus looking at its limb), for some wavelengths, and for some configurations (alignments) of polaroid filters that only let polarised light in one direction pass through.

Even though the observational approach by Dijkstra & Loeb (2008) has proved to yield results that later were reproduced observationally, the details of the scattering process is not quantum mechanically accurate. Despite being somewhat inaccurate, the implementation of polarisation by Dijkstra & Loeb (2008) is rather unique, in a time where other numerical radiative transfer codes increase in complexity and physical realism, but ignore polarisation.

In the unpublished article by Lee & Ahn (2002) is a quantum mechanical correct treatment of scattering of Lyα radiation presented. It allows for scattering of photons with various degrees of polarisation with various polarisation vectors.

The aim of this thesis is to incorporate the quantum mechanical method devised by Lee & Ahn (2002) into an existing Monte Carlo radia-
tive transfer routine developed by Gronke & Dijkstra (2014). However, the quantum mechanical method could yield polarisation properties that are restricted to observations of the type of idealised scattering media investigated by Lee & Ahn (2002), and the properties of the method is therefore analysed using a top-down approach.

The quantum mechanical method is applied to both theoretical scattering cases, numerical single scattering cases and in the full radiative transfer routine, thus treating multiple scatterings of photons. The obtained polarised properties are analysed to assess the inner workings of the quantum mechanical method and its applicability. The effects of having fully polarised photons on the distribution of scattering angles are also investigated.

1.2 Structure

A general introduction to cosmology is given in Chapter 2. Chapter 3 deals with cosmological sources of Lyα radiation, whereas Chapter 4 describes the framework needed to work with radiative transfer and polarisation. Chapter 5 describes the methods used to implement the density matrix formalism into an existing radiative transfer routine. Chapter 6 reports the results and comments them, and Chapter 7 summarises the results and provides an outlook.

1.3 Supervision

Ass. Prof. Dr. Mark Dijkstra at the Institute of Theoretical Astrophysics, University of Oslo, Norway has been the supervisor of this Msc. project.
Chapter 2

Cosmological Prelude

Perhaps, some day we will discover that space and time are simpler than the human equation.

Cpt. Jean-Luc Picard

2.1 Introduction

Space and time, or spacetime, is intimately intervened with its contents through the Einstein field equation,

\[ E_{\mu \nu} = \kappa T_{\mu \nu} \]  

(2.1)

where the Einstein tensor \( E_{\mu \nu} \) describes the curvature of spacetime and equates it to the stress-energy tensor \( T_{\mu \nu} \), which describes the content (represented as stress, energy and momentum), multiplied by the constant \( \kappa = 8\pi G/c^4 \).

This thesis does not encompass general relativity, as it does not delve into the properties of spacetime. What it does encompass, is a description of some of spacetime’s content. Thus will this text mainly reside at the right hand side of the Einstein field equation.

Which questions would it make sense to raise, should one be interested in understanding the contents of the Universe?

\(^1\)where \( G \) is the gravitational constant, and \( c \) is the speed of light in vacuum.
2. Cosmological Prelude

2.2 What is out there?

Throughout the history of mankind, several explanations of the contents, or building blocks, of the Universe have been presented.

From being the four elements earth, water, fire and the æther which the heavenly objects must have been made of in ancient Greece, today, we have the invisible cold dark matter, the visible baryonic matter, radiation (including traditional radiation and the more lucid neutrinos) and the driving force of the expanding Universe, the dark energy represented in the equations through the cosmological constant. These four (five, with neutrinos) elements make up the LCDM-model, which is the generally accepted cosmological model describing the contents and evolution of the universe.

However, our physical understanding of the Universe is strongly restricted by what we are able to measure or observe. It was observations of receding galaxies or (then) nebulæ, cepheid variable and supernovæ that made Hubble and Lemaître conclude independently that the Universe was expanding, (Livio 2011), and it is observations of the velocities of stars, and their luminosity that led to the conclusion that most of the galactic matter cannot be seen—hence its name, the dark matter.

Bright matter, or more precisely, baryonic matter, which in astrophysics include the electrons, which are leptons, and not baryons, is thus the origin of most of the observable quantities in astronomy. And these physical observables are used to test theoretical models as well as fundamental physics.

Can the very nature of the Universe be deduced from observations of baryonic structures? To answer this, we need a way of describing the nature of the Universe.

Cosmological models

The Einstein field equation, eq. (2.1), provide a starting point for describing the nature of the universe. In this section, the curvature of spacetime will be equated with an approximation of the contents of the universe.
2.2. What is out there?

The components of the stress-energy tensor,

\[
T^{\mu \nu} = \begin{bmatrix}
T^{00} & T^{01} & T^{02} & T^{03} \\
T^{10} & T^{11} & T^{12} & T^{13} \\
T^{20} & T^{21} & T^{22} & T^{23} \\
T^{30} & T^{31} & T^{32} & T^{33}
\end{bmatrix}
\]  

(2.2)

should give a full description of the components of the universe that cause spacetime to bend. Recalling that a 4-vector has four components

\[\mathbf{V} = \{\text{timelike component, three spatial coord.}\} = \{V^0, V^1, V^2, V^3\},\]

(2.3)

that can be written in terms of unit vectors, see App. A for a definition of the Einstein summation convention and other relevant concepts,

\[\mathbf{V} = V^\alpha \mathbf{e}_\alpha\]

(2.4)

and that an outer product of two vectors (or two one-forms where a one-form is a vector’s dual, or a mix of both, both being of rank-1) is needed to construct a tensor of rank-2,

\[A^{\mu \nu} \mathbf{e}_\mu \otimes \mathbf{e}_\nu = V^{\mu} \mathbf{e}_\mu \otimes W^{\nu} \mathbf{e}_\nu,\]

(2.5)

It should now be clear what the different components of \(T^{\mu \nu}\) of eq. (2.2) mean.

- Any component with a 0-superscript indicates that it is a magnitude of a vector product with at least one vector that has a direction in time,

- Whereas any component where either or both of the superscripts are different from 0 represent a spatial dependence, or the magnitude of a vector product where at least one vector has a spatial direction.

From special relativity (Taylor & Wheeler 1992), we recall that energy is a physical quantity which is purely determined from the observer’s experience of time, whereas the momentum is an effect of the observer being in a different rest frame from a massive object (the object can be said to be “moving”, which then reciprocally holds for the observer). The elements are (Grøn & Hervik 2007):

\(^2\)Greek sub-/superscripts are used for tensors of any rank which is represented in spacetime, whereas Latin is used for spatial components, and 0 for temporal components.
2. Cosmological Prelude

- $T^{00}$ represents energy density
- $T^{0i} = T^{0i}$ represents momentum density
- $T^{ii} > 0$ represents pressure
- $T^{ii} < 0$ represents stress
- $T^{ij} = T^{ji}$ represents shear forces

Assuming that the Universe can be described as an ideal fluid, and that we observe it in its rest frame, all off-diagonal elements ($T^{\alpha\beta}$, $\alpha \neq \beta$) disappear as there are no shear forces nor effects giving a non-zero 3-momentum.

A description of the curvature of spacetime is now needed, for this, a metric comes into aid. A metric provides an invariant description of distance in terms of a line element given a certain set of basis vectors,

$$ds^2 = \text{insert geometry here}$$  \hspace{1cm} (2.6)

where one can insert a sum of scalar products of basis vectors times products of coordinate differential by taking the inner product between differential vectors tangential to the manifold.

The simplest metric is that of flat spacetime, which is the spacetime version of an Euclidian metric, the Minkowski metric;

$$ds^2 = -c^2dt^2 + dx^2 + dy^2 + dz^2,$$  \hspace{1cm} (2.7)

which is the inner product of an infinitesimal distance vector (being a 4-vector) with itself, giving a scalar value that is independent of the observer's coordinate system. We have already treated the inner product of components which give the geometry of a manifold in eq. (2.8), and can understand the line element to consist of vector components

$$ds^\mu = (dt, dx, dy, dz)$$  \hspace{1cm} (2.8)

which does not reveal anything about the geometry, this information is embedded in the unit vectors,

$$e_0 \cdot e_0 = -c^2$$

$$e_i \cdot e_j = \delta_{ij}$$  \hspace{1cm} (2.9)

emphasising that they are tangential to the Minkowski manifold.

<+BRIDGE THE GAP HERE++>
2.2. What is out there?

Defining the metric tensor as
\[ g = g_{\mu\nu} \, dx^\mu \otimes dx^\nu \]  
(2.10)

it immediately follows that the elements \( g_{\mu\nu} \) of the Minkowski metric are
\[
\begin{pmatrix}
-c^2 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]
(2.11)

To wrap things up: one cannot leave out the geometry (which is represented through the metric) when dealing with vectors or one-forms. The inner product between two vectors is thus
\[
V \cdot W = V^\mu e_\mu \otimes W^\nu e_\nu = V^\mu W^\nu g_{\mu\nu}
\]  
(2.12)

which is invariant under coordinate transformations.

Challenge 2.1: Pick a vector in an orthonormal basis with an easy-to-find length. Now, construct a non-orthonormal basis and represent the same vector in this. Take the inner product with itself. Did it change?

The next step is to compare the curvature of spacetime to its contents.

The Einstein tensor can be expanded in terms of the Ricci scalar \( R \) and the Ricci curvature tensor \( R_{\mu\nu}; \)
\[
E_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R.
\]  
(2.13)

The Ricci curvature tensor is a contraction of the Riemann tensor, which consists of connection coefficients and their derivatives. These describe the curvature of the metric by means of parallel transport of vectors tangential to it (walk a round on a metric, keeping the unit vectors pointing in the same direction all the time—are they pointing where they did when you come back to where you started?). The Ricci scalar is a contraction of the Ricci tensor.

Then, to find the curvature part of the Einstein field equation, the metric is examined using the Riemann tensor and its contractions. But what metric should we use?

The most familiar choice has been given above, but, as we need the derivatives of the connection coefficients, we know that one or more of the metric components must be dependent (a function) of the coordinates, otherwise we will end up with an empty left hand side of eq. (2.1).

Assuming that the Universe can expand (or contract), the scale-factor \( a(t) \) makes the spatial coordinates become time-dependent giving this metric for the case of a flat universe described in Cartesian coordinates
\[
g_{\mu\nu} \, dx^\mu \otimes dx^\nu =
\]  
(2.14)
2. Cosmological Prelude

Now that we have ensured that the curvature part of the Einstein field equation will not be zero (which would imply that the right hand side also became zero, corresponding to an empty universe), we need to fill the stress-energy tensor.

As already assumed, if the universe is described as a perfect fluid, and observed from its rest frame, then $T_{\mu\nu}$ is on diagonal form. Following Grøn & Hervik (2007) and Zee (2013), who give the stress-energy tensor as

$$T_{\mu\nu} = \left( \rho + \frac{p}{c^2} \right) U_\mu U_\nu + p g_{\mu\nu}$$

(2.15)

where $\rho$ once more is the mass density, $p$ is the pressure (which does not have any preferred direction, allowing it to be put simply as $p$), and $U_\alpha$ are the components of the 4-velocity of the fluid, which has to oblig the identity

$$U^\mu U^\nu g_{\mu\nu} \equiv U^\mu U_\mu = -c^2$$

(2.16)

and, as we are comoving with the fluid, the spatial components of the 4-velocity must be zero, leaving

$$U^\mu = (1, 0, 0, 0)$$

(2.17)

and, lowering the index,

$$U_\nu \equiv U^\mu g_{\mu\nu} = \left(-c^2, 0, 0, 0\right).$$

(2.18)

The time-time (00) component is thus

$$T_{00} = \left( \rho + \frac{p}{c^2} \right) c^4 - pc^2 = \rho c^4$$

(2.19)

which can be compared to the curvature part of the Einstein field equation, which is obtained from contraction of the Riemann tensor,

$$R_{00} - \frac{1}{2} R g_{00} = -3 \frac{\ddot{a}}{a} + \frac{1}{2} \frac{6}{c^2} \left( \left( \frac{\dot{a}}{a} \right)^2 + \frac{\ddot{a}}{a} \right) c^2$$

$$= 3 \left( \frac{\dot{a}}{a} \right)^2.$$

(2.20)

Here, $R \equiv R^\mu_\mu$ is the trace of the Ricci tensor, and where the 00-components of the Ricci tensor, $R_{00}$, were obtained by using the antisymmetry of the Riemann tensor, $R^\gamma_\beta\gamma_\delta = -R^\gamma_\delta\beta_\gamma$, when contracting it; $R_{00} = R^\alpha_\alpha_{00} = -R^\alpha_\alpha_{00}$. The dot(s) over the scale factor denote derivative with respect to time.
2.2. What is out there?

From the Einstein field equation for the \(00\)-component, we get

\[
3 \left( \frac{\dot{a}}{a} \right)^2 \equiv 3 \left( H(t) \right)^2 = \frac{8\pi G}{c^4} \rho c^4 = 8\pi G \rho \tag{2.21}
\]

which is the first Friedmann equation for a flat universe.

To make use of the spatial components of the Ricci tensor (the contraction of the Riemann tensor), we could take the trace of both sides of the Einstein field equation by first raising one index,

\[
g^{\mu \nu} R_{\mu \nu} - \frac{1}{2} R g^{\mu \nu} g_{\mu \nu} = \kappa g^{\mu \nu} T_{\mu \nu}
\]

\[
R^\mu_\mu - \frac{1}{2} \mathcal{R} \delta^\mu_\mu = \kappa T^\mu_\mu \tag{2.22}
\]

where the metric identity \( g^{\alpha \beta} g_{\beta \gamma} \equiv \delta^\alpha_\gamma \) was used, where \( \delta^\alpha_\beta \) is the Kronecker delta, and then summing over the same indices,

\[
R^\mu_\mu - \frac{1}{2} R^\mu_\mu \delta^\mu_\mu = \kappa T^\mu_\mu
\]

\[
\mathcal{R} - \frac{4}{3} \mathcal{R} = \kappa \mathcal{T}
\]

\[
\mathcal{R} = -\kappa \mathcal{T}
\]

\[
\frac{6}{c^2} \left( \left( \frac{\dot{a}}{a} \right)^2 + \frac{\ddot{a}}{a} \right) = -\kappa \left( \frac{-\rho c^4}{c^2} + 3 \frac{\dot{a} \rho}{a} \right) = -\frac{8\pi G}{c^4} \left( 3\rho - \rho c^2 \right) \tag{2.23}
\]

Using that \( (\dot{a}/a)^2 \) is given in eq. (2.21), we get

\[
\frac{\ddot{a}}{a} = -\frac{4\pi G}{3c^2} \left( 3\rho - \rho c^2 \right) - \frac{8\pi G}{3} \rho
\]

\[
= -\frac{4\pi G}{3} \left( \rho + \frac{3\rho}{c^2} \right) \tag{2.24}
\]

which is the second Friedmann equation for a flat universe.

A more common metric, is one that allows spacetime to have an intrinsic curvature. This is represented through the parameter \( k = -1, 0, +1 \) which corresponds to a closed universe (walking in a straight line will get you where you started), a flat universe (two friends who start out walking in parallel, will not move away from each other), and an open universe.
2. **Cosmological Prelude**

(The two friends walking in parallel would move away from each other). This metric is called the Friedmann-Lemaître-Robertson-Walker, and is given as

\[
\text{FLRW-metric} \quad ds^2 = -c^2 dt^2 + a^2(t) \left[ \frac{1}{1 - kr^2} dr^2 + r^2 d\Omega^2 \right]
\] (2.25)

where we have the scale factor \( a \) and the curvature parameter \( k \) which can take on any value \([-1, 1]\).

The right hand side gives the contents of the universe. As stated, we have dark matter, visible matter, radiation (and neutrinos). Each of these are represented by different stress-energy tensors.

**Archaic cosmological models**

In the category *archaic* cosmological models fall the models that either have been observationally falsified, or are unstable in their very nature, making them unable to explain the stable universe. A note of caution is in place, however, as belief, and not science, has condemned models to be archaic, only to be rediscovered later.

Currently accepted archaic models include the Einstein universe (closed, static), the Einstein-de Sitter universe (dust-filled, flat), the de Sitter universe (flat, empty with cosmological constant), etc. (Elgarø y 2009).

An example of a central theoretical feature that was abandoned and revived, is the cosmological constant \( \Lambda \). Introduced by Einstein (1917) as an additional term to a pressure-free \( (p = 0) \), thus consisting of dust) universe, which either was empty or of zero size (Elgarø y 2009), Einstein deduced a static, closed universe. This *Einstein universe* is highly unstable—any perturbation away from its equilibrium radius would make it either expand or collapse.

Einstein regretted introducing the cosmological constant, in light of the discovery of the Hubble expansion. It remained unpopular among authors, but gained usage as an integration constant (without any *a-priori* value), an energy difference (between the *true* energy density and the one deduced laboratory physics) and a zero-energy (Peebles & Ratra 2003).

In modern cosmology, the cosmological constant is revived, providing the cosmological models with a time-independent vacuum energy that provides the needed age to explain the oldest stars. In the currently accepted cosmological model the ΛCDM model, the current (our!) epoch is *dominated* by the \( \Lambda \)-term.
2.2. What is out there?

The cosmological $\Lambda$CDM model

Listed in the previous subsection were different archaic cosmological models. Alone, they do not explain the evolution of the universe, but a combination of concepts from these into a large unified model, a cosmological model appears that is able to explain both the evolution of the universe at early times, to the current accelerating expansion.

The act of “combining several concepts” from the other models can be done by working with the Friedmann equations. The stress-energy tensor of eq. (2.1) can be decomposed into the individual components $x$ with densities $\rho_x$ that comprise the universe. Assuming it consists of

- $\Lambda$: a vacuum energy/dark energy/quintessence that drives the current accelerating expansion of the universe, represented through the cosmological constant which is added to the left hand side of eq. (2.1), with $\rho_{\Lambda}$,
- Cold, dark matter: cold, non-baryonic matter that only interacts with other matter through gravitation, with $\rho_{\text{CDM}}$,
- Baryonic matter: visible (interacts electromagnetically) matter, with $\rho_{b}$,
- Radiation: electromagnetism, or light, with $\rho_{r}$,
- Neutrinos: low-mass particles (leptons) that only weakly interacts with baryonic matter, making them in practice belong to the category “radiation”, with $\rho_{\nu}$.

We may introduce a parameter that is relative to a critical density (the density needed to sustain a flat, $k = 0$, Universe) and attempt to write the 1. Friedmann equation in terms of it,

$$\Omega_x = \frac{\rho_x}{\rho_c}$$ (2.26)

where the critical density is

$$\rho_c = \frac{3H^2(t)}{8\pi G}.$$ (2.27)

The evolution of each component can be integrated separately, yielding different dependencies on the scale factor $a$. Even the curvature term $k$ of Eq. (2.25) can be considered a separate component with a separate evolution history.
2. Cosmological Prelude

Denoting present-day values with the subscript “0”, the Friedmann equation can be simplified to

\[
\frac{H(t)}{H_0} = \left[ \frac{\Omega_{\text{CDM}} + \Omega_b}{a^3} + \Omega_\Lambda + \frac{\Omega_\gamma + \Omega_\nu}{a^4} + \Omega_k \right] (2.28)
\]

but, observationally, only the relevant parameters for the cosmological ΛCDM-model are estimated.

The parameters are estimated by Planck Collaboration et al. (2015). Previous results from WMAP (Hinshaw et al. 2013) give the baryon density \(\Omega_b h^2 = 0.02240\), the cold dark matter density \(\Omega_{\text{CDM}} h^2 = 0.1146\) and the dark energy density \(\Omega_\Lambda = 0.7181\), with \(H_0 = 100 h\ \text{km s}^{-1} \text{Mpc}^{-1}\) being the present-epoch Hubble constant, with \(H_0 = 69.7\).

2.3 Are we special?

What facilitates our existence? And are our observations dependent (or affected) by the fact that the observations are carried out by us?

These questions may seem archaic, but does have wide-ranging implications. Copernicus challenged the Aristotelean geocentric cosmology, where existence must be understood in terms of the causes of things. Following Aristotle (Falcon 2015), it is insufficient to understand the composition of things (which differs from the atomists’ perspective), as proper knowledge is only obtained when the final cause of things, that is: their reason, are understood.

Even if Copernicus explained the motion of planets according to a heliocentric model (opposing Aristotle and much of the contemporary scientific community), he did not oppose the contemporary idea that man was the final cause of nature (Barrow & Tipler 1986). Yet, the move to a heliocentric world-view, can be thought of as a major move towards reducing the role of the observer in the universe.

How far has this reduction gone? To investigate this, the guiding principles for current cosmological models can be discussed. These are:

1. The Copernican principle: our position in the universe is typical (ie., not special in any way),

2. The cosmological principle: at sufficient large scales, the universe is isotropic (the properties have no preferred directionality) and homogeneous (the constituents of the universe are uniformly distributed across it).
The Aristotelean model of the universe violates both principles. It gives the observer the preferred position, and has a structure that neither is isotropic nor homogeneous.

While the principles, at first glance, reduce the significance of the observer to nothing (which is in stark contrast to the quantum mechanical perspective, where an observation alters the observed system), they also act as safety mechanisms. They ensure that something can be inferred about the universe from observations of its contents.

An important note on the cosmological principle is needed—it only applies on large scales. It is then possible to have both significant overdensities at small scales, as a unique planetary system, but also that this planetary system is a part of a more uniform, isotropic structure on cosmological scales.

A philosophical possibility that would violate the Copernican principle is that the universe takes on different properties dependent on the position of the observer. If the laws and constants of physics are different throughout universe, the models that only adhere to the subset that we observe would fail to describe the universe observed from any other location. In essence would observations be specific to the observer.

The last statement is, however, to a large extent true. To understand why, the initial question, how far the reduction of the importance of the observer can continue, must be given some lower bound. The weak anthropic principle (Barrow & Tipler 1986) is a good candidate:

The observed values of all physical and cosmological quantities are not equally probable but they take on values restricted by the requirements that there exist sites where carbon-based life can evolve and by the requirement that the Universe be old enough for it to already have done so.

The properties of the Universe must thus be such to allow humans to (exist and) observe it. As humans are constrained by space and time, we may for instance only observe a fraction of the thought infinite universe, that is, the parts of it from which light reaches Earth, which is called the observable universe.

The weak anthropic principle thus gives a lower bound on the significance of the observer on the observed universe. It acts as a constraint on the age (old enough to allow intelligent life to develop) and size (it must be large enough to the matter to reach an equilibrium where intelligent life is supported) (Barrow & Tipler 1986). It also provides a clue on the importance of the properties of the observer, which determine what is seen.
Chapter 3

Hydrogen transitions in astrophysics

3.1 Some astrophysical sources and applications

As hydrogen is the most abundant element in the universe, strong emission and absorption features originating from hydrogen transitions are expected and observed throughout the universe from various astrophysical objects.

On the largest scales are hydrogen lines used for both constraining the Big Bang nucleosynthesis (Burles & Tytler 1998) and to trace out the distributions of dark matter (Cen & Ostriker 1999). Hydrogen lines are also crucial in the determination of emission systems, the transition Hα, corresponding to the de-excitation from the third level of hydrogen to the second ground level yielding radiation with the laboratory wavelength 6562.8 Å, is often very dominant (Kennicutt 1998). As mentioned in the introductory Ch. (1), are some of the most distant galaxies observed in Lyα emission.

Following the Big Bang, the universe was a hot and dense place, but with few structures. Quantum fluctuations seeded the initial density per-
turbations that would later on lead to gravitationally bound structures, but before these came into existence, the Universe was mostly dark and opaque. This period between the (re)combination of protons and electrons into neutral hydrogen around 400,000 years after the Big Bang, and the formation of the first galaxies around 400 million years after the Big Bang, is called the dark ages (Zaroubi 2013).

The end of the dark ages were marked by the ionisation of the intergalactic medium, driven by luminous UV-emitting sources. Possible sources of this reionisation process are the first and second generations of stars, (Pop. III and II, respectively) and (mini-) quasars. Accretion disks around supermassive black holes where the origins of the mass is somewhat unknown could also provide wealths of ionising UV- and X-ray radiation (Zaroubi 2013). The earliest stars, Pop. III stars, were also vigorous emitters of ionising radiation, producing up to five orders of magnitude more radiation in certain wavelengths than the more metal rich, long-lived Pop. II stars (Ciardi & Ferrara 2005).

Some of the main evidences of a reionisation epoch where the Universe went from consisting of mostly neutral HI to ionised HII, are observations of the Gunn-Peterson trough, yielding an increasing column density (and hence more absorption or scattering out of the line of sight) of neutral HI for increasing redshifts (Ciardi & Ferrara 2005; Zaroubi 2013). Fan et al. (2006) did a systematic study of multiple, increasingly distant quasars and found results indicating increasing IGM absorption in the hydrogen transitions related to the ground state, the Lyman-series, for increasing redshifts. See Fig. (3.1) for the hallmark figure by Fan et al. (2006) showing decreasing fluxes for wavelengths shorter than the Ly$\alpha$ emission line, indicating presence of neutral hydrogen.

The driving process of recombination can be mapped using the hydrogen 21 cm-line, which is intrinsically coupled to the local Ly$\alpha$ radiation field. As the wavelength (21 cm) is much larger than the local Ly$\alpha$ emission wavelength (1.2 $\times$ 10$^{-5}$ cm), it is much less likely to be scattered or absorbed by local (and distant) HI. Current and future low-frequency radio-interferometers as LOFAR (Low-Frequency Array, Jelić et al. 2008), MWA (Murchison Widefield Array, Bowman et al. 2013) and the SKA (Square Kilometre Array Mellema et al. 2013) may thus provide insight into the reionisation process using observations of the 21 cm line.
3.1. Some astrophysical sources and applications

**Figure 3.1:** Fluxes from 19 SDSS quasars sampled by Fan et al. (2006) showing decreasing fluxes bluward of the Lyα emission line, indicating increasing amounts of neutral hydrogen in the early Universe, consistent with the view that the Universe was reionised from a neutral, opaque state, to the current ionised, transparent state.
3. Hydrogen transitions in astrophysics

3.2 Hydrogen lines

In Fig. (3.2) are different level splittings plotted for the Ly\(\alpha\) transition, which is the transition a hydrogen atom undergoes when it de-excites from the first excited state \(n = 2\) to the ground state \(n = 1\).

The Lyman series are transitions from the excited levels \(n = 2, 3, 4, 5, \ldots\) to the ground state \(n = 1\) and are denoted Ly\(\alpha\), Ly\(\beta\), Ly\(\gamma\), Ly\(\delta\), etc., respectively. Ly\(\alpha\) is the transition corresponding to an emission/absorption of the longest wavelength in the Lyman series, where the higher order transitions correspond to larger energy differences and hence more energetic emitted/absorbed radiation.

The 21 cm line corresponds to a forbidden transition between the two hyperfine levels \(F = 1 \rightarrow 0\), corresponding to a spin flip. The decay rate is low, approximately \(\sim 10^{-15} \text{s}^{-1}\), but due to the large amounts of hydrogen it can still be an important astrophysical observable.

The H\(\alpha\) line was mentioned earlier, it is the transition from the \(n = 3\) level to the \(n = 2\) level. The series with transitions to the \(n = 2\) level are named the Balmer series, and denoted H\(\alpha\), H\(\beta\), H\(\gamma\), etc., for transitions \(n = 3 \rightarrow 2, n = 4 \rightarrow 2, n = 5 \rightarrow 2\), etc., respectively.

Other series, corresponding to de-excitations/excitations from higher \(n > 2\), also exist. The Paschen series are transitions where the lower level is \(n = 3\), the Bracket series has the lowest \(n = 4\), the Pfund series has \(n = 5\) and the Humphrey series has \(n = 6\).
Figure 3.2: Possible levels associated with the Lyα transition where the lower level is $n = 1$ and the upper level is $n = 2$, from Brasken & Kyrola (1998). The notation is on the form $nLJ$ where $n$ denotes energy level, $L$ denotes orbital angular momentum and $J$ denotes total angular momentum, see Ch. 4. $F$ denotes hyperfine levels, and give the difference between the magnetic moments from the spin of the nucleus and the electron. Degenerate hyperfine levels are denoted $m_F$. The 21 cm line corresponds to a forbidden (extremely rare) transition between the $F = 0$ and $F = 1$ levels in the ground state, $n = 1$. Higher order Lyman series transitions correspond to transitions where the upper level is $n > 2$. Other transition series where the lower level $n > 1$ are given in the text. Hα is the $n = 3$ to $n = 2$ transition, being the strongest transition in the Balmer series (where the lower $n = 2$).
Chapter 4

Lyman alpha transfer and polarisation

Resistance is futile.

The Borg

This chapter will deal with the methods involved in transfer of Lyman alpha photons, with a particular emphasis on polarised radiative transfer. Methods for dealing with polarisation on a quantum mechanical scale, observational scale, and in numerics are presented.

4.1 Radiative transfer

Einstein relations

The Einstein coefficients are used to describe the quantum mechanical processes leading to emission or absorption of radiation.

To explain the coefficients, it is necessary to distinguish between radiative process that are caused by changes in the atomic configurations (excitations, de-excitations, ionisation and recombination) and those who are caused by (de-)acceleration of particles. Following Rutten (2003),

- **Bound-bound (bb)** processes lead to emission, scattering or absorption of radiation from excitations and de-excitations of atoms and molecules. These processes are hence dependent on the energy differences between the discrete different atomic configurations. The relevant atomic processes are
4. Lyman Alpha Transfer and Polarisation

- Radiative and collisional excitation
- Spontaneous, induced/stimulated and collisional de-excitation

• **Bound-free (bf)** processes involve ionisation or recombination of atoms and molecules, and the energy differences can thus be continuous. The relevant processes are
  - Radiative and collisional ionisation
  - Recombination, collisional and induced/stimulated recombination

• **Free-free (ff)** processes, strictly speaking only consists of thermal bremsstrahlung. It is *thermal* as kinetic energy is lost as radiation, and the kinetic energy is lost due to *bremsung* (braking) of a particle in an electric field. Should the acceleration be in a *magnetic field*, then the resulting radiation is *cyclotron* or *synchrotron* radiation.

The Einstein coefficients are given per particle with unit s⁻¹, and are defined as:

- \( A_{ul} \) is the transition probability that a particle goes from an upper state (subscript \( u \)) to a lower state (subscript \( l \)) spontaneously.

- \( B_{lu} J_{\nu_0} \) is the transition probability for a particle going from a lower to an upper level given an incident radiation field \( J_{\nu_0} \) (angle and frequency averaged intensity). This corresponds to radiative excitation.

- \( B_{ul} J_{\nu_0} \) is the opposite of \( B_{lu} \), now, it is the transition probability of a particle being de-excited given an incident radiation field. This corresponds to induced/stimulated de-excitation.

- \( C_{ul} \) and \( C_{lu} \) are the probabilities for collisional de-excitation (from level \( u \) to level \( l \)) and collisional excitations (from \( l \) to \( u \)).

Note that the angle and frequency averaged intensity \( J_{\nu_0} \) is dependent on the core (resonance) frequency of the transition, thus will deviations in frequency from the core frequency decrease the overall transition probability. See Rutten (1988) for further details on the related profile functions.

The Einstein relations can be used to give a precise description of the processes involved in both emission and transport of radiation. The *transport equation* and its dependent variables can be used to relate the quantum processes to large scale observables.
4.1. Radiative transfer

Transport equation

The central equation in radiative transfer is the transport (or transfer) equation, which gives how the intensity changes as a function of geometric stretch $s$ travelled,

$$\frac{dI_\nu}{ds} = j_\nu - \alpha_\nu I_\nu$$  \hspace{1cm} (4.1)

where the subscript $\nu$ denotes a frequency dependence of the related quantity, thus can they be called monochromatic. The quantities involved are the intensity $I_\nu$, the differential geometric stretch $ds$, the emission coefficient $j_\nu$ and the extinction coefficient $\alpha_\nu$.

However, an additional term may be added to Eq. (4.1) that accounts for contributions from redistributed radiation. This term, the redistribution function $R$, redistributes radiation propagating an arbitrary direction $n'$ into the beam direction $n$, as well as any frequency $\nu'$ into $\nu$. Its total contribution to the transport equation would then be

$$\int d\nu' \int dn' I(\nu', n') R(\nu', \nu, n', n)$$  \hspace{1cm} (4.2)

which is an integral over all possible frequencies and all possible directions radiation could be scattered from. The direction $n$ of the beam in the transport equation would then have to be given explicitly,

$$n \cdot \nabla I_\nu(n) = j_\nu(n) - \alpha_\nu I_\nu(n) + \int d\nu' \int dn' I_\nu(n') R(\nu', \nu, n', n)$$  \hspace{1cm} (4.3)

where $n \cdot \nabla$ reduces to $d/ds$ in the case where the directional dependence can be ignored. This makes the transport equation become an integro-differential equation, see eg. (Dijkstra (2014)). The redistribution function has been discussed by eg. Unno (1952) who introduced an approximation that could account for the thermal motion of the scattering particles, by Adams (1972) who applied the approximation of Unno (1952), and by Harrington (1973) who generalised the results.

The integro-differential equation is only solvable in a few idealised cases, and numerical methods are needed to deal with more realistic scenarios.

Emission and absorption coefficients

Following Rutten (1988), the emission coefficient is the proportionality constant $j_\nu$ in the expression between a change in energy $E_\nu$ given a
change in volume $V$, time $t$, frequency $\nu$ and solid angle $\Omega$,

$$dE_\nu \equiv j_\nu \, dV \, dt \, d\nu \, d\Omega$$  \hspace{1cm} (4.4)

a positive change in a monochromatic bundle of light, in form of photons from spontaneous de-excitation processes. The relevant Einstein coefficient is $A_{ul}$. It can be useful to introduce the intensity $I_\nu$,

$$dE_\nu \equiv I_\nu(x, n, t) \, n \cdot a \, dA \, dt \, d\nu \, d\Omega$$  \hspace{1cm} (4.5)

which is the proportionality constant where energy is transported in the direction $n$ through a surface $dA$ with area vector $a$, rather than a volume $dV$. It can be related to a change in intensity (Rutten 1988) over a path length $ds$,

$$dI_\nu(s) = j_\nu(s) \, ds$$  \hspace{1cm} (4.6)

which thus is a function of path length traversed $s$.

Similarly is the absorption coefficient the proportionality constant $\alpha_\nu$ in the case of a negative change in energy, or reduction in intensity,

$$dI_\nu \equiv -\alpha_\nu \, ds$$  \hspace{1cm} (4.7)

The monochromatic optical thickness $\tau_\nu$ can be defined in terms of the extinction given in Eq. (4.7),

$$d\tau_\nu(s) \equiv \alpha_\nu(s) \, ds$$  \hspace{1cm} (4.8)

which can be integrated, given that the absorption coefficient is constant in the medium, yielding a relation between physical distance and the optical thickness light perceives,

$$\tau_\nu(s) = \alpha_\nu s.$$  \hspace{1cm} (4.9)

### Photon creation, scattering and destruction

In the previous subsections were processes that govern creation, destruction and scattering of photons presented.

- **Photon creation** is the process where photons are created through collisional excitation of an atom followed by radiative de-excitation. The photons will have no recollection of the events or processes that lead to the creation of it. The relevant Einstein coefficients are $C_{lu}$, $A_{ul}$ and $B_{ul}J_{nu}$. 

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4.2 Polarisation

- **Photon scattering** is the process where photons retain their identity after interacting with an atom. The process thus requires a radiative excitation of an atom, followed by radiative de-excitation. The relevant Einstein coefficients are $B_{lu}J_{v0}$, $A_{ul}$ and $B_{ul}J_{v0}$.

- **Photon destruction** is the process where an incoming photon excites an atom whereas the atom is de-excited collisionally. The relevant Einstein coefficients are $B_{lu}J_{v0}$ and $C_{ul}$.

The definitions do not account for processes where photons are created by acceleration of particles (bremsstrahlung, cyclo- and synchrotron radiation), but are given as in Rutten (1988). To understand the reason, it is possible to differ between thermal and non-thermal processes, which photon creation and destruction both are.

Thermal processes "couple the radiation energy to the local kinetic energy" (Rutten, 2003), whereas non-thermal processes depend on the local radiation field which not necessarily reflects the local (kinetic) temperature.

Scattering of photons are hence non-thermal, and so are bremsstrahlung, cyclo- and synchrotron radiation.

4.2 Polarisation

Polarisation is a property of the electric field of the radiation, describing the preferred oscillation direction of the field. It is loosely defined by Chandrasekhar (1960) as

> [A] known amount of retardation in the phase of vibrations in one direction relative to the phase of vibrations in a direction at right angles to it, and then measure the intensity in all directions in the transverse plane.

This definition is suitable for both observational use as well as theoretical use, with a slight interpretative difference. Observationally, the polarisation is measured as a collective phenomenon, being the statistical average of the direction of the electric field of the photons that arrive at the detector during the integration time. Theoretically, however, the polarisation can be described as a possible time-dependent orientation of the electric field $\mathbf{E}$, always being perpendicular to the Poynting vector $\mathbf{S} = \mathbf{E} \times \mathbf{H}$ with $\mathbf{H}$ being the magnetic field. $\mathbf{S}$ points in the direction of energy flow.
Polarisation in observations: Stokes parameters

The four Stokes parameters $I, Q, U$ and $V$ provide an observational formalism for handling polarisation, but can also be described in terms of properties of the radiation field. They provide an unambiguous description of the radiation and *Mueller calculus* can be used to describe for instance polarisation effects from observational filters and prisms.

The Stokes parameters are described in detail in *e.g.* Chandrasekhar (1960); Rybicki & Lightman (1979); del Toro Iniesta (2003). From an observational viewpoint, the Stokes parameters can be obtained by comparing the intensity through different polarisation filters aligned at different angles $\theta$ to each other and by comparing the constant phase lag $\delta$ between the intensity along one polarisation direction and another that is perpendicular in the image plane to the former. Denoting the measured intensity $I_{\text{meas}}(\theta, \delta)$, the measurable Stokes parameters are

\[
\begin{align*}
I & = I_{\text{meas}}(0, 0) + I_{\text{meas}}(\pi/2, 0), \\
Q & = I_{\text{meas}}(0, 0) - I_{\text{meas}}(\pi/2, 0), \\
U & = I_{\text{meas}}(\pi/4, 0) - I_{\text{meas}}(3\pi/4, 0), \\
V & = I_{\text{meas}}(\pi/4, \pi/2) - I_{\text{meas}}(3\pi/4, \pi/2)
\end{align*}
\]

(4.10)

where $I$ denotes the total intensity, $Q$ the degree of linear polarisation along the coordinate axes of the image plane, $U$ the degree of linear polarisation from two axes that are rotated $\pi/4$ compared to the image plane axes, and $V$ the degree of circular polarisation (del Toro Iniesta 2003).

By following del Toro Iniesta (2003), who introduces a set of basis vectors that allows for the helicity of photons to be accounted for, it is possible to relate the Stokes parameters to the physical properties of the ray.

The choice of a complex coordinate system is closer to the physical reality than a real coordinate system in which the helicity as a fundamental property must be derived as a linear combination of unit vectors. The complex basis vectors are

\[
\begin{align*}
e^{\ell} & \equiv \frac{1}{\sqrt{2}}(e_x + ie_y), \\
e^r & \equiv \frac{1}{\sqrt{2}}(e_x - ie_y), \\
e^z & \equiv e_z
\end{align*}
\]

(4.11)
4.2. Polarisation

where \( \{ \mathbf{e}_e, \mathbf{e}_r, \mathbf{e}_z \} \) form a Cartesian basis. A similar definition is also used by Lee et al. (1994) as the ion basis \( \{ \mathbf{e}_q \} \) (their Eq. (2.2)). The subscript \( l \) and \( r \) denotes left and right-handed helicity, respectively. The vectors are perpendicular to each other, note that a \( \pi/2 \) rotation in the complex plane gives \( \pm i = e^{\pm i\pi/2} \). A electromagnetic wave at a location \( x \) propagating in the \( \mathbf{e}_z \)-direction may be written as

\[
\mathbf{E}(x,t) = E_r(x,t)\mathbf{e}_r + E_l(x,t)\mathbf{e}_l
\]

(4.12)

and the Stokes parameters can be defined as

\[
\begin{align*}
I &\equiv \kappa \langle |E_r|^2 + |E_l|^2 \rangle, \\
Q &\equiv \kappa \langle (E_rE_l^*) + (E_lE_r^*) \rangle, \\
U &\equiv i\kappa \langle (E_lE_r^*) - (E_rE_l^*) \rangle, \\
V &\equiv \kappa \langle |E_r|^2 - |E_l|^2 \rangle,
\end{align*}
\]

(4.13)

where \( \kappa \) is a normalisation factor “that translates the Stokes parameters into intensity units” (del Toro Iniesta 2003) and the brackets denote time-averaged values.

The \( I \) parameter gives the total intensity of a beam, whereas the \( V \) parameter give the total circular polarisation (maximum if the beam either is right- or left-handed). The \( Q \) and \( U \) parameters give the degree of linear polarisation, which in this formalism is represented as a superposition of the left- and right circular components of the ray.

For further discussions and more elaborate derivations of the Stokes parameters, see eg. paragraph 15 of Chandrasekhar (1960), chapter 2.4 of Rybicki & Lightman (1979). See also del Toro Iniesta (2003) for Mueller calculus, the Jones vector, instrumental effects and the Poincaré sphere \( \mathbb{P} \) as a representation of the Stokes parameters.

Polarisation in theory

Each polarisation state can be understood in terms of the two possible spin states of light, the helicity of photons, being either clockwise (right-handed) or counter-clockwise (left-handed) around the propagation direction of the photon. The polarisation (space) of each photon can thus be described (spanned) by two complex 4-vectors \( \mathbf{e}^{\mu}(\mathbf{k}, \sigma) \) where \( \mathbf{k} = \mathbf{k}/|\mathbf{k}| \) is the unit vector pointing in the photon momentum direction and \( \sigma = \pm \) corresponding to a right \((\sigma = +)\) or left circularly polarised photon. Fol-
4. Lyman alpha transfer and polarisation

Following Weinberg (1995), the polarisation vectors also adhere to

\[ \mathbf{k} \cdot \varepsilon(\mathbf{k}, \sigma) = 0 \]  
(4.14)  
\[ \varepsilon^0(\mathbf{k}, \sigma) = 0 \]  
(4.15)

which are the formal requirements for orthogonality to the momentum direction (Eq. (4.14)) and for being in the rest frame of the system (Eq. (4.15)).

Following Weinberg (2013), the wave function of a photon with momentum \( \hbar \mathbf{k} \)
is

\[ \Psi_{k, \xi} \equiv (\xi_+ a^\dagger(\mathbf{k}, +) + \xi_- a^\dagger(\mathbf{k}, -)) \Psi_0\gamma \]  
(4.16)

which corresponds to a superposition of the states obtained by using the ladder operator \( a(\mathbf{k}, \sigma) \) for the two possible helicities of the photon, \( \sigma = \pm \) (the ladder operators \( a^\dagger \) and \( a \) raises and lowers the energy, respectively). The subscript \( 0\gamma \) of the eigenstate \( \Psi_0\gamma \) denotes that it is the radiative (\( \gamma \)) eigenstate for the ground state (0) of the corresponding radiative Hamiltonian operator, opposed to the possible matter eigenstate.

The factors \( \xi_\pm \) are bound by the constraint

\[ |\xi_+|^2 + |\xi_-|^2 = 1 \]  
(4.17)

and the factors are generally complex. Equality, \( \xi_+ = \xi_- = 1/\sqrt{2} \), give a linearly polarised photon, whereas having \( \xi_\pm = 1 \) and \( \xi_\mp = 0 \) give a circularly polarised photon with defined helicity. Any other combination give rise to elliptical polarisation.

**Polarisation of Ly\( \alpha \): origins**

The degree and direction of polarisation a wave packet—a photon—obtains after a scattering event is intimately related to the quantum mechanics of the scattering process.

There are two relevant scattering domains, given by the frequency offset from the line centre of the core transition: resonance or core scattering; and wing scattering. Core scattering events are characterised by the incoming photons having energies close to the energy needed to excite the atom, whereas wing scattering events are closer related to scattering off free electrons, as the frequency of the photons differs from the resonance frequency.

Ly\( \alpha \)-radiation corresponds as earlier noted to the energy released from a de-excitation to the ground state from the first excited level of
4.2. Polarisation

a hydrogen atom. There are two possible sublevels of the first excited state: the $2P_{1/2}$ level and the $2P_{3/2}$ level, following a notation (Griffiths (2005), Dijkstra & Loeb (2008)) on the form “$nL_J$” where $n$ is the principal quantum number, $L$ is the orbital angular momentum number ($S; P, D, F, \cdots$ for $L = 0, 1, 2, 3, \cdots$) and $J$ is the total angular momentum, with $J \equiv L + S$ where $S$ is the electron spin which may take on the values $\pm 1/2$.

Quantum mechanical selection rules restrict the available transitions: $\Delta S = 0$, $\Delta L = 0, \pm 1$, $\Delta J = 0, \pm 1$ with the requirement that $J = 0 \not\leftrightarrow J = 0$ (Lee et al. 1994). Thus, a transition $1S_{1/2} \rightarrow 2S_{1/2} \rightarrow 1S_{1/2}$ is not possible.

The configuration of the excited state affects both the preferred direction of the scattered photon and its polarisation. This can be understood as a consequence of the angular part of the wave-function of the excited states. The angular part of the wave-function for a hydrogen atom is given by the spherical harmonic $Y^m_L(\theta, \phi)$ (with $m$: the magnetic quantum number). For $2P_{1/2}$ or $(n, L, m) = (2, 0, 0)$, the angular part is $Y^0_0 = \sqrt{1/4\pi}$, which is a constant, whereas for $2P_{3/2}$ or $(n, L, m) = (2, 1, 0)$, $Y^0_1 = \sqrt{3/4\pi \cos \theta}$.

The emitted photon from the de-excitation will thus “remember” the configuration of the excited atom: in the case of de-excitation from the $2P_{3/2}$ state, there are scattering directions that are more likely than others.

In the case of de-excitation from the $2P_{1/2}$ state, where the angular wave function is constant, the scattered photon has no such memory and should scatter isotropically. In the latter case, the polarisation will also be zero as the outgoing photon has no memory of the polarisation of the incoming photon and the excited state does not induce any preferred polarisation directions.

Polarisation of Ly$\alpha$: relating physics to observables

Following Rybicki & Lightman (1979), it is now possible to define the degree of polarisation by decomposing the Stokes parameters into two states,

$$
\begin{bmatrix}
I \\
Q \\
U \\
V
\end{bmatrix} = \begin{bmatrix}
I - \sqrt{Q^2 + U^2 + V^2} \\
0 \\
0 \\
0
\end{bmatrix} + \begin{bmatrix}
\sqrt{Q^2 + U^2 + V^2} \\
Q \\
U \\
V
\end{bmatrix}
$$  (4.18)

where the first is that of a completely unpolarised wave, and the second is that of a completely polarised wave. The degree of polarisation is then the
ratio of the intensity of the completely polarised state to the total intensity,

\[ \Pi \equiv \frac{I_{\text{polar}}}{I} = \frac{\sqrt{Q^2 + U^2 + V^2}}{I}. \] (4.19)

Following Brasken & Kyrola (1998), the phase function can be defined. It is a measure on relative intensity for different solid angle elements to the total intensity,

\[ p(\theta, \phi) = \frac{I(\theta, \phi)}{\langle I \rangle} \] (4.20)

where the angles denote the scattering angles, and the brackets denote angle-averaged intensity, divided by \(4\pi\).

Note that Brasken & Kyrola (1998) only had a single angle-dependence, which can be interpreted as an assumption of rotational symmetry in scattering events.

### Relations between Stokes parameters and scattering process

Chandrasekhar (1960) thoroughly treats scattering in radiative transfer using mathematical physics and linear algebra. He also gives the transport equation on forms that can be numerically solved. Detailed solution strategies to the polarised transport equations are given by Phillips & Meszaros (1986).

Dijkstra & Loeb (2008) recaps some of the relevant equations from Chandrasekhar (1960) and apply them to obtain a phase function that can govern numerical scattering of unpolarised Lyα radiation. Central is the scattering matrix \(R\) that consists of two components: Rayleigh scattering and isotropic ("\(J = 0 \to 1\)") scattering. It governs the components of the intensities parallel and perpendicular to the scattering plane,

\[
\begin{bmatrix}
I_\parallel' \\
I_\perp'
\end{bmatrix} = R \begin{bmatrix}
I_\parallel \\
I_\perp
\end{bmatrix}
\] (4.21)

where primes denote scattered quantities. Unpolarised light has \(I_\parallel = I_\perp = 1/2\) and the total intensity is given as \(I = I_\parallel + I_\perp\). The scattering matrix for the parallel and perpendicular components is given in Dijkstra & Loeb (2008) (which is taken from Eq. (259), p. 51 in Chandrasekhar (1960)),

\[
R = \frac{3}{2} E_1 \begin{bmatrix}
\cos^2 \theta & 0 \\
0 & 1
\end{bmatrix} + \frac{1}{2} E_2 \begin{bmatrix}
1 & 1 \\
1 & 1
\end{bmatrix}.
\] (4.22)
4.2. Polarisation

Table 4.1: From Chandrasekhar [1960], the constants $E_1$ and $E_2$ that weigh the contributions from Rayleigh and isotropic scattering, respectively, can be calculated by considering the change in total angular momentum $\Delta J$ and the total angular momentum of the initial level, $J$.

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<thead>
<tr>
<th>$\Delta J$</th>
<th>$E_1$</th>
<th>$E_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\frac{(2J+5)(J+2)}{10(J+1)(2J+1)}$</td>
<td>$\frac{3J(6J+7)}{10(J+1)(2J+1)}$</td>
</tr>
<tr>
<td>0</td>
<td>$\frac{(2J-1)(2J+3)}{10J(J+1)}$</td>
<td>$\frac{3(2J^2+2J+1)}{10J(J+1)}$</td>
</tr>
<tr>
<td>-1</td>
<td>$\frac{(2J-3)(J-1)}{10J(2J+1)}$</td>
<td>$\frac{3(6J^2+5J-1)}{10J(2J+1)}$</td>
</tr>
</tbody>
</table>

The coefficients $E_1$ and $E_2$ denote the relative contribution from Rayleigh and isotropic scattering, respectively. They can be calculated for a change in total angular momentum, $\Delta J$, for the initial level having the quantum number $J$ in tab. (4.1). The origin of the angle is $\cos \theta = e_k \cdot e'_k$ with $e_k$ pointing in the momentum propagation direction of the incoming wave.

An attempt to derive the phase function for the different transitions can be done by using the definition,

$$p(\theta) = \frac{I'_\parallel + I'_\perp}{\langle I \rangle}$$ \hspace{1cm} (4.23)

with

$$I'_\parallel = \frac{3}{2} I_\parallel E_1 \cos^2 \theta + \frac{1}{2} E_2 \left( I_\parallel + I_\perp \right)$$ \hspace{1cm} (4.24)

$$I'_\perp = \frac{3}{2} E_1 I_\perp + \frac{1}{2} E_2 \left( I_\parallel + I_\perp \right)$$ \hspace{1cm} (4.25)

$$\langle I \rangle = \int_{-1}^{1} I'_\parallel + I'_\perp \, d(\cos \theta)$$

$$= E_1 \left( I_\parallel + 3I_\perp \right) + 2E_2 \left( I_\parallel + I_\perp \right)$$ \hspace{1cm} (4.26)

such that the (polarisation and scattering type) general, normalised (to unity) phase function becomes

$$p(\theta) = \frac{(3/2)E_1 I_\parallel \cos^2 \theta + (3/2)E_1 I_\perp + E_2 \left( I_\parallel + I_\perp \right)}{E_1 I_\parallel + 3E_1 I_\perp + 2E_2 \left( I_\parallel + I_\perp \right)}$$ \hspace{1cm} (4.27)

which for scattering of unpolarised light, $I_\parallel = I_\perp = 1/2$, reduces to

$$p(\theta) = \frac{3E_1 + 3E_1 \cos^2 \theta + 4E_2}{8 (E_1 + E_2)}$$ \hspace{1cm} (4.28)
which is found in Dijkstra & Loeb (2008) in un-normalised form, and in derived forms in Laursen (2010).

An attempt to find the relevant degree of linear polarisation is done by comparing the ratio between the Stokes $Q$ and $I$ parameters, using that $Q = I_\parallel - I_\bot$ as these quantities are negatively proportional,

$$\Pi(\theta) = \frac{Q}{I} = \frac{I_\parallel - I_\bot}{I_\parallel + I_\bot}$$  \hspace{1cm} (4.29)

such that the general expression for the degree of linear polarisation becomes

$$\Pi(\theta) = \frac{(3/2) (I_\parallel \cos^2 \theta I_\bot)}{(3/2) (I_\parallel \cos^2 \theta I_\bot) + (E_2/E_1) (I_\parallel + I_\bot)}$$ \hspace{1cm} (4.30)

which, for scattering of unpolarised light, readily reduces to

$$\Pi(\theta) = \frac{\sin^2 \theta}{1 + 4E_2/(3E_1) + \cos^2 \theta}.$$  \hspace{1cm} (4.31)

This expression is found in Dijkstra & Loeb (2008) and derived expressions (for combinations of $E_1$ and $E_2$) are found in Lee & Blandford (1997).

The phase functions and polarisation degree are calculated below for different transitions.

- **K-transition:** for $J = 1/2 \rightarrow 1/2$, as in scattering between the levels $1S_{1/2} \rightarrow 2P_{1/2} \rightarrow 1S_{1/2}$. As earlier shown is this scattering type isotropic and displays no scattering angle preference, nor gives rise to any degree of polarisation. The coefficients are $(E_1, E_2)_K = (0, 1)$ such that

$$p_K(\theta) = \frac{1}{2}$$ \hspace{1cm} (4.32)

$$\Pi_K(\theta) \rightarrow 0$$ \hspace{1cm} (4.33)

- **H-transition:** for $J = 1/2 \rightarrow 3/2$, as in scattering between the levels $1S_{1/2} \rightarrow 2P_{3/2} \rightarrow 1S_{1/2}$. This transition has a strong angle dependence. The coefficients are $(E_1, E_2)_H = (1/2, 1/2)$ such that

$$p_H(\theta) = \frac{7}{16} + \frac{3}{16} \cos^2 \theta$$  \hspace{1cm} (4.34)

$$\Pi_H(\theta) = \frac{\sin^2 \theta}{7/3 + \cos^2 \theta}$$  \hspace{1cm} (4.35)
where the maximum degree of polarisation is $\Pi_H = 3/7$ for scattering at $\theta = \pm \pi/2$, corresponding to scattering at right angles. The phase function is maximised for $\theta = (0, 1)\pi$, corresponding to forward and backward scattering, respectively.

- **Wing-scattering**, or Rayleigh scattering: can be treated as $J = 0 \rightarrow 1$ scattering with coefficients $(E_1, E_2)_{\text{wing}} = (1, 0)$ such that

$$p_{\text{wing}}(\theta) = \frac{3}{8} + \frac{3}{8} \cos^2 \theta$$  \hspace{1cm} (4.36)

$$\Pi_{\text{wing}}(\theta) = \frac{\sin^2 \theta}{1 + \cos^2 \theta}$$  \hspace{1cm} (4.37)

where the maximum degree of polarisation is $\Pi_{\text{wing}} = 1$ for scattering at $\theta = \pm \pi/2$, and the minimum is $\Pi_{\text{wing}} = 0$ for $\theta = (0, 1)\pi$. The phase function is maximised when the polarisation degree is minimised, and vice versa.

- **Core-scattering**: cannot be treated as either a K- or a H-transition, as the interference between the upper levels must be accounted for. Stenflo (1980) calculates the ratio between the K and H lines, and finds that the oscillator strength of the K line is a factor 2 stronger than the oscillator strength of the H line. The phase function and degree of polarisation can be found as a superposition of the relevant phase functions for the H- and K-transitions, weighting the H-transition twice as much as the K-transition,

$$p_{\text{core}} = \frac{1}{3}p_K + \frac{2}{3}p_H = \frac{11}{24} + \frac{1}{8} \cos^2 \theta$$  \hspace{1cm} (4.38)

$$\Pi_{\text{core}} = \frac{1}{3}\Pi_K + \frac{2}{3}\Pi_H = \frac{2 \sin^2 \theta}{7 + 3 \cos^2 \theta}$$  \hspace{1cm} (4.39)

where the angle preferences from the H-transition has been retained, but the effect is damped—scattering at right angles only gives a maximum degree of polarisation of $\Pi_{\text{core}} = 2/7$.

Note that these relations only applies for scattering of unpolarised light.
Density matrix formalism

Following the single-photon polarisation description by [Weinberg (2013)], a note of caution is in place. The overall measured degree of polarisation does not correspond to a certain preferred combination of $\xi_+$ and $\xi_-$. This combination only describes a single (possibly mixed) state, whereas the observed polarisation is a collective phenomenon of an ensemble of photons.

To describe the ensemble of photons, some notation is required. A particular wave function of Eq. (4.16) is denoted $|\Psi_{k,\chi}^j\rangle$ with $\chi$ denoting a polarisation direction given a momentum propagation direction $\hat{k}$. An ensemble can consist of several combinations of $|\Psi_{k,\chi}^j\rangle$.

The hermitian density matrix

\[
\rho \equiv \sum_i p_i |\Psi_{k,\chi}^j\rangle \langle \Psi_{k,\chi}^j | \tag{4.40}
\]

holds all obtainable information on a quantum mechanical ensemble of states, each weighted by a factor $p_i$, with $\sum p_i = 1$. See App. B for detailed properties of density matrix formalism.

The density matrix formalism is especially beneficial in numerical Monte Carlo radiative transfer codes. Each photon can be described as a qubit, consisting of a superposition of the two possible circular polarisation states. Observing unpolarised radiation means that one is as likely to obtain one polarisation configuration as another. This can accurately be represented by using a density matrix, where the factors $p_i$ allows for each polarisation state to have some probability of being observed (or drawn from the ensemble).

Highly polarised radiation means that $p_i$ is larger for some states than for others. The choice of expansion of the state $|\Psi_{k,\chi}^j\rangle$ in Eq. (4.40) determines what kind of polarisation the weight represents. One can choose to represent the polarisation in terms of the circular polarisation states, in terms of an orthogonal representation, or in terms of linear polarisation states (which for photons is a superposition of the two helical photon states).

Density matrix: Lyman $\alpha$-scattering

In Ch. 5, the density matrix formalism described by the unpublished article by [Lee & Ahn (2002)] is implemented numerically. Their work is

\[\text{Dirac: } \langle \Psi | A | \Phi \rangle \equiv \int \Psi^*(x) A \Phi(x) \, d^3N_x \text{ for an operator } A \text{ acting on } N\text{-particle wave functions, } \text{[Sethna (2011)]}\]
similar to that in the published article of Ahn et al. (2002), and base their formalism on time-dependent perturbation theory. The relation between the time-dependent perturbation theory is examined in App. C.

Ahn et al. (2002) states that the “density matrix element associated with the scattered photon \( \rho_{\beta\beta'} \) is related with that of the incident photon \( \rho_{\alpha\alpha'} \) by”:

\[
\rho_{\beta\beta'} \propto \sum_{I, I'} \frac{(\hat{r} \cdot \varepsilon^{(\beta')})_{AI} (\hat{r} \cdot \varepsilon^{(\alpha)})_{IA}}{E_I - E_A - \hbar \omega} \\
\times \rho_{\alpha\alpha'} \frac{(\hat{r} \cdot \varepsilon^{(\alpha')})_{I'A} (\hat{r} \cdot \varepsilon^{(\beta)})_{AI'}}{E_{I'} - E_A - \hbar \omega}
\]

(4.41)

and neglect \( n > 2 \) terms and treat the radial part of the wave function as a constant. The sub-/superscripts of Eq. (4.41) are not given in Ahn et al. (2002). The notation with parentheses that are subscripted \( AI, IA, I'A \) and \( AI' \) can be interpreted as shorthand for a bra-ket description, where the subscripts denote the final and initial state that the enclosed dipole, or in the notation applied in App. C perturbation, operator works on. The position operator is denoted \( \hat{r} \) rather than \( x \) in Eq. (4.41), while the polarisation vectors are given as \( \varepsilon \) rather than \( \epsilon \), compared to Eq. (C.5).

The calculated elements of the 2 \( \times \) 2 hermitian density matrix that are generated from Eq. (4.41) are given in Ahn et al. (2002), and also in Lee & Ahn (2002), but there without reference to the generating function. The calculated elements are also given below.

In the following are unprimed quantities associated with incoming radiation, primed quantities associated with outgoing radiation and \( \Delta \phi = \phi' - \phi \). Due to the density operator being hermitian, the density matrix element \( \rho_{21} \) is not given, as \( \rho_{12} = \rho_{21}^* \).

For wing scattering, which is Rayleigh scattering, but treated as scattering between the \( J = 0 \rightarrow J = 1 \) levels, the density matrix elements
4. **Lyman Alpha Transfer and Polarisation**

are

\[
\begin{align*}
\rho'_{11} &= \rho_{11} \cos^2 \Delta \phi \\
&\quad - \rho_{12} \cos \theta \sin 2\Delta \phi \\
&\quad + \rho_{22} \sin^2 \Delta \phi \cos^2 \theta, \\
\rho'_{12} &= \frac{1}{2} \rho_{11} \cos \theta' \sin (2\Delta \phi) \\
&\quad + \rho_{12} [\cos \theta \cos \theta' \cos (2\Delta \phi) + \sin \theta \sin \theta' \cos \Delta \phi] \\
&\quad - \rho_{22} \cos \theta \left[ \sin \theta \sin \theta' \sin \Delta \phi + \frac{1}{2} \cos \theta \cos \theta' \sin (2\Delta \phi) \right], \\
\rho'_{22} &= \rho_{11} \cos^2 \theta' \sin^2 \Delta \phi \\
&\quad + \rho_{12} \cos \theta' (2 \sin \theta \sin \theta' \sin \Delta \phi + \cos \theta \cos \theta' \sin (2\Delta \phi)) \\
&\quad + \rho_{22} (\cos \theta \cos \theta' \cos \Delta \phi + \sin \theta \sin \theta')^2
\end{align*}
\]

(4.42)

For resonance scattering between the \( J = 1/2 \rightarrow J = 3/2 \) levels, the density matrix elements are

\[
\begin{align*}
\rho'_{11} &= \rho_{11} (5 + 3 \cos (2\Delta \phi)) \\
&\quad - 6 \rho_{12} \cos \theta \sin (2\Delta \phi) \\
&\quad + \rho_{22} [(5 - 3 \cos (2\Delta \phi)) \cos^2 \theta + 2 \sin^2 \theta] \\
\rho'_{12} &= 3 \rho_{11} \sin (2\Delta \phi) \cos \theta' \\
&\quad + 6 \rho_{12} (\cos \theta \cos \theta' \cos (2\Delta \phi) + \sin \theta \sin \theta' \cos \Delta \phi) \\
&\quad - 3 \rho_{22} \cos \theta (2 \sin \theta \sin \theta' \sin \Delta \phi + \cos \theta \cos \theta' \sin (2\Delta \phi)) \\
\rho'_{22} &= \rho_{11} [(5 - 3 \cos (2\Delta \phi)) \cos^2 \theta' + 2 \sin^2 \theta'] \\
&\quad + \rho_{12} (6 \sin (2\Delta \phi) \cos \theta \cos^2 \theta' + 2 \sin \Delta \phi \cos \theta' \sin \theta \sin \theta') \\
&\quad + \rho_{22} [(5 + 3 \cos (2\Delta \phi)) \cos^2 \theta \cos^2 \theta' \\
&\quad + 2 \cos^2 \theta \sin^2 \theta' + 12 \cos \Delta \phi \cos \theta' \cos \theta \sin \theta \sin \theta'] \\
&\quad + 2 \cos^2 \theta' \sin^2 \theta + 8 \sin^2 \theta \sin^2 \theta']
\end{align*}
\]

(4.43)

and for resonance scattering between \( J = 1/2 \rightarrow J = 1/2 \) which a \( 1S_{1/2} \) to \( 2P_{1/2} \) transition is, the density matrix is that of a completely unpolarised case, giving an isotropic angular distribution,

\[
\begin{align*}
\rho'_{11} &= \frac{1}{2}, \quad \rho'_{12} = 0, \quad \rho'_{22} = \frac{1}{2}
\end{align*}
\]

(4.44)

These matrix elements assumes a right-handed coordinate system, and introduces the momentum propagation direction vector \( \mathbf{k} \) and two
4.2. Polarisation

polarisation vectors $\epsilon_1$ and $\epsilon_2$ associated with the *incoming* photon,

$$
\begin{align*}
\mathbf{k} &= \begin{bmatrix} \sin \theta \cos \phi \\
\sin \theta \sin \phi \\
\cos \theta \end{bmatrix}, \\
\epsilon_1 &= \begin{bmatrix} -\sin \phi \\
\cos \phi \end{bmatrix}, \\
\epsilon_2 &= \begin{bmatrix} \cos \theta \cos \phi \\
\cos \theta \sin \phi \\
-\sin \theta \end{bmatrix}
\end{align*}
(4.45)
$$

that are perpendicular to each other. The outgoing photon is described with the primed vectors, $\mathbf{k}', \epsilon_1', \epsilon_2'$. See Fig. (4.1) for a sketch of the coordinate system and the angles involved.

**Figure 4.1:** (a): Sketch of the right-handed coordinate system applied in Eqs. (4.42, 4.43, 4.44) and (b): the set of basis vectors $\{\epsilon_1, \epsilon_2, \mathbf{k}\}$ of Eq. (4.45) that form a left-handed coordinate system.

The interpretation of the density matrices introduced in Eqs. (4.42, 4.43, 4.44) from their dimension $(2 \times 2)$ is that they are polarisation density matrices on the form of Eq. (C.25) and are thus comprised of the Fourier transformed components of the incoming and outgoing electric vector.

The normalisation factor of Eq. (C.25) appears in Lee & Ahn (2002) through the requirement of “unit trace”.

The density matrix elements are related to the Stokes parameters that are presented in the next section.

**Stokes parameters and the density matrix formalism of Lee & Ahn (2002)**

The unpublished article by Lee & Ahn (2002) gives the following relations between the Stokes parameters and the density matrix elements of
4. Lyman alpha transfer and polarisation

Eqs. (4.42, 4.43, 4.44):

\[
\begin{align*}
\rho_{11} &= \frac{I + Q}{2}, & \rho_{22} &= \frac{I - Q}{2}, & \rho_{12} &= \frac{U + iV}{2}, & \rho_{21} &= \rho_{12}^*,
\end{align*}
\]

but the relations are unmotivated and are not part of the published paper by Ahn et al. (2002).

An attempt to see whether the density matrix elements are related to the polarisation density matrix of Eq. (C.25) given by Lee et al. (1994), as theorised earlier, can be done by representing an arbitrarily polarised electromagnetic wave propagating in the \( z \)-direction in terms of the helical unit vectors as in Eq. (4.12).

Then, the (Fourier components of the) electric field has to be transformed from the ion basis \( \{ e_i \} \) to the two-component photon basis \( \{ e_a \} \), as the density matrix of Eq. (C.25) is given for that basis. This requires rotations \( \phi \) and \( \theta \) in the complex and real plane, respectively, by using the rotation matrix \( S_{aq} \) of Eq. (C.23) whose elements are given in Eq. (2.4) in Lee et al. (1994),

\[
\tilde{E}_a = S_{aq} \tilde{E}_q
\]

where the definitions of the helical basis vectors of Eq. (4.11) were used, and that \( \tilde{E}_z = 0 \) as there is no field in the propagation direction.

Furthermore, the polarisation components of Eq. (C.25) are given as the product of the real and complex conjugated photon basis electric vectors,

\[
\begin{align*}
\tilde{E}_\perp \tilde{E}_\perp^* &= \frac{1}{2} \cos^2 \theta \left( |\tilde{E}_r|^2 + |\tilde{E}_l|^2 \right), \\
\tilde{E}_\parallel \tilde{E}_\parallel^* &= \frac{1}{2} \left( |\tilde{E}_r|^2 - |\tilde{E}_l|^2 \right), \\
\tilde{E}_\perp \tilde{E}_\parallel^* &= \frac{1}{2} i \cos \theta \left( |\tilde{E}_l|^2 - |\tilde{E}_r|^2 \right), \\
\tilde{E}_\parallel \tilde{E}_\parallel^* &= (\tilde{E}_\perp \tilde{E}_\perp^*)^*
\end{align*}
\]

divided by some normalisation factor \( \tilde{E}_a \cdot \tilde{E}_a^* \). Lee et al. (1994) defines the polarisation density matrix by using the product between the real
4.2. Polarisation

component of the incoming wave and the complex conjugate component of the outgoing wave. The choice of rotation angles ϕ and θ determines what coordinate representation the photon basis will have.

Above it was assumed that the density matrix elements of Eqs. (4.42, 4.43, 4.44) were given in the parallel/perpendicular basis the notation in Lee et al. (1994) implied.

However, if it is attempted to interpret the density matrix of Eq. (C.25) as to be consisting of the linear electric field components in a Cartesian basis, where the electric field components are linear combinations of the helical components (del Toro Iniesta 2003):

\[
E_x(x, t) = \frac{1}{\sqrt{2}} [E_r(x, t) + E_l(x, t)]
\]
\[
E_y(x, t) = \frac{i}{\sqrt{2}} [E_l(x, t) - E_r(x, t)]
\]

(4.49)

the elements of Eq. (C.25) become (omitting functional dependencies and working with the Fourier components):

\[
\tilde{E}_x \tilde{E}_x^* = \frac{1}{2} \left[ \tilde{E}_r \tilde{E}_r^* + \tilde{E}_l \tilde{E}_l^* + \tilde{E}_r \tilde{E}_l^* + \tilde{E}_l \tilde{E}_r^* \right] = \frac{I + Q}{2}
\]
\[
\tilde{E}_y \tilde{E}_y^* = \frac{-i}{2} \left[ \tilde{E}_r \tilde{E}_r^* + \tilde{E}_l \tilde{E}_l^* - \tilde{E}_r \tilde{E}_l^* - \tilde{E}_l \tilde{E}_r^* \right] = \frac{I - Q}{2}
\]
\[
\tilde{E}_x \tilde{E}_y^* = -\frac{i}{2} \left[ \tilde{E}_r \tilde{E}_l^* - \tilde{E}_l \tilde{E}_r^* + \tilde{E}_l \tilde{E}_r^* - \tilde{E}_r \tilde{E}_l^* \right] = \frac{U + iV}{2}
\]
\[
\tilde{E}_y \tilde{E}_x^* = \frac{i}{2} \left[ \tilde{E}_r \tilde{E}_l^* + \tilde{E}_l \tilde{E}_r^* - \tilde{E}_l \tilde{E}_r^* - \tilde{E}_r \tilde{E}_l^* \right] = \frac{U - iV}{2}
\]

(4.50)

where brackets denoting time averages are skipped and the definitions of the Stokes parameters of Eq. (4.13) were used with κ = 1. The above relations are equal to those given in Eq. (4.46) and correspond to a rotation in the complex plane by ϕ = −π/2 and in the real plane by θ = 0.

Lee & Ahn (2002) and Ahn et al. (2002) define the relations between the density matrix elements ρ_{11}, ρ_{12} and ρ_{22} and the phase function as

\[
p(\theta, \phi, \theta', \phi') = \rho_{11} + \rho_{22}
\]

(4.51)

and the degree of polarisation can be derived from the definition of Eq. (4.19) and the relations between the Stokes parameters and the density

**Challenge 4.1:**

Set \( \phi = -\pi/2 \) and \( \theta = 0 \) in Eq. (4.47). Which Cartesian component does \( E_\perp \) represent: \( E_x \) or \( E_y \) (and vice versa for \( E_\parallel \)?)
matrix elements of Eq. (4.46),

\[
\Pi = \frac{I_{\text{pol}}}{I} = \frac{\sqrt{Q^2 + U^2 + V^2}}{I} = \frac{\sqrt{(\rho_{11} - \rho_{22})^2 + 4\rho_{21}\rho_{12}}}{\rho_{11} + \rho_{22}} = \frac{\sqrt{Q^2 + 4\left(\frac{1}{4}(U^2 + V^2)\right)}}{I},
\]

(4.52)

however, if \( V = 0 \), which corresponds to no circular polarisation, and the detection axes are rotated such that all the polarisation information is embedded in \( Q \), the expression reduces to the one used in the definition of Lee & Ahn (2002);

\[
\Pi = \frac{\sqrt{Q^2}}{I} = \frac{\rho_{11} - \rho_{22}}{\rho_{11} + \rho_{22}}.
\]

(4.53)

As there are no sources of circularly polarised Ly\(\alpha\) radiation, nor will scattering off hydrogen atoms induce circular polarisation, the assumption \( V = 0 \) is sensible.
Chapter 5

Including polarisation in radiative transfer

What’s a knockout like you doing in a computer-generated gin joint like this?

Cmdr. William T. Riker

This chapter will present the numerical implementation of the polarisation methods presented in Ch. 4, as well as the Monte Carlo algorithm that is used to in practice solve the integro-differential radiative transfer equation.

The first section will deal with the main features of Monte Carlo radiative transfer, before describing briefly the approaches taken by Lee & Ahn (2002) and Gronke & Dijkstra (2014). Finally, the modifications done to the code by Gronke & Dijkstra (2014) are presented, these both allow for scattering of polarised light and provides a quantum mechanical treatment of the process that makes light become polarised.

5.1 Monte Carlo radiative transfer

Monte Carlo methods are based on sampling random numbers according to some underlying distribution, see eg. Press et al. (2007). In the context of radiative transfer, the physical process of scattering is approximated as a diffusion process in real space and frequency space, where each photon is a random walker.

Each photon is given a set of characteristics, as position and direction in real space, position in frequency space, polarisation (degree and
5. Including polarisation in radiative transfer

direction), travel time (since emission), scattering counts, and travel
distance (since last scattering). When the photons escapes the scattering
medium, statistics can be created from their collective properties. These
statistics often correspond to astrophysical observables.

The Monte Carlo photon diffusion process is described and applied
in eg. Avery & House (1968); Lee & Lee (1997); Loeb & Rybicki (1999);
Ahn et al (2000); Zheng & Miralda-Escude (2002); Dijkstra & Loeb (2008);
Pierleoni et al. (2009); Laursen (2010). See also Dijkstra (2014) for an
extensive overview.

The Monte Carlo part of a radiative transfer routine is embedded in
several steps of the random walk process:

1. A photon is emitted: it is given a random position in the frequency
   space, distributed according to the local temperature, and a random
direction, distributed uniformly on a sphere (uniform in each solid
angle element).

2. The photon propagates before it scatters: the stretch the photon
   travels before scattering is determined by drawing a random optical
depth

   \[ \tau = -\ln R \]  \hspace{1cm} (5.1)

   where \( R \sim \text{Unif}(0, 1) \). The travel distance \( r \) is found (Laursen 2010)

   \[ r = \frac{\tau}{n_H \sigma_H(a, x) + n_d \sigma_d} \]  \hspace{1cm} (5.2)

   where the optical depth was defined in eq. (5.19) and \( n_H, n_d \) are the
   number densities (particles per volume) of neutral hydrogen and
dust, respectively, with corresponding cross sections \( \sigma_H \) and \( \sigma_d \). The
   rest frame cross section of a hydrogen atom is both temperature
   and the frequency displacement \( x \) from the core frequency of the
   incoming photon,

   \[ \sigma_H(a, x) = f_{12} \frac{\sqrt{\pi} e^2}{m_e c \Delta \nu_D} H(a, x) \]  \hspace{1cm} (5.3)

   where \( f_{12} \) is the oscillator strength for a transition from the \( n = 1 \) to
   \( n = 2 \) state of hydrogen, \( e \) is the unit charge, \( m_e \) is the electron mass
   and \( \Delta \nu_D \) is the Doppler width:

   \[ \Delta \nu_D = \frac{\nu_{th}}{c} \nu_0 \]  \hspace{1cm} (5.4)
5.1. Monte Carlo radiative transfer

where \( v_{th} \) is the thermal velocity of the particle, effectively Doppler shifting the frequency away from the resonance frequency \( \nu_0 \),

\[
v_{\text{th}} = \frac{2k_B T_g}{m_H}
\]  

(5.5)

with \( k_B \) as the Boltzmann constant, \( T_g \) as the gas temperature and \( m_H \) as the hydrogen mass (Ahn et al. 2000). Furthermore was the Voigt-Hjerting function introduced,

\[
H(a, x) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-y^2}}{(x - y)^2 + a^2} \, dy
\]  

(5.6)

where the \( a \)-parameter is given as

\[
a \equiv \frac{\Gamma}{4\pi \Delta \nu_D} = 4.7 \times 10^{-4} \left( \frac{T_g}{10^4 \, \text{K}} \right)^{-1/2}
\]  

(5.7)

according to Ahn et al. (2000), where \( \Gamma = A_{21} \). This natural line width can be rewritten in terms of radiative and collisional line broadening (Rutten 2003), but Laursen (2010) concludes that collisional line broadening contributes negligibly. The frequency offset is also used,

\[
x \equiv \frac{\Delta \nu}{\Delta \nu_D} = \frac{\nu - \nu_0}{\Delta \nu_D}.
\]  

(5.8)

As the dust density is assumed zero in the numerical calculations, in-depth descriptions of dust interactions are omitted. Some notes regarding dust scattering are still kept in this summary.

3. The photon scatters: it interacts with a moving particle, a random number determines whether the interaction is with a dust particle or a hydrogen atom (Laursen 2010), if the random number is greater than the ratio

\[
r_{\text{dust--vs--hyd}} = \frac{n_d \sigma_d}{n_H \sigma_H(a, x) + n_d \sigma_d}
\]  

(5.9)

then, the photon scatters off a hydrogen atom.

4. Furthermore, if the photon interacts with a hydrogen atom, Ahn et al. (2000) suggests that the scattering type is determined before determining the velocity component of the scattering atom in the photon propagation direction. They suggest that core scattering
only happens if the frequency offset $x$ is approximately the same as the velocity parameter

$$u \equiv \frac{v_k \nu_0}{c \Delta \nu_D}$$ (5.10)

where $v_k$ is the velocity component in the photon momentum propagation direction. [Ahn et al. (2000)] proceeds to derive the probability of having a resonance scattering, with the result being

$$P_r = \frac{e^{-x^2}}{H(a, x)}$$ (5.11)

and consequently, the probability that the scattering is non-resonant (wing scattering) is given as

$$P_{nr} = 1 - P_r.$$ (5.12)

[Ahn et al. (2001)] modifies the above approach, and consider level splitting between the $2P_{3/2}$ and $2P_{1/2}$ levels by considering the resonance frequencies of the two levels in terms of the Doppler width,

$$u_H \equiv \frac{\nu - \nu_H}{\Delta \nu_D}, \quad u_K \equiv \frac{\nu - \nu_K}{\Delta \nu_D}$$ (5.13)

where the subscripts H and K denote a H-line and a K-line, respectively. Thereafter, [Ahn et al. (2001)] considers the probabilities of scattering to each level, with the probability of H-line scattering given as

$$P_H = \frac{2 e^{-u_H^2}}{H(a, u_K) + 2H(a, u_H)},$$ (5.14)

the probability of K-line scattering given as

$$P_K = \frac{e^{-u_K^2}}{H(a, u_K) + 2H(a, u_H)},$$ (5.15)

and the probability of wing scattering is then

$$P_{nr} = 1 - P_H - P_K.$$ (5.16)

Note that the frequency separation between the levels $2P_{1/2}$ and $2P_{3/2}$ are $\nu_{2P_{3/2}} - \nu_{2P_{1/2}} = 1.1 \times 10^{10}$ Hz, and are observationally blended by the much smaller natural line width of the line for both transitions, $\Gamma \sim 10^8$ Hz [Dijkstra & Loeb (2008)].
5.1. Monte Carlo radiative transfer

A random number $\mathcal{R} \sim \text{Unif}(0, 1)$ can then be drawn to determine whether the scattering was in the wing ($P_{nr} > \mathcal{R}$) and the kind of transition, if the scattering was resonant.

Dijkstra et al. (2006); Dijkstra & Loeb (2008) applies a different approach, they compare the frequency offset $x$ to the parameter $x_{\text{cr}} = 0.2$ motivated by the quantum interference explored by Stenflo (1980), whereas Laursen (2010) calculates an analytical formula dependent on the $a$-parameter, $x_{\text{cw}}(a)$.

Here, a possible computational speed up is possible. Avery & House (1968) remark that photons with frequencies near the core frequency undergo many scatterings in the vicinity of the scattering event (both in frequency and position space) before eventually obtaining a single, large enough frequency shift (making the medium efficiently much more transparent for the photons), allowing for significant spatial displacement.

A frequency offset threshold can be defined, $x_{\text{crit}}$ (Laursen, 2010), which separates core ($x \leq x_{\text{crit}}$) from wing ($x > x_{\text{crit}}$) scatterings for each photon. Photons that are subject to core scatterings, only interact with fast-moving particles whose velocity component in the incoming scattering direction is larger than that one a Gaussian distribution would have procured.

This acceleration scheme is not applied by Ahn et al. (2000), who use that the parallel velocity component $u \approx x_i$ in the case of core scatterings, but Ahn et al. (2002) apply it.

5. The velocity component of the scattering particle parallel to the momentum propagation direction of the photon plays an important role in determining the effective frequency of the photon in the rest frame of the scattering particle. The distribution of parallel velocities $u_\parallel$ is given as

$$f(u_\parallel) = \frac{a}{\pi H(a, x)} \frac{e^{-a^2 u_\parallel^2}}{(x - u_\parallel)^2 + a^2}$$

(5.17)

see eg. Ahn et al. (2002); Laursen (2010). As this function is not analytically integrable and invertible, which would have allowed direct sampling random numbers distributed according to $f(u_\parallel) \ du_\parallel$, the parallel velocities are obtained by using a Monte Carlo method: acceptance-rejection sampling, described by eg. Zheng & Miralda-Escude (2002) or Press et al. (2007). By using an integrable
and invertible enveloping function, velocities can be sampled from the distribution \( f(u_i) \).

Note that Ahn et al. (2000) samples velocity components directly from a Maxwell-Boltzmann velocity distribution, where the velocities along each axis is normally distributed.


If a phase function is given, the scattering direction can be determined using rejection sampling described in eg. Zheng & Miralda-Escude (2002). A new random outgoing direction (or angle) is drawn, and then plugged into the phase function before drawing a random number \( \mathcal{R} \sim \text{Unif}[0,1] \) which is compared to the scalar value the phase function returns. If \( p(k_{\text{out}}) \geq \mathcal{R} \), the new direction \( k_{\text{out}} \) is accepted. Otherwise, a new random direction is drawn.

7. Once the new direction has been found, the frequency offset yielded by the scattering in the rest frame of the scattering particle has to be transformed back to the photon basis. This coordinate transformation accounts for the thermal velocity of the scattering particle, Doppler shifting the frequency of the outgoing photon from the particle rest frame.

8. The loop continues from the second step until the photon escapes the scattering medium.
5.2 Numerical approach by Lee & Ahn (2002)

This section will feature the main numerical concepts of Lee & Ahn (2002), who introduced a quantum mechanical description of the polarisation of scattered Ly$\alpha$ radiation. This theoretical formalism was presented in Ch. 4.

Geometry

Lee & Ahn (2002) utilises the Monte Carlo radiative transfer code which was developed by Ahn et al. (2000), Ahn et al. (2001) and Ahn et al. (2002).

Lee & Ahn (2002) consider the case of an optically thick ($\tau \gg 1$) semi-infinite plane-parallel slab of neutral hydrogen (HI) where photons can escape once they reach the optical depth along the slab normal, which is taken to be in the $z$-direction:

$$\tau_0 > |z|. \quad (5.18)$$

Note that this implies that the slab size (or height) is given in units of optical depth, and that the total slab height is $2\tau_0$. Also, this means that the slab is infinite in the $x$- and $y$-directions.

At the centre of the slab, a single illuminating source is placed, this acts as the location where photons are emitted.

The numerical value for the vertical column density of the slab can be estimated from observations, see eg. Cantalupo et al. (2014) who observes Ly$\alpha$ emission around a quasar and infer a neutral hydrogen column density of $N_{\text{HI}} \approx 10^{22} \text{ cm}^{-2}$. Lee & Ahn (2002) operate with column densities in the range $N_{\text{HI}} \in (10^{19}, 10^{22}) \text{ cm}^{-2}$. The recent observations by Cantalupo et al. (2014) thus lie in the upper range of the expected column densities used by Lee & Ahn (2002).

The column density and gas temperature gives the optical depth of a system (Ahn et al. 2000),

$$\tau (a, x) = 1.41 \times 10^{-13} \left( \frac{T_g}{10^4 \text{K}} \right)^{-1/2} N_{\text{HI}} H (x, a) \quad (5.19)$$

which can be rewritten in terms of the line center optical depth

$$\tau_0 \equiv 1.41 \times 10^{-13} \left( \frac{T_g}{10^4 \text{K}} \right)^{-1/2} N_{\text{HI}} \quad (5.20)$$

such that

$$\tau (a, x) = \tau_0 H (x, a). \quad (5.21)$$
Another general quantity that can be used to describe the system is

\[
\alpha \tau_0 = 6.63 \times 10^{-17} \frac{N_{\text{HI}}}{T_g/10^4 \text{K}}
\]  

(5.22)

which decreases for increasing temperatures and increases for increasing column densities. Lee & Ahn (2002) use \( a = 1.49 \times 10^{-2} \), corresponding to \( T_g = 10 \text{ K} \) in their simulations.

Scattering

Lee & Ahn (2002) implement the density matrix formalism presented in Ch. 4. An incoming photon is described by the propagation vector \( \mathbf{k} \), and the two polarisation vectors \( \mathbf{\epsilon}_1 \) and \( \mathbf{\epsilon}_2 \) of eq. (4.45) that together form an orthogonal set of basis vectors that span \( \mathbb{R}^3 \) using polar coordinates.

They consider scattering from the \( 1S_{1/2} \)-level to the two possible upper levels \( 2P_{1/2} \) and \( 2P_{3/2} \), corresponding to K- and H-transitions, respectively. The scattering type is determined in accordance with the method proposed by Ahn et al. (2000), which was given through eqs. (5.14; 5.15; 5.16).

K-transitions are described with the density matrix elements of eq. (4.44), H-transitions with the elements of eq. (4.43). Also, they consider wing scattering described with the density matrix elements of eq. (4.42).

The outgoing propagation direction is determined from the phase function given in eq. (4.51). Each photon also retains the density matrix elements from the last scattering to be used in the next scattering event, see this dependence in eqs. (4.42; 4.43; 4.44). The degree of polarisation is also obtainable from the density matrix elements associated with each photon, from eq. (4.53).

Lee & Ahn (2002) remark that the degree of polarisation is related to the slab geometry,

- \( \Pi > 0 \) correspond to polarisation in the direction perpendicular to the slab normal,
- \( \Pi < 0 \) correspond to polarisation in the direction parallel to the slab normal.
5.3 “tlac” – Tiny Lyman alpha Code

Gronke & Dijkstra (2014) have developed an independent radiative transfer routine, which is based in part on the thorough description by Laursen (2010). They call it the “Tiny Lyman alpha Code”, abbreviated tlac. Its relevant features are briefly explained in this section.

Geometry

Under initialisation, a 3D grid is set up consisting of cells filled with gas (and optionally dust) that is distributed according to the given temperature $T_{\text{gas}}$ and optical depth. Each cell is given a neighbouring cell as a boundary, or optionally, the surface is set as the escape surface of the photons. It is also possible to construct (semi-)infinite slabs by imposing a periodic boundary where the neighbour of the “outermost” cells are the outermost cells on the opposite side of the grid.

Another possibility is to set up a 3D grid using polar coordinates, with the scattering medium either distributed inside a radius or inside distinct shells at given radii. It is also possible to specify a global velocity for the scattering medium, making it possible to construct expanding or contracting shells.

The source of emission of Ly$\alpha$ radiation can be set to be a point source, random sources inside each cell, according to an exponential distribution, along a plane in the center of the cell, or in clouds.

Scattering

Photons are emitted according to the user-specified input, each holding a set of physical and statistical characteristics. Each photon is tracked as it propagates through the scattering medium, and its characteristics are written to file when it escapes.

The scattering process follows that of Laursen (2010), and a scattering angle is drawn according to phase functions similar to those of Ch. 4. When the scattering angle $\chi$ has been chosen, a random outgoing direction $\mathbf{k}_{\text{out}}$ is chosen such that $\mathbf{k}_{\text{in}} \cdot \mathbf{k}_{\text{out}} = \cos \chi$. Note that this implies rotational symmetry in 3D.

Acceleration scheme

To accomodate the core skipping scheme outlined by Laursen (2010), tlac allows for a $x_{\text{crit}}$ to be specified by the user. Laursen (2010) concludes with
5. Including polarisation in radiative transfer

the following formula for the core skipping parameter, “from numerous tests”,

\[ x_{\text{crit}} = \begin{cases} 
0 & \text{for } a\tau_0 \leq 1 \\
0.02 \exp \left[ \xi \ln \chi a\tau_0 \right] & \text{for } a\tau_0 > 1
\end{cases} \] (5.23)

where the two scalar parameters \((\xi, \gamma) = (0.6, 1.2)\) or \((1.4, 0.6)\) for \(a\tau_0 \leq 60\) and \(a\tau_0 > 60\), respectively (Laursen 2010).

Dijkstra (2014) concludes that \(x_{\text{crit}} \approx 3.2\) for \(T_g = 10^4\) K, whereas Ahn et al. (2002) use \(x_{\text{crit}} = \sqrt{\pi}\) for \(a\tau_0 > 10^3\), and smaller \(x_{\text{crit}}\) for smaller values of \(a\tau_0\). See fig. (5.1) for a comparison of the resonance probabilities calculated from eq. (5.11) for \(T_g = (10, 100, 10^4, 10^8)\) K.

![Figure 5.1: Comparison of different resonance scattering probabilities calculated from eq. (5.11) for \(a\)-parameters given by the gas temperature \(T_g = (10, 100, 10^4, 10^8)\) K. The limits given by Dijkstra (2014) \((x_{\text{crit}} = 3.2)\) and Ahn et al. (2002) \((x_{\text{crit}} = \sqrt{\pi})\) are also plotted as dot-dashed and dashed lines, respectively. Note that the resonance probability decreases at lower \(x\) with decreasing gas temperatures. Note also that the probability of core scattering \(P_r > 1\) for small \(x\) for \(T = 10\) K.](image)

5.4 Adding polarised transfer to tlac

To enable creating, scattering and transport of polarised Lyα, the stand-alone radiative transfer routine tlac written in the programming language C by Gronke & Dijkstra (2014) has to be modified.
5.4. Adding polarised transfer to \textit{tlac}

**Photon properties**

Each photon is described using a density matrix $\rho$. In practice does this reduce to the photon being given three extra parameters corresponding to the density matrix elements $\rho_{11}$, $\rho_{12} = \rho_{21}$ and $\rho_{22}$. At initialisation, $\rho_{11} = \rho_{22} = 0.5$ and $\rho_{12} = \rho_{21} = 0$, which corresponds to unpolarised light.

The density matrix elements can change under each scattering event and are used both for inferring the phase function and the degree of polarisation.

Additional parameters that are added to the photon are: count of wing scatterings before escape $N_{\text{wing}}$, the total travel distance before escape $r_{\text{esc}}$, and the last scattering angle $\cos \chi = \mathbf{k}_{\text{in}} \cdot \mathbf{k}_{\text{out}}$.

**Scattering**

The scattering routine in \textit{tlac} is completely replaced by an acceptance-rejection routine where the phase function of the proposed outgoing photon is calculated and accepted (or rejected). The algorithm consists of the following steps:

1. An incoming photon with direction $\mathbf{k}_{\text{in}}$ is determined to scatter. The photon frequency offset, $x$, is compared to the transition frequency between core and wing scatterings that \textit{Laursen} (2010) calculates,

$$x_{\text{cw}}(a) = 1.59 - 0.60 \log a - 0.03 (\log a)^2$$

where $a$ is the temperature dependent parameter defined in eq. (5.7). If $x < x_{\text{cw}}$, then the photon scatters resonant. A random number $R \sim \text{Unif}(0, 1)$ is drawn to determine the transition type. If $R > 1/3$, the transition is H-type, otherwise it is K-type. This is in accordance with \textit{Stenflo} (1980).

If the frequency offset $x \geq x_{\text{cw}}$, the scattering happens in the damping wing.

2. According to the scattering type, the correct density matrix formalism is chosen.

3. Before calculating a proposed density matrix, a normalisation constant has to be estimated. As forward and backward scatterings are the most likely scattering directions in the dipole approximation, the maximum obtainable phase function should be that which appears from applying the density matrix formalism on a photon that
5. **Including polarisation in radiative transfer**

is forward or backward scattered. The normalisation constant can be denoted \( \langle I \rangle = (\rho_{11} + \rho_{22})_{\text{max}} \) and is different for the different scattering types. An analytical calculation of this constant would require an integration of the phase function over the incoming and outgoing set of angles, and the phase function is a non-linear function of these as well as the density matrix elements of the incoming photon.

4. If the scattering happens in the wing, the relevant density matrix elements are those of eq. (4.42).

If the scattering is resonant H-type, the relevant density matrix elements are those of eq. (4.43), and for K-type, the elements are found in eq. (4.44).

5. The density matrix requires a set of incoming and outgoing angles. The incoming angles are the polar coordinates \((\theta, \phi)\) of \(k_{\text{in}}\), and the outgoing angles \((\theta', \phi')\) are determined from a randomly drawn \(k_{\text{out}}\) from the unit sphere.

6. When a proposed outgoing \(k_{\text{out}}\) has been drawn, the (proposed) density matrix \(\rho'\) associated with the scattering \(k_{\text{in}} \rightarrow k_{\text{out}}\) is calculated.

7. The phase function for this scattering is calculated,

\[
p(\theta, \phi, \theta', \phi') = \frac{\rho'_{11} + \rho'_{22}}{\langle I \rangle} \quad (5.25)
\]

and compared to a random number \(\mathcal{R} \sim \text{Unif}[0,1]\). If \(p(\theta, \phi, \theta', \phi') \geq \mathcal{R}\), the proposed \(k_{\text{out}}\) and \(\rho'\) are accepted. Note that the normalisation constant makes it possible to compare the phase function with \(\mathcal{R}\), as \(\rho'_{11} + \rho'_{22} > 1\) for some combinations of \(\rho\) and \((\theta, \phi, \theta', \phi')\) for H-transitions.

8. The last scattering angle \(\chi\) is stored and the total travel distance \(r_{\text{esc}}\) is increased.
Chapter 6

Results

This chapter will present analytical and numerical results based on application of the density matrix formalism for radiative transfer of polarised light, introduced by Lee & Ahn (2002) and Ahn et al. (2002).

6.1 Density matrix formalism

Before proceeding to numerical investigations of the density matrix formalism and an application of it on an idealised astrophysical case of a plane-parallel semi-infinite optically thick slab of neutral hydrogen, some theoretical scattering cases are explored.

Phase function

The phase function was defined in Eq. (4.51), and it gives, if normalised, the probability of a scattering event in a direction specified by the outgoing angles \( \theta', \phi' \) given the set of incoming angles \( \theta, \phi \).

In idealised cases where an incoming wave propagates along some axis (with \( \theta, \phi \) specified) and scatters, the phase function derived from Eqs. (4.42, 4.43, 4.44) can be written in a simplified form.

In the case of scattering of unpolarised (\( \rho_{11} = \rho_{22} = 1/2, \rho_{12} = \rho_{21}^* = 0 \)) light, the phase functions for the different scattering types become:

- **Wing-scattering**: the density matrix elements are given in Eq. (4.42), and yield a phase function dependent only on \( \theta' \) as an outgoing
angle, given that the incoming light propagates along the $z$-axis. Hence the incoming angles are $\theta = \phi = 0$, and the phase function becomes

$$p_{\text{wing}} (\theta' | \theta = \phi = 0, \text{unpolarised}) \langle I \rangle = \frac{1}{2} (1 + \cos^2 \theta') , \quad (6.1)$$

but is, however, un-normalised. The normalisation factor is found to be

$$\langle I \rangle = \int_{-1}^{+1} p_{\text{wing}} (\theta' | \theta = \phi = 0, \text{unpolarised}) \, d (\cos \theta') = \frac{4}{3}$$

such that the phase function becomes

$$p_{\text{wing}} (\theta' | \theta = \phi = 0, \text{unpolarised}) = \frac{3}{8} (1 + \cos^2 \theta') \quad (6.2)$$

which is on the exact same form as Eq. (4.36) derived from Chandrasekhar [1960]. The most likely scattering directions are given by the maximum of the phase function, and $\max (p_{\text{wing}}) = 3/4$ for $\theta' = (0, 1)\pi$, corresponding to forward and backward scattering, respectively. The least likely scattering direction is found by the minimum, which is $\min (p_{\text{wing}}) = 1/2$ for scattering at right angles, i.e. when $\theta' = \pm \pi/2$.

In the case of unpolarised light propagating along the $x$-axis, the phase function becomes different. Following the same procedure as above, but with $\theta = \pi/2$ and $\phi = 0$, the un-normalised phase function becomes

$$p_{\text{wing}} (\theta', \phi' | \theta = \pi/2, \phi = 0, \text{unpolarised}) \langle I \rangle = \frac{1}{2} (\cos^2 \phi' + \cos^2 \theta' \sin^2 \phi' + \sin^2 \theta' ) \quad (6.3)$$

however, to assess any symmetries, as found in the case above, where the phase function was constant in rotations around the $z$-axis, a constraint has to be placed on the phase function in the current case.
6.1. Density matrix formalism

A scattering where the incoming wave $k_{\text{in}}$ propagates along the $z$-axis can be described in a fixed coordinate system, as above with $\theta = \pi/2$ and $\phi = 0$, or using the coordinate-invariant scattering angle $\cos \chi = k_{\text{in}} \cdot k_{\text{out}}$.

To investigate whether the phase function is solely dependent on the scattering angle $\chi$, variations of $\theta'$ and $\phi'$ that yield $\chi$ can be plugged into the phase function. If the phase function is constant for these combinations of $\theta'$ and $\phi'$, the scattering can be described solely by the scattering angle $\chi$.

Such combinations of $\theta'$ and $\phi'$ would trace out a circle in the $yz$-plane, see Fig. 6.1. Any point along the rim of the circle corresponds to the same scattering angle $\chi$, but with different combinations of $\theta'$ and $\phi'$.

![Diagram](image)

Figure 6.1: Scattering with $\theta = \pi/2$ and $\phi = 0$ and a fixed scattering angle $\chi$ traces out a circle in the $yz$-plane where $\chi$ is constant. If the phase function only depends on the scattering angle $\chi$ it will not vary along the circle.

Each point of the circle can be described using two coordinates,

$$
\begin{align*}
y &= r \sin \phi' \\
z &= r \cos \theta'
\end{align*}
$$

(6.4)

fulfilling the constraint

$$
y^2 + z^2 = r^2 (\sin^2 \phi' + \cos^2 \theta') = r^2 \sin^2 \chi
$$

(6.5)

where the radius $r$ is the length of the hypotenuse in the triangle with one side being the radius of the outlined circle, and the other
side being the distance from the line centre to the origin. The angle between the line from the circle to origin and the hypotenuse is the scattering angle $\chi$.

In this representation, the un-normalised phase function of Eq. (6.3) becomes, after some algebra,

$$p_{\text{wing}}(\phi'|\theta = \pi/2, \phi = 0, \text{unpolarised, fixed } \chi) \langle I \rangle$$

$$= 1 - \frac{1}{2} \sin^2 \chi + \frac{1}{2} \sin^2 \phi' \left( \sin^2 \chi - \sin^2 \phi' \right)$$

(6.6)

and is thus dependent on both the scattering angle $\chi$ and the coordinate-specific angle $\phi'$ (and $\theta'$ which is determined once the other two are given).

- **H-type scattering**: the density matrix elements are given in Eq. (4.43). The phase function with $\theta = \phi = 0$ is only dependent on one scattering angle, $\theta'$ and is in un-normalised form

$$p_{H}(\theta'|\theta = \phi = 0, \text{unpolarised}) \langle I \rangle$$

$$= 5 + 5 \cos^2 \theta' + 2 \sin^2 \theta'$$

$$= 7 + 3 \cos^2 \theta'$$

(6.7)

where it was used that $\sin^2 \theta' = 1 - \cos^2 \theta'$. The normalisation factor is

$$\langle I \rangle = \int_{-1}^{+1} p_{H}(\theta'|\theta = \phi = 0, \text{unpolarised}) \, d(\cos \theta')$$

$$= 16$$

such that the phase function becomes

$$p_{H}(\theta'|\theta = \phi = 0, \text{unpolarised})$$

$$= \frac{7}{16} + \frac{3}{16} \cos^2 \theta'$$

(6.8)

which is identical to the phase function of Eq. (4.34). The maximum phase function is $\max (p_{H}) = 5/8$ for $\theta' = (0, 1)\pi$. The minimum is $\min (p_{H}) = 7/16$ for $\theta' = \pm \pi/2$.

In the case where the incoming wave propagates along the $x$-axis, and hence $\theta = \pi/2$ and $\phi = 0$, the un-normalised phase function becomes

$$p_{H}(\theta', \phi'|\theta = \pi/2, \phi = 0, \text{unpolarised}) \langle I \rangle$$

$$= \frac{1}{2} \left[ 7 + 3 \cos (2\phi') \sin^2 \theta' + 7 \cos^2 \theta' + 10 \sin^2 \phi' \right].$$

(6.9)
To assess whether the phase function is independent of the coordinate representation, the procedure outlined above for the wing scattering case can be repeated. This yields, after some algebra, a un-normalised phase function that is dependent on both scattering angle $\chi$ and the coordinate-representation specific angle $\phi'$,

$$p_{\text{wing}} (\phi'|\theta = \pi/2, \phi = 0, \text{unpolarised, fixed } \chi) \langle I \rangle = 10 - 3 \sin^2 \chi + 3 \sin^2 \phi' \left( \sin^2 \chi - \sin^2 \phi' \right).$$  \hspace{1cm} (6.10)

- **K-type scattering**: the density matrix elements for this transition are given in Eq. (4.44) and yield unpolarised, isotropic scattering. Hence, the normalised phase function is

$$p_K = \frac{1}{2}$$  \hspace{1cm} (6.11)

which is on the same form as Eq. (4.32).

### Degree of polarisation

For the first of the two theoretical scattering cases above, where unpolarised light ($\rho_{11} = \rho_{22} = 1/2, \rho_{12} = \rho_{21} = 0$) propagates along the z-axis ($\theta = \phi = 0$), the degree of polarisation can be found by using Eq. (4.53).

- **Wing scattering**: the density matrix elements are given in Eq. (4.42), and the un-normalised phase function is given in Eq. (6.1), yielding

$$\Pi_{\text{wing}} (\theta'|\theta = \phi = 0, \text{unpolarised}) = \frac{\rho_{11} - \rho_{22}}{\rho_{11} + \rho_{22}}$$

$$= \frac{1/2}{1 + \cos^2 \theta'}$$

$$= \frac{\sin^2 \theta'}{1 + \cos^2 \theta'}$$  \hspace{1cm} (6.12)

which is angle-dependent and equal to Eq. (4.36). The maximum degree of polarisation is found for $\theta' = \pm \pi/2$, yielding max ($\Pi_{\text{wing}}$) = 1, and min ($\Pi_{\text{wing}}$) = 0 for $\theta' = (0, 1)\pi$.

- **H-type scattering**: the density matrix elements are given in Eq. (4.43) and the un-normalised phase function is given in Eq. (6.7),
yielding

\[
\Pi_{H}(\theta'|\theta = \phi = 0, \text{unpolarised}) = \frac{5 - 5 \cos^2 \theta' - 2 \sin^2 \theta'}{7 + 3 \cos^2 \theta'} = \frac{3 - 3 \cos^2 \theta'}{7 + 3 \cos^2 \theta'}
\]

(6.13)

which has a maximum value \( \max(\Pi_H) = 3/7 \) for \( \theta' = \pm \pi/2 \), and a minimum value \( \min(\Pi_H) = 0 \) for \( \theta' = (0, 1) \). The extrema and function are equal to those of the polarisation function derived from Chandrasekhar (1960) in Eq. (4.35).

### 6.2 Single scattering events

This section describes single scattering of photons using numerical methods.

**Directional dependent phase function**

The analytical phase functions for scattering of unpolarised light that propagated along either the \( z \)- or the \( x \)-axis were found in the above section to depend on the propagation direction.

This investigation was numerically extended to encompass scattering events where the incoming radiation was propagating along all the coordinate axes, for both wing and H-type resonance scattering. In addition, scattering of radiation propagating along an arbitrary incoming direction was analysed.

See Fig. (4.1) for a sketch of the scattering coordinate system that the density matrix formalism requires. The set of incoming momentum propagation directions were \( \{k_{in}\} = e_x, e_y, e_z, k_{in, \text{random}} \), where \( e_i \) denotes the unit vector along coordinate axis \( i \), and \( k_{in, \text{random}} \) denotes a random incoming direction.

\( N = 10^5 \) unpolarised photons were scattered once for each of the two possible scattering types and for four possible incoming directions \( k_{in} \). The outgoing directions were chosen in accordance with the acceptance-rejection sampling algorithm for scattering direction, outlined in Ch. 5.

See Fig. (6.2) for the distribution of accepted scattering angles \( \cos \chi \equiv k_{in} \cdot k_{out} \) given the incoming propagation direction, for *wing scattering*.

See Fig. (6.3) for the distribution of accepted scattering angles \( \cos \chi \), given the incoming propagation directions, for *H-type resonance scattering*. 

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6.2. Single scattering events

The accepted angles were binned and the histogram was normalised. Overplotted in Fig. (6.2) is the analytical phase function for Rayleigh scatterings of Eq. (4.36), and the distributions of accepted angles all trace out this phase function.

Similarly, in Fig. (6.3), is the analytical phase function for H-type scatterings of Eq. (4.34) overplotted. The four distributions all trace out this phase function.

\[ \cos \chi \equiv k_{\text{in}} \cdot k_{\text{out}} \]

Figure 6.2: Distribution of accepted angles after single scatterings of unpolarised \((\rho_{11} = \rho_{22} = 1/2, \rho_{12} = \rho_{21}^* = 0)\) photons that propagated along either of the coordinate axes \(e_x, e_y, e_z\) or along a random direction. The scattering angle is given from the direction of the incoming and outgoing photon, \(\cos \chi = k_{\text{in}} \cdot k_{\text{out}}\). The outgoing photons were drawn uniformly from the unit sphere and accepted/rejected according to their scattering probability. The solid line is the analytical phase function for Rayleigh scatterings derived by Dijkstra & Loeb (2008), and the normalised distributions of accepted angles trace out this phase function.

Preferred scattering angles, polarisation and analytical phase functions

The similarity between the distributions that the scattering angles trace out and the analytical phase functions shown in the previous subsection was analysed using statistical methods. The analysis was extended to also include distributions of preferred scattering angles where the incoming radiation was fully polarised.
Figure 6.3: Distribution of accepted angles after single H-type scatterings of unpolarised photons that propagated along either of the coordinate axes. The scattering angle is $\chi$, and as for single wing scatterings, was an outgoing direction accepted if the scaled phase function derived from the density matrix elements was larger than a random number. Overplotted is the analytical phase function for H-type scatterings of Eq. (4.34). All the distributions trace out the analytical phase function.

$N = 10^5$ photons were scattered once for each incoming propagation direction and for three possible polarisation states:

- **completely unpolarised**: where the non-zero density matrix elements of the incoming photon were $\rho_{11} = \rho_{22} = 0.5$;

- **maximally polarised**: where the incoming radiation was fully polarised along either of the polarisation axes, and hence were the associated density matrix elements $(\rho_{11}, \rho_{22}) = (1, 0)$ or $(\rho_{11}, \rho_{22}) = (0, 1)$ (and $\rho_{12} = \rho_{21} = 0$ for both cases).

The outgoing direction was drawn randomly from a unit sphere, and accepted in accordance with the acceptance-rejection sampling method outlined in Ch. (5). The accepted scattering angles $\cos \chi = k_{\text{in}} \cdot k_{\text{out}}$ were stored.

Tab. (6.1) presents mainly the similarity between the distributions of the scattered angles given a defined $k_{\text{in}}$ and a random $k_{\text{out}}$. These distributions are compared to the analytical phase function using the Kolmogorov-Smirnov (abbreviated “KS”) statistic and its associated $p$-value.
6.2. Single scattering events

The Kolmogorov-Smirnov statistic is calculated by comparing the empirical distribution functions that the data points are sampled from. Denoting $x'_1, x'_2, \ldots, x'_m$ and $y'_1, y'_2, \ldots, y'_n$ realisations of two independent random variables $X$ and $Y$, respectively, with associated empirical cumulative distribution functions $F_m(x)$ and $G_n(x)$, respectively, the Kolmogorov-Smirnov statistic is

$$D_{m,n} = \sup_j |F_m(x) - G_n(x)|$$ (6.14)

if $X$ and $Y$ share a common continuous distribution $F(x)$ (Feller 1948).

The KS-statistic can be interpreted as the greatest separation between the empirical cumulative distribution functions. If the separation goes to zero for $m, n \to \infty$, the sampling distributions are the same. A null hypothesis can be defined, $H_0$: $X$ and $Y$ share the same distribution.

To compare the distribution that the scattered photons were drawn from, given an incoming direction and polarisation state, a suitable null hypothesis can be given. For this purpose it can be defined to be $H_0$: the distribution of scattered photons is the same as the analytical phase function for related scattering type.

The scattering types, incoming direction and polarisation state are all given in tab. (6.1). The $p$-values of $H_0$ failing to be rejected are given as "KS: p-value", and were calculated using the stats.ks_2samp function of SciPy.

For a significance level $\alpha = 0.05$, $H_0$ fails to be rejected and all the scattered angles can be said to be distributed according to the transition-type corresponding analytical phase function. The Kolmogorov-Smirnov method was tested by comparing the distributions of angles to an arbitrary phase function, and yielded insignificant $p$-values when the phase function was for another transition that the one the photons had been scattered through.

**Polarisation after single scattering events**

The degree of polarisation was calculated for $N = 10^5$ photons that had scattered once and binned according to scattering angles. The incoming photons were given a fixed incoming direction and polarisation state.

The incoming directions were the same as investigated above, with $\{k_{in}\} = e_x, e_y, e_z$ and randomly (for each scattering event). The three possible polarisation states were the same as above: either fully unpolarised, polarised with $\rho_{11} = 1$ (other density matrix elements zero), polarised with $\rho_{22} = 1$ (other density matrix elements zero).
6. Results

Table 6.1: Comparison of the distribution of scattered angles to the analytical phase functions for the corresponding transition. The unpolarised cases are plotted in Figs. 6.2, 6.3 for wing and H-type core scatterings, respectively. The vector notation for the incoming direction denotes which coordinate axis the incoming photon was propagating along. The direction “random” denotes that the incoming direction was drawn randomly from the unit sphere for each scattering event. The $p$-values denotes the probability of failure to reject the null hypothesis, which is that the scattering angles are sampled from the same distribution as the corresponding analytical phase function for the transition. The related analytical phase functions are those of Eqs. (4.34, 4.36) for K-type core scattering events and wing scattering events, respectively. The distributions of accepted angles for core and wing scatterings of fully polarised photons (either $\rho_{11} = 1$ or $\rho_{22} = 1$ with the other zero) were also compared to the analytical phase functions for unpolarised light.

<table>
<thead>
<tr>
<th>Inc. rad. polarisation state</th>
<th>Scatter. type</th>
<th>Incoming vector dir.</th>
<th>KS: $p$-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unpolarised</td>
<td>Core</td>
<td>[1, 0, 0]</td>
<td>$4.1 \times 10^{-1}$</td>
</tr>
<tr>
<td>Unpolarised</td>
<td>Core</td>
<td>[0, 1, 0]</td>
<td>$6.6 \times 10^{-1}$</td>
</tr>
<tr>
<td>Unpolarised</td>
<td>Core</td>
<td>[0, 0, 1]</td>
<td>$7.52 \times 10^{-1}$</td>
</tr>
<tr>
<td>Unpolarised</td>
<td>Core</td>
<td>random</td>
<td>$3.09 \times 10^{-2}$</td>
</tr>
<tr>
<td>Unpolarised</td>
<td>Wing</td>
<td>[1, 0, 0]</td>
<td>$1.29 \times 10^{-1}$</td>
</tr>
<tr>
<td>Unpolarised</td>
<td>Wing</td>
<td>[0, 1, 0]</td>
<td>$1.95 \times 10^{-1}$</td>
</tr>
<tr>
<td>Unpolarised</td>
<td>Wing</td>
<td>[0, 0, 1]</td>
<td>$3.76 \times 10^{-1}$</td>
</tr>
<tr>
<td>Unpolarised</td>
<td>Wing</td>
<td>random</td>
<td>$6.06 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Core</td>
<td>[1, 0, 0]</td>
<td>$1.12 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Core</td>
<td>[0, 1, 0]</td>
<td>$9.98 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Core</td>
<td>[0, 0, 1]</td>
<td>$8.61 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Core</td>
<td>random</td>
<td>$2.7 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Wing</td>
<td>[1, 0, 0]</td>
<td>$1.17 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Wing</td>
<td>[0, 1, 0]</td>
<td>$9.34 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Wing</td>
<td>[0, 0, 1]</td>
<td>$5.33 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{11} = 1.0$</td>
<td>Wing</td>
<td>random</td>
<td>$9.24 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Core</td>
<td>[1, 0, 0]</td>
<td>$9.21 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Core</td>
<td>[0, 1, 0]</td>
<td>$3.41 \times 10^{-1}$</td>
</tr>
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<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Core</td>
<td>[0, 0, 1]</td>
<td>$1.08 \times 10^{-2}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Core</td>
<td>random</td>
<td>$8.99 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Wing</td>
<td>[1, 0, 0]</td>
<td>$6.79 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Wing</td>
<td>[0, 1, 0]</td>
<td>$4.68 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Wing</td>
<td>[0, 0, 1]</td>
<td>$5.7 \times 10^{-1}$</td>
</tr>
<tr>
<td>Polarised - $\rho_{22} = 1.0$</td>
<td>Wing</td>
<td>random</td>
<td>$7.61 \times 10^{-1}$</td>
</tr>
</tbody>
</table>
The different degrees of polarisation given a scattering type and incoming polarisation state are plotted as functions of scattering angle $\cos \chi = \mathbf{k}_{\text{in}} \cdot \mathbf{k}_{\text{out}}$ in Fig. 6.4. The degree of polarisation for the outgoing photon was calculated in accordance with Eq. (4.53). In the third subplot, where the incoming radiation was pointing in the $z$-direction, are the analytical polarisation degrees for wing, H- and K-type resonance scattering, given by Eqs. (4.37), (4.35), (4.33), respectively, overplotted.

The polarisation degrees for the different scattering types are both dependent on the direction of the incoming radiation, the scattering angle and the scattering type. K-type transitions yield zero polarisation in all scattering cases (green line), whereas the other transitions give different degrees of polarisation for different choices of incoming directions and polarisation states.

In the case where the incoming photon points in the $z$-direction, the degree of polarisation goes as the analytic solution for both K-, H- and Rayleigh-type scattering. The degrees of polarisation have the same scattering angle dependence in the case where the incoming photon propagates in the $x$- or $y$-direction (top two subplots of Fig. 6.4) for the different scattering types and polarisation states. This similarity does not exist for scattering where the incoming photon was propagating in the $z$-direction.

The effect of having an incoming photon that is fully polarised affects the degree of polarisation of the outgoing photon.

For wing scattering events (red, purple and yellow lines) where the incoming photons propagates along either the $x$- or $y$-direction (upper two plots), are maximally polarised outgoing photons obtained when the incoming photons are polarised. When the incoming photon is polarised with $\rho_{22} = 1$, the polarisation of the outgoing photon is $\Pi = -1$, irrespective of scattering angle. This corresponds to a case where the outgoing $\rho_{11} = 0$ and $\rho_{22}$ has an arbitrary non-zero value (see Eq. (4.53)).

For H-type core scattering events (blue, orange and brown lines), will unpolarised photons become up to $|\Pi_{H}| \sim 40\%$ polarised in the cases where the incoming photons are propagating along the $x$, $y$- or $z$-directions and scatters at right angles. However, when both the incoming and the outgoing photons are drawn randomly from the unit sphere (fourth subplot, direction denoted “random”), the net polarisation is zero for all scattering angles.

The degree of polarisation for the different scattering types where the incoming vector is drawn randomly from the unit sphere is symmetric around zero polarisation for the different scattering types. Incoming radiation being positively polarised ($\rho_{11} = 1$) prior to scattering is also
positively polarised after scattering, and likewise for negatively polarised radiation ($\rho_{22} = 1$). The degree of polarisation is also larger for forward- and backward scatterings than for scattering at right angles for polarised light in the case with random incoming and outgoing directions.

However, due to the asymmetries in the polarisation profiles, it is of interest to also include the Stokes $U$-parameter, thus deviating from the treatment by Lee & Ahn (2002). By using Eq. (4.52), and disregarding the Stokes $V$-parameter, the total degree of polarisation becomes

$$
\Pi_{Q,U} = \frac{\sqrt{Q^2 + U^2}}{I} = \frac{\sqrt{(\rho_{11} - \rho_{22})^2 + 4\rho_{12}\rho_{21}^*}}{\rho_{11} + \rho_{22}}
$$

(6.15)

which also is compatible with the observationally based degree of polarisation given in Eq. (3) in the supplementary information of Hayes et al. (2011).

The total, non-negative, degree of polarisation $\Pi_{Q,U}$ for the single scattering cases presented above, are plotted in Fig. (6.5). The total polarisation is distributed alike for all incoming scattering directions, including random incoming photon propagation directions.

Fully polarised photons ($\rho_{11} = 1$ or $\rho_{22} = 1$, purple line and yellow dot-dashed line, respectively) that undergo wing scattering, retain their degree of polarisation. Unpolarised photons that undergo K-type scattering, does not obtain any polarisation (green line).

H-type scattering of fully polarised photons result in outgoing photons that have maximally $\Pi_{Q,U} \sim 60\%$ and minimally $\Pi_{Q,U} \sim 40\%$ (brown and orange lines).

Unpolarised photons that undergo wing scattering (red lines) scatter obtain a degree of polarisation following the analytical function of Eq. (4.37) (compare with analytical solutions overplotted in third subplot) with a maximum of $\Pi_{Q,U} \sim 100\%$.

Photons that undergo H-type scattering obtain a total degree of polarisation comparable to the analytical function of Eq. (4.35) with a maximum of $\Pi_{Q,U} \sim 40\%$ for scattering at right angles ($\cos \chi = 0$).

### 6.3 Radiative transfer

In the previous sections were analytical and numerical implications from describing single scattering events using the density matrix formalism explored. In this section is the modified radiative transfer routine tlac used to solve radiative transfer problems and thus deals with multiple scattering events.
6.3. Radiative transfer

A solution to the transport equation for the angle-averaged frequency dependent intensity $J_{\nu}$ in the case of a semi-infinite plane-parallel, optically thick slab with the light source being a thin sheet was presented by Neufeld (1990). Laursen (2010) notes that due to symmetries, the emission sheet can be approximated as a point source.

The mean intensity at the surface of a semi-infinite slab, $J(\pm \tau_0, x)$, at a frequency offset $x$ from the line centre, with photons emitted at the frequency offset $x_{\text{inj}}$ at a location $\tau'_s$ in the slab, is

$$J(\pm \tau_0, x) = \frac{\sqrt{6}}{24} \frac{x^2}{\sqrt{\pi a\tau_0}} \frac{\cos (\pi \tau'_s/2\tau_0)}{\cosh \left( \sqrt{\pi^3/54} \left( x^3 - x_{\text{inj}}^3 \right) / a\tau_0 \right) \mp \sin (\pi \tau'_s/2\tau_0)}$$

from Neufeld (1990). For $x_{\text{inj}} = 0$ and $\tau'_s = 0$, this expression reduces to the Eq. (35) in Harrington (1973) who approached the problem as a analytical diffusion problem that was governed by a Poisson equation.

Using the polarisation enabled tlac, a point source in a plane-parallel semi-infinite slab was simulated. The gas temperature was set $T_g = 10$ K, and two simulations with different line centre optical thickness were run: $\tau_0 = (2 \times 10^4, 2 \times 10^6)$. The core skipping parameter was chosen to be $x_{\text{crit}} = \sqrt{\pi}$.

In Fig. (6.6) are the binned frequency offsets plotted against the analytical solution given by Eq. (6.16). In both cases does tlac reproduce the expected spectrum.

The Neufeld solution fits the optically thickest case ($\tau_0 = 2 \times 10^6$) better than the thinner case ($\tau_0 = 2 \times 10^4$). In the latter case has the Neufeld solution a smaller spread and higher peaks than the simulated spectrum (from the normalised histogram made of binned frequency offsets), see Fig. (6.7).

**Polarisation from scatterings in semi-infinite plane-parallel slab**

The polarisation enabled tlac was above used to describe scatterings in semi-infinite plane-parallel slabs. Using the same setups, where only the line centre optical thickness differed, were scattering in two slabs simulated. For both slabs where $\tau_0 = 2 \times 10^4$ and $\tau_0 = 2 \times 10^6$ were $N = 1.6 \times 10^6$ photons emitted from a point source at a frequency offset $x_{\text{inj}} = 0$ in a slab that was infinite in the x- and y-directions, having a
gas temperature $T_g = 10$ K. The core-skipping parameter was in both simulations set $x_{crit} = \sqrt{\pi}$.

The polarisation of the escaped radiation for the two simulations were calculated using Eq. (4.53) and binned.

In Fig. (6.8) is the degree of polarisation plotted as a function of positive frequency offsets $x > 0$ for the simulation where $\tau_0 = 2 \times 10^4$ and $T_g = 10$ K, with the photons emitted at the frequency $x_{inj} = 0$ from a point source in the middle ($r_s' = 0$) of the slab. Overplotted are the results that Lee & Ahn (2002) obtained for the same scattering case, but without error bars as these were incomplete and unsalvageable from the article. The results match.

For $\tau_0 = 2 \times 10^4$, the degree of polarisation decreases from zero as the frequency offset increases. The maximum obtainable degree of polarisation $|\Pi(x)|$ is reached when $x > 15$, with $\Pi(x \sim 15) = -0.13$ corresponding to 13% polarisation in the direction parallel to the slab normal. The preferred escape frequency offset was $x \sim \pm 8$, according to Fig. (6.7). The highly polarised photons thus belong to the upper tail of the frequency distribution.

In Fig. (6.9) is the degree of polarisation plotted as a function of positive frequency offsets, as above, but for the simulation with $\tau_0 = 2 \times 10^6$. The polarisation is constant slightly positive within the error bars for all frequency offsets. The preferred escape frequency was $x \sim \pm 30$, see Fig. (6.6).

**Viewing-angle dependent polarisation**

From the simulations outlined in the previous paragraphs, it was also possible to obtain the degree of polarisation for different viewing angles relative to the slab surface.

The polarisation as function viewing angle $\mu \equiv \cos \theta$, being the angle between the slab normal ($e_z$) and the outgoing propagation direction ($k_{out}$) is plotted for a semi-infinite plane-parallel slab with line centre optical thickness $\tau_0 = 2 \times 10^4$ in Fig. (6.10) and for a similar slab differing only in optical thickness, being $\tau_0 = 2 \times 10^6$, in Fig. (6.11).

Due to symmetry, $\theta$ can be considered the viewing angle, even though the photon might escape in a direction that is not towards the observer, but with the same angle relative to the slab normal.

For the simulation with $\tau_0 = 2 \times 10^4$, the degree of polarisation is plotted for viewing angles $\mu \in [-1,1]$, where $\mu > 0$ corresponds to photons escaping at $+\tau_0$, whereas $\mu < 0$ corresponds to photons escaping at the other side of the slab, at $-\tau_0$. The degree of polarisation is
6.3. Radiative transfer

symmetric around $\mu = 0$, and reach a maximum of $|\Pi| \sim 5\%$ for $\mu \to 0$. This corresponds to photons that has an escape direction that is almost parallel to the slab surface. Photons that escape at $\mu \sim \pm 0.7$ has the most negative polarisation, $\Pi \sim -1\%$, whereas $\Pi \to 0$ for $\mu \to \pm 1$.

For the simulation with $\tau_0 = 2 \times 10^6$, the degree of polarisation is plotted for $\mu \in [0, 1]$. Overplotted are the numerical results of Lee & Ahn (2002) who ran an equivalent simulation with a plane-parallel slab infinite in the $x$- and $y$-directions, with $T_g = 10$ K and line centre optical thickness $\tau_0 = 2 \times 10^6$. Overplotted are also the results of Chandrasekhar (1960) (table XXIV) for scattering of free electrons. The results match those of Lee & Ahn (2002) and follow the curve from Chandrasekhar (1960). The maximum degree of polarisation is $|\Pi| \sim 11\%$ obtained when $\mu \to 0$, and $\Pi \to 0$ for $\mu \to 1$.

Wing scattering events and polarisation

For the previous simulations where a semi-infinite plane-parallel slab that only differed in optical thickness, being either $\tau_0 = 2 \times 10^4$ or $\tau_0 = 2 \times 10^6$, some observable quantities were estimated. From the simulations was it also possible to create statistics on the scattering process.

In Fig. (6.12) is the polarisation degree for escaping photons binned and plotted as a function of the number of wing scattering events $N_{\text{wing}}$, this for the slab with $\tau_0 = 2 \times 10^2$. The polarisation is divided into two categories, $\Pi > 0$ which corresponds to polarisation in the perpendicular direction to the slab normal, and $\Pi < 0$ which corresponds to polarisation in the parallel direction to the slab normal.

The degree of polarisation for the two polarisation directions have the same absolute value, and the scattering events are distributed similarly in scattering frequency. The average absolute value are for most photons $|\Pi| \sim 55\%$.

In Fig. (6.13) is the absolute value of the polarisation degree for escaping photons from multiple simulations binned and plotted as function of wing scattering events $N_{\text{wing}}$. All the simulations were of a plane-parallel slab that was infinite in the $x$- and $y$-directions, with temperature $T_g = 10$ K. $N = 1.6 \times 10^6$ photons were emitted from a point source in the centre with $x_{\text{init}} = 0$. The following line centre optical thicknesses and core skipping parameters were used:

- $\tau_0 = 2 \times 10^2$: with $x_{\text{crit}} = \sqrt{\tau}, 0$,
- $\tau_0 = 2 \times 10^3$: with $x_{\text{crit}} = \sqrt{\tau}, 0$,
6. Results

- $\tau_0 = 2 \times 10^4$: with $x_{\text{crit}} = \sqrt{\pi}, 0$.
- $\tau_0 = 2 \times 10^6$: with $x_{\text{crit}} = \sqrt{\pi}$.

The average absolute value of the polarisation degree increases for increasing line centre optical depth $\tau_0$, with highest polarisation degrees obtained by photons scattered in the medium with $\tau_0 = 2 \times 10^6$. For the thinner media $\tau_0 = 2 \times 10^2, \tau_0 = 2 \times 10^3$, there is larger variability in the polarisation degree as function of scattering events. For $\tau_0 = 2 \times 10^3$, the degree of polarisation increases with the number of wing scattering events.

The number of wing scattering events also increases for increasing line centre optical thickness. The spread in scattering frequency indicates the lower and upper bounds for the number of wing scattering events a photon must undergo before it may escape the medium. Core scattering events are not included.

Note also that there are small differences between the polarisation degrees obtained from the simulations with core skipping enabled and set to $x_{\text{crit}} = \sqrt{\pi}$ and those simulations that did not use the acceleration scheme.

Photon escape direction

In Fig. (6.14) are the distribution of preferred escape angles $\cos \theta$ plotted, from simulations of semi-infinite, plane-parallel slabs of $T_g = 10$ K with photons emitted from a point source and at a frequency offset $x_{\text{inj}} = 0$, with line centre optical thicknesses $\tau_0 = 2 \times 10^2, 2 \times 10^3, 2 \times 10^4, 2 \times 10^6$. For the line centre optical thicknesses $\tau_0 = 2 \times 10^2$ and $2 \times 10^3$ were the core-skipping acceleration scheme disabled.

The escape angle $\mu = \cos \theta$ is relative to the slab normal. Photons with $\mu > 0$ escaped at the top of the slab, $\tau_0$, whereas photons with $\mu < 0$ escaped at $-\tau_0$.

The preferred escape angles are parallel to the slab normal. Lower optical thicknesses reduces this preference, and in those simulations, more photons escape perpendicular to the slab normal.

In Fig. (6.15) are the distributions of the last scattering angles $\cos \chi = k_{\text{in}} \cdot k_{\text{out}}$ plotted for the same simulations as above.

In the media with lower optical thickness, there is a more uniform distribution of last scattering angles than in the media with higher optical thickness. For the simulation with $\tau_0 = 2 \times 10^6$ is forward scattering strongly preferred, both over scattering at right angles, but also over backward scattering.
Figure 6.4: The degree of polarisation, denoted $II$, given as a function of scattering angle $\cos \chi$ where $\cos \chi = \mathbf{k}_{\text{in}} \cdot \mathbf{k}_{\text{out}}$ for the incoming vectors $\{\mathbf{k}_{\text{in}}\} = \mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ and "random" (with plot subplot title indicating $\mathbf{k}_{\text{in}}$). The latter denotes an incoming vector drawn uniformly from the unit sphere. The polarisation degrees were obtained by binning the accepted scattering angles. Overplot in the third subplot, where $\mathbf{k}_{\text{in}} = \mathbf{e}_z$, are the analytical degrees of polarisation for Rayleigh, H-type and K-type transitions.
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Figure 6.5: The total degree of polarisation $\Pi_{Q,U}$ plotted as a function of the last scattering angle $\cos \chi = k_{\text{in}} \cdot k_{\text{out}}$ from single scattering events, as in Fig. (6.4). The total degree of polarisation is found from Eq. (6.15). The degree of polarisation for unpolarised photons goes as the analytical functions given in Eqs. (4.33; 4.35; 4.37) for K-, H- and Rayleigh-type scattering, respectively. These functions are overplotted in the third subplot. Scattering of polarised light photons make them either retain their full degree of polarisation (wing scattering) or reduces the polarisation degree (H-type scattering, zero polarisation for K-type scatterings by definition).
6.3. Radiative transfer

Figure 6.6: Binned escape frequency offsets for photons from two simulations, one with $\tau_0 = 2 \times 10^4$, another with $\tau_0 = 2 \times 10^6$, and both with $T_g = 10$ K. The emission originated in a point source in a semi-infinite plane-parallel slab and escaped at the surface defined by the optical thickness $\tau_0$. The analytical solution is given by Harrington (1973); Neufeld (1990). The analytical solution fits the optically thicker case better than the thinner, see Fig. (6.7) for a plot of the latter case alone.

Figure 6.7: Simulated spectrum from binned frequency offsets plotted against the analytical solution by Harrington (1973); Neufeld (1990). $N = 1.6 \times 10^6$ photons were emitted from a point source in a semi-infinite plane-parallel slab with temperature $T_g = 10$ K and line centre optical thickness $\tau_0 = 2 \times 10^4$. Note that the analytical solution does not fit the data perfectly in the peaks or at the base, as the Neufeld solution only applies for very optically thick media. For $\tau_0 = 2 \times 10^6$, the fit is excellent.
6. Results

Figure 6.8: Binned polarisation degrees calculated using Eq. (4.53) for increasing frequency offsets $x > 0$. The degree of polarisation reach a maximum of $|\Pi(x \sim 15)| \sim 0.13$, being approximately zero for $x = 0$. The preferred escape frequency offset was $x \sim 8$, according to Fig. (6.7) and the highly polarised photons do then belong to the upper tail of the frequency distribution. Overplotted as green circles are the results Lee & Ahn (2002) obtained for the same setup, with $\tau_0 = 2 \times 10^4$, $T_g = 10$ K and radiation emitted at the centre of a plane-parallel, semi-infinite slab in the $xy$-directions with the slab normal pointing in the $z$-direction. The error bars of the green points were not obtainable, but the reproduced results are well within the results of Lee & Ahn (2002).

Figure 6.9: Binned polarisation degrees for increasing frequency offsets $x$, as in Fig. (6.8), but for a simulation that differed only in line centre optical thickness $\tau_0 = 2 \times 10^6$. Most photons escaped the slab at a frequency offset $x \sim 30$, see Fig. (6.8). The degree of polarisation is constant, slightly positive within the error bars for the frequency offsets plotted.
6.3. Radiative transfer

Figure 6.10: Binned polarisation degrees as function of the escape angle $\mu \equiv \cos \theta$ with respect to the slab normal which points in the $z$-direction for a semi-infinite plane-parallel slab with $\tau_0 = 2 \times 10^4$ and setup as in Figs. (6.7, 6.8). The escape angle may also be considered the viewing angle. The degree of polarisation is symmetric around $\mu = 0$, and $\mu < 0$ correspond to escape at $-\tau_0$, whereas $\mu > 0$ corresponds to escape at the top, $\tau_0$. The maximum degree of polarisation is $|\Pi| \sim 5\%$ for $\mu \rightarrow 0$.

Figure 6.11: Binned polarisation degrees as a function of viewing angle $\mu \equiv \cos \theta$ where $\theta$ is the angle between the escaping photon direction and the slab normal, defined to be in the $z$-direction. The simulation was equal in setup as in Fig. (6.10), but differ in line centre optical depth $\tau_0 = 2 \times 10^6$. Overplotted are the results of Lee & Ahn (2002) obtained for an equal setup (green circles), and also, the analytical results obtained by Chandrasekhar (1960) for free electron scattering (solid black line). The maximum degree of polarisation is $|\Pi| \sim 11\%$ for $\mu \rightarrow 0$, and $|\Pi| \rightarrow 0$ when $\mu \rightarrow 1$. 
6. Results

Figure 6.12: Degree of polarisation calculated and binned for photons that scattered in a plane-parallel, semi-infinite medium with line centre optical thickness $\tau_0 = 2 \times 10^4$. Negative polarisation is associated with polarisation directions parallel to the slab normal, and positive polarisation is associated with polarisation directions perpendicular to the slab normal. The mean absolute value of the degree of polarisation is $|\Pi| \sim 55\%$.

Figure 6.13: Absolute values of the degree of polarisation calculated and binned linearly for simulations of a plane-parallel, semi-infinite slab with different optical thicknesses and with core skipping enabled ($x_{ crit} = \sqrt{\pi}$) or disabled. The degree of polarisation for each photon increases for increasing optical thickness, as does the mean number of scatterings.
6.3. Radiative transfer

Figure 6.14: Distributions of preferred escape angles $\cos \theta$ for simulations of plane-parallel semi-infinite slabs that only differ in optical thickness. For $\tau_0 = 2 \times 10^2, 2 \times 10^3$ were the core skipping acceleration scheme disabled. The escape angle is defined with respect to the slab normal. In media with larger optical thickness, the photons have stronger preference for escaping parallel to the slab normal than for systems with lower optical thickness, where more photons escape perpendicular to the slab normal.

Figure 6.15: Distributions of last scattering angles $\cos \chi = k_{\text{in}} \cdot k_{\text{out}}$ from the same set of simulations as in Fig. (6.14). There is a strong preference for forward scattering in the media with $\tau_0 = 2 \times 10^4, 2 \times 10^6$, whereas the last scattering angle in the thinner media are distributed more uniformly. Core skipping was disabled for $\tau_0 = 2 \times 10^2, 2 \times 10^3$. 
7.1 Conclusion

The density matrix formalism for scattering of light with various polarisation states, devised by Ahn et al. (2002); Lee & Ahn (2002) has been implemented into tlac, a Monte Carlo Ly\textalpha radiative transfer routine originally developed by Gronke & Dijkstra (2014).

A detailed comparison of phase functions for different types of scattering for both polarised and unpolarised light, has been presented.

Some of the main results from Lee & Ahn (2002) have been successfully reproduced. The results from scattering in extremely optically thick media produce polarisation in accordance with analytical results obtained by Chandrasekhar (1960).

It has been shown that the degree of polarisation presented by Lee & Ahn (2002) is coordinate dependent, with their Stokes $Q$-parameter defined for a plane-parallel slab that is infinite in the $x$- and $y$-directions, and that has a slab normal along the $z$-direction. It is also shown that a coordinate-independent degree of linear polarisation can be obtained by using both the Stokes $Q$ and $U$-parameters.

The coordinate-independent degree of polarisation follows theoretical functions derived by eg. Dijkstra & Loeb (2008) for single scatterings of
unpolarised photons. However, scattering of maximally polarised photons does not reproduce the polarisation degrees expected from scattering of unpolarised photons, and it is shown that unpolarised photons after a single scattering in the damping wing may obtain 100 % polarisation, or 60 % polarisation in the case of resonance H-type scattering events. Wing scattering events of maximally polarised photons does not alter their total degree of polarisation.

It was also shown that maximally polarised and unpolarised photons were distributed according to the same phase functions, without any dependence on the incoming angle, see Tab. (6.1), even though analytical derivations indicated that the phase function was dependent on the incoming direction, see Eqs. (6.6, 6.10). However, the analytical solutions were not representative for a physical process, as the latter in practice involves averaging over all incoming and outgoing scattering directions. An analytical calculation would require estimations of four-dimensional integrals over all incoming and outgoing scattering angles.

It is shown that the degree of polarisation photons obtain increase as a function of wing scattering events. The range of wing scattering events required before a photon escapes a scattering medium is dependent on the line centre optical depth of the slab. An increase in slab optical thickness also increases the mean number of wing scatterings the escaped photons underwent.

Even though the degree of polarisation associated with each photon is high in the case of extremely optically thick media, with $\Pi > 60\%$ for $\tau_0 = 2 \times 10^6$, the observed degree of polarisation depends on the observation method.

It was shown that the distribution between polarisation directions parallel and perpendicular to the slab normal was approximately equal in magnitude and opposite in sign. Had all these photons been observed, would the net $Q$-polarisation have been approximately zero. It was thus of interest to bin the polarisation as a function of other observables, as viewing angle $\theta$ and frequency offset $x$.

It was shown that the polarised photons in a semi-infinite plane-parallel slab with $\tau_0 = 2 \times 10^4$ originate in the upper tail of the frequency distribution, whereas in a thicker slab where $\tau_0 = 2 \times 10^6$, this frequency dependence was washed out and the net polarisation was only slightly positive and constant for all frequency offsets.

The polarisation as a function of viewing angle increased for $\cos \theta \to 0$, where $\theta = 0$ corresponds to observations of a plane-parallel slab nadir. Thus, a generalisation from the slab to a sphere where the scattering medium can be considered plane-parallel, the polarisation should be
A cautionary note is in place: it was shown that the total polarisation \( \Pi_{Q, U} = \sqrt{Q^2 + U^2} \) and the degree of linear polarisation \( Q \) applied by Lee & Ahn (2002) differs. This difference is caused by differences in the observational methods used to obtain the polarisation. Furthermore was it shown that the intrinsic polarisation of each photon (a quantum mechanical property) could be large (60%) but still yield insignificant observational signatures. The overall geometry also has an effect on the observed polarisation, as symmetries may smear out a polarisation signal that otherwise would have been observable. The cautionary note is then to not mix up intrinsic photon polarisation with the observed polarisation (from an ensemble of photons), and to be aware of the differences between the measure of polarisation in a numerical code (and the underlying geometric dependencies) and the (external) geometry an observer would adapt.

7.2 Outlook

The papers by Lee et al. (1994); Lee & Lee (1997); Lee & Blandford (1997); Lee & Ahn (1998); Ahn et al. (2002) that lead to the formalism in the unpublished paper by Lee & Ahn (2002) were all ahead of their time. The instrumental capabilities required to detect polarisation have not until recent times been reached, with the detection of tangential polarisation up to \( \Pi = 11.9 \pm 2\% \) by Hayes et al. (2011) around a Ly\( \alpha \) blob located at \( z = 3.09 \) marking an observational watershed.

Hayes et al. (2011) compared their results to the numerical results by Dijkstra & Loeb (2008), who simulated a geometrically more complex scattering medium than Lee & Ahn (2002), treating an outflowing scattering shell around a central point source, but with a simplified polarisation treatment. Dijkstra & Loeb (2008) applied the polarisation strategy of Rybicki & Loeb (1999) where each photon was assigned a polarisation vector (and assumed it to be 100% polarised).

The method of Rybicki & Loeb (1999) provided only two Stokes parameters, \( I \) and \( Q \), but due to the geometry applied by Dijkstra & Loeb (2008) where their polarisation degree was defined to be relative to the radius vector, the results were comparable to the polarisation measure \( \Pi_{Q, U} = \sqrt{Q^2 + U^2} \) used by Hayes et al. (2011). The Stokes \( Q \)-parameter which was obtained in this thesis, on the other hand, is defined relative to a semi-infinite plane-parallel slab where the slab
normal points in the $z$-direction. This stringent definition is suitable from an observational perspective, given that the geometry of the setup matches the one an observer would require. Otherwise, the results can be misleading. However, the degree of total polarisation $\Pi_{Q,U}$ is more flexible, and should allow for the routine to treat more realistic scattering media.

Without polarisation data, it is much harder to specify the origins of the observed Ly$\alpha$ radiation. Cantalupo et al. (2014) observed Ly$\alpha$ radiation far beyond the possible dark matter halo virial radius of a scattering system around a radio-quiet quasar at $z \approx 2.3$, concluding that the observed radiation was scattered, not produced in-situ. As shown in this thesis, would radiation scattered in highly optically thick media obtain large degrees of polarisation, and could therefore act as a constraining observable on both the geometry of the scattering medium and the origins of the observed Ly$\alpha$ radiation.

However, high signal-to-noise ratios and rigorous observational techniques are required to obtain a usable polarisation signal. Prescott et al. (2011) were the first to attempt to measure the degree of polarisation around a Ly$\alpha$ blob, and did it to a high-redshift one at $z \approx 2.656$, but obtained an insignificant signal, with $\Pi = 2.6 \pm 2.8\%$. Prescott et al. (2011) noted that observational and methodological effects made it difficult to constrain the signal. Humphrey et al. (2013) obtained a polarisation signal of $\Pi = 16.4 \pm 4.6\%$ in the Ly$\alpha$ radiation around a radio-loud quasar at $z = 2.34$, with lower polarisation signal in the brightest regions and for small frequency offsets.

The field of using Ly$\alpha$ polarimetry is thus in its infancy, but observations show promising results. With the advent of the 30 metre ground based telescopes, much enhanced polarisation signals should be obtainable. There are plans of supplying polarimetric instruments to the Thirty Meter Telescope (Atwood et al. 2014), as well as to the European Extremely Large Telescope (E-ELT). For E-ELT, however, is the main motivational factor observations of exoplanets, and not the polarisation of high-redshift galaxies (Keller et al. 2010). The mentioned observations, and the results of thesis showing that highly scattered photons may obtain large degrees of intrinsic polarisation that may be observed given a suitable geometry, should also motivate future polarimetric observations of high-$z$ Ly$\alpha$ sources.

The need is large for polarisation enabled radiative transfer routines, and in this thesis have a method that is quantum mechanically accurate been numerically implemented. However, the method was only applied to simple geometrical models where testable results existed, but will be
extended to more complex and physically accurate models in the future.
Appendix A

Concepts from Relativity

Spacetime Spacetime is a geometric interpretation that unifies time with space. Distances are measured between events in spacetime, where an event has both a temporal coordinate as well as spatial coordinates.

Event An event in spacetime can be thought of as the time and place at which somethings happens.

If you want to measure your own height, you could define two events that you perceived to be simultaneous, like two firecrackers going off, one situated at your feet, the other at your head.

In your reference frame is the difference between the two events merely the spatial difference, i.e., the difference between the spatial coordinates \((x, y, z)\) of the first firecracker and \((x', y', z')\) of the other. This difference should be a good approximation to your height!

Another example is the duration of your life. Say you choose to remain at one fixed spatial position throughout your life. Define the first spacetime event to be your birth, and the last one to be your death. As you have not moved, the difference between the two events is merely the time that has passed, i.e., the length of your life.

Position four-vector A position four-vector, or position 4-vector, is a vector that specifies the coordinates of an event in spacetime.

The ordering of coordinates is

\[
V^\alpha = \{1 \text{ temporal, 3 spatial}\} \\
= \{V^0, V^1, V^2, V^3\}.
\]  

(A.1)
Note that a vector's components only make sense if they are given with respect to some basis vectors \( \mathbf{e}_\alpha \), so that the 4-vector becomes

\[
\mathbf{V} = \sum_{\alpha=0}^{3} V^\alpha \mathbf{e}_\alpha = V^0 \mathbf{e}_0 + V^1 \mathbf{e}_1 + V^2 \mathbf{e}_2 + V^3 \mathbf{e}_3 \equiv V^\alpha \mathbf{e}_\alpha. \tag{A.2}
\]

see Einstein summation for description of the last equivalency.

Why does a vector need the basis vectors? (Hint: what happens to the components \( V^\alpha \) if you choose a new set of coordinate vectors?)

**One-form** A one-form, or a covector or cotangent, is the dual of a vector. Whereas a vector can be thought of as an arrow with a direction, the one-form can be thought of as a sheet (a hyperplane) with an inherent magnitude that is perpendicular to its dual vector.

Suggestion: think of it as the area an area vector is pointing from.

If we represent a vector as a column vector in linear algebra, then the equivalent to a one-form would be the row vector.

A one-form can be represented as

\[
\Omega = \sum_{\alpha=0}^{3} w_\alpha \omega^\alpha \equiv w_\alpha \omega^\alpha \tag{A.3}
\]

where \( w_\alpha \) are the components given a set of basis one-forms \( \omega^\alpha \). See Einstein summation for the last equivalency.

The product between a one-form \( \Omega \) and a vector \( \mathbf{V} \) is a scalar,

\[
\Omega \otimes \mathbf{V} = w_\alpha \omega^\alpha \otimes V^\beta \mathbf{e}_\beta \tag{A.4}
\]

\[
= w_\alpha V^\beta \omega^\alpha \otimes \mathbf{e}_\beta \tag{A.5}
\]

\[
= w_\alpha V^\beta \delta^\alpha_\beta \tag{A.6}
\]

\[
= \sum_{\alpha=0}^{3} \sum_{\beta=0}^{3} w_\alpha V^\beta \delta^\alpha_\beta \tag{A.7}
\]

\[
= w_0 V^0 + w_1 V^1 + w_2 V^2 + w_3 V^3 \tag{A.8}
\]

where \( \omega^\alpha \otimes \mathbf{e}_\beta = \delta^\alpha_\beta \) if they are each other's dual. The Kronecker delta \( \delta^\gamma_\sigma = 1 \) if \( \sigma = \gamma \) and 0 otherwise.

Does a one-form need its basis one-forms, or can it survive with only its components \( w_\alpha \)?

What happens if the basis one-forms are not the duals of the basis vectors? (Hint: \( \omega^\alpha \otimes \mathbf{e}_\beta \neq \delta^\alpha_\beta \), but the product is still a scalar! Could perhaps other elements sneak in?)
Einstein summation  Any index that appears more than once in an additive term is implicitly summed over,

\[ a_i b^i \equiv \sum_{i=1}^{3} a_i b^i = a_1 b^1 + a_2 b^2 + a_3 b^3. \]  \hspace{1cm} (A.9)

An index that is not repeated is a free index or a dummy index, e.g. \( \alpha \) in

\[ c_{\alpha} = a_{\alpha \beta} b_{\beta} = \sum_{\beta=0}^{3} a_{\alpha \beta} b_{\beta} = a_{\alpha 0} b_0 + a_{\alpha 1} b_1 + \cdots + a_{\alpha 3} b_3. \]

The choice of character also plays a role:

- Latin characters, a–z, denote spatial coordinates and are thus running from 1, and not 0, to 3,
- The index 0 denotes the temporal coordinate,
- Greek letters, \( \alpha–\omega \), denote spacetime coordinates and are running from 0 to 3.

World line  A world line is the path of a particle through spacetime. It is a geodesic if the particle is moving at a constant speed.

As spacetime appears locally to be Lorentzian (flat) everywhere, the paths of free-falling particles appear to be straight lines for local observers. For non-local observers, spacetime can appear curved (eg. Schwarzschild metric), and a particle can appear to follow a curved geodesic.

Invariant  An invariant quantity is a quantity that does not change under coordinate transformations.

Line element  The line element \( d x^\alpha \) is the gradient of the coordinates which are given for a point along a world line of a particle. It is a one-form, and if it works on a vector, it will give the rate of change of the coordinates in the vector’s direction.

Interpreting the one-form \( d x^\alpha \) using the notion of hyperplanes, are these the planes of constant \( x^\alpha \).

The line element squared, which often denoted \( ds^2 \), is an invariant quantity. This quantity is often abbreviated “the line element”. The physical interpretation of the (scalar quantity, the squared)
A. Concepts from Relativity

Line element is a composite description of the geometry (given by the metric) and the choice of coordinate system (given by the components of the one-form $d\sigma^a$ working on the same unit vectors that procured the metric), providing a “measuring rod”.

The sign of the line element can be:

- $d\sigma^2 > 0$: for events that are separated at a greater spatial distance than temporal distance, that thus are causally connected. Such events are time-like,
- $d\sigma^2 = 0$: for events where spatial and temporal difference is the same. This is the case for light, and thus are they called light-like,
- $d\sigma^2 < 0$: for events where the temporal separation is larger than the spatial separation. Either are the events causally disconnected, or are they connected through faster-than-light particles (tachyon-like particles). These events are called space-like.

**Metric**

A metric provides a geometrical description of a manifold. It is represented as the tensor $g_{\mu\nu}$, or its inverse, $g^{\mu\nu}$.

It is related to the line element $d\sigma^2$ using that the metric elements are given from this definition

$$g = g_{\alpha\beta} \, dx^\alpha \otimes dx^\beta,$$

and then treating the line element as vector components,

$$d\sigma^2 = g_{\alpha\beta} dx^\alpha dx^\beta$$

which is identical to let the metric tensor $g$ act on the basis vectors that provides it with its components,

$$g_{\mu\nu} dx^\mu \otimes dx^\nu = g(dx^\mu e_\mu, dx^\nu e_\nu) = e_\mu \cdot e_\nu \, dx^\mu dx^\nu.$$  

**Covariant and contravariant indices**

A vector is associated with contravariant components, that are the components where the index is raised, as $i$ in $V^i$.

A one-form is associated with covariant components, where the index is lowered, as $j$ in $\omega_j$.

Lowering and raising of indices can be done with help from the metric;

$$\alpha$$

<+++>
Kronecker delta The Kronecker delta is defined

\[
\delta^{\alpha \beta} \text{ or } \delta^\alpha_\beta = \begin{cases} 
1 & \text{for } \alpha = \beta \\
0 & \text{for } \alpha \neq \beta
\end{cases}
\]  

(A.14)

and the metric satisfies

\[
g_{\alpha \beta} g^{\beta \gamma} = \delta^\gamma_\alpha.
\]  

(A.15)

Riemann tensor The Riemann tensor is a rank-(1, 3) tensor which describe the intrinsic curvature of of a manifold. It is given in terms of the connection- and structure coefficients as

\[
R^\alpha_{\beta \gamma \delta} = \Gamma^\alpha_{\beta \gamma, \delta} + \Gamma^\mu_{\beta \gamma} \Gamma^\alpha_{\mu \delta} - \Gamma^\mu_{\beta \delta} \Gamma^\alpha_{\mu \gamma} - \Gamma^\mu_{\gamma \delta} \Gamma^\alpha_{\beta \mu}
\]  

(A.16)

where, $\rho \equiv \partial/\partial x^\rho$ is the derivative operator, $c_{\gamma \delta}^\mu e^\mu_\nu \equiv [e_\gamma, e_\delta]$ are the structure coefficients and $\Gamma^\alpha_{\beta \gamma}$ are the connection coefficients (see Christoffel symbol).

Its definition is derived from parallel transport of a vector on the manifold, and represents the change of the vector after the transport.

It is antisymmetric in its third and fourth indices, $R^\alpha_{\beta \gamma \delta} = -R_{\beta \delta \gamma}^\alpha$, and also $R^\alpha_{\alpha \gamma \delta} = 0$. Using a coordinate basis, the structure coefficients vanish.

4-velocity The 4-velocity is defined as

\[
U^\alpha = \frac{dx^\alpha}{d\lambda}
\]  

(A.17)

where $x^\alpha = (x^0, x^1, x^2, x^3)$ are the coordinates of an event along a trajectory in spacetime parametrised with the parameter $\lambda$. 
Appendix B

Density matrix formalism

The density matrix formalism allows all the obtainable information on a quantum system to be written in form of a matrix, and not in terms of wave functions.

To apply the density matrix on an ensemble of photons, some notation, that was previously introduced, is required. A particular wave function of eq. (4.16) is denoted

\[ |\Psi_{k,\chi}\rangle \]  

(B.1)

with \( \chi \) denoting a polarisation direction given a momentum propagation direction \( \hat{k} \). An ensemble can consist of several combinations of \( |\Psi_{k,\chi}\rangle \).

The expectation value of an operator \( \mathbf{A} \) acting on an ensemble is then given as

\[ \langle \mathbf{A} \rangle = \sum_i p_i \langle \Psi_{k,\chi_i} | \mathbf{A} | \Psi_{k,\chi_i} \rangle \]  

(B.2)

where the weights are real and oblige \( \sum_i p_i = 1 \) and \( 0 \leq p_i \leq 1 \). Each weight can be interpreted as the probability of drawing the corresponding state from a statistical ensemble. The ensemble does not have to span the entire vector space, nor does its components have to be orthogonal.

Introducing an orthonormal basis spanning the 4-dimensional com-
plex vector space of eq. (B.2), \( \sum_n |\Phi_n\rangle\langle \Phi_n| = 1 \),
\[
\langle A \rangle = \sum_i p_i \langle \Psi_{k,\chi_i} | \left( \sum_n |\Phi_n\rangle\langle \Phi_n| \right) A |\Psi_{k,\chi_i}\rangle
\]
\[
= \sum_i p_i \sum_n \langle \Psi_{k,\chi_i} | \Phi_n\rangle \langle \Phi_n| A |\Psi_{k,\chi_i}\rangle
\]
\[
= \sum_i p_i \sum_n \langle \Phi_n| A |\Psi_{k,\chi_i}\rangle \langle \Psi_{k,\chi_i} | \Phi_n\rangle
\]
\[
= \sum_n \langle \Phi_n| A \left( \sum_i p_i |\Psi_{k,\chi_i}\rangle \langle \Psi_{k,\chi_i}| \right) |\Phi_n\rangle
\]
(B.3)
(B.4)
(B.5)
(B.6)

where the hermitian density matrix is defined as:
\[
\rho \equiv \sum_i p_i |\Psi_{k,\chi_i}\rangle \langle \Psi_{k,\chi_i}|
\]
(B.7)
such that
\[
\langle A \rangle = \sum_n \langle \Phi_n| A \rho |\Phi_n\rangle
\]
(B.8)

but, this is only the sum of the diagonal elements as the basis vectors \( |\Phi_n\rangle \) span the vector space,
\[
\langle A \rangle = \text{Tr} (A \rho),
\]
(B.9)

see for example Sakurai & Napolitano (2011), Sethna (2011), Weinberg (2013). The density matrix holds all obtainable information on a system and has no phase ambiguity. Defining the density operator \( \rho \) for the state \( |\Psi_{k,\chi_j}\rangle \),
\[
\rho \equiv |\Psi_{k,\chi_j}\rangle \langle \Psi_{k,\chi_j}|
\]
(B.10)

and rotating the state an angle \( \theta \),
\[
|\Psi_{k,\chi_j}\rangle \rightarrow e^{i\theta} |\Psi_{k,\chi_j}\rangle
\]
(B.11)
does not affect the density operator,
\[
\rho \rightarrow \rho' = e^{i\theta} |\Psi_{k,\chi_j}\rangle \langle \Psi_{k,\chi_j}| e^{-i\theta}
\]
(B.12)
\[
= \rho.
\]
(B.13)

An ensemble consisting of one state (with probability coefficient \( p_j = 1 \)) is said to be pure. The density matrix of a pure ensemble is \( \rho = \rho^2 \).
and hence $\text{Tr}(\rho^2) = 1$. An incoherent mixture of states would yield $0 < \text{Tr}(\rho^2) < 1$.

Another feature of the density matrix is the ability to describe the time-evolution of a system. The classical probability density for Hamiltonian systems does not change with time,

$$\frac{d\rho_{\text{classical}}}{dt} = 0 \quad (B.14) \text{ Liouville theorem}$$

which is the Liouville theorem, with upright “d” denoting total derivative. The quantum mechanical version for an arbitrary wave function $|\psi\rangle$,

$$\frac{\partial \rho}{\partial t} = \sum_i p_i \left( \frac{\partial |\psi_i\rangle}{\partial t} \langle \psi_i | + |\psi_i\rangle \frac{\partial \langle \psi_i |}{\partial t} \right)$$

$$= \frac{1}{i\hbar} (H\rho - \rho H)$$

$$= \frac{1}{i\hbar} [H, \rho] \quad (B.15) \text{ Quantum Liouville}$$

can be cast into an equivalent form using relations between the commutator and Poisson brackets, see Sethna (2011).
Appendix C

Understanding the density matrix elements: relation to time-dependent perturbation theory

Lee et al. (1994) derives the transition rates from a general excited state to a ground state in a hydrogen atom (or, more generally “an ion” following their notation). This formalism was applied specifically for scattering of Lyα photons in a certain geometry by Lee & Ahn (2002) (unpublished) and Ahn et al. (2002). In this appendix it is shown that the density matrix elements of Lee & Ahn (2002) should be understood in terms of the formalism devised by Lee et al. (1994). This formalism uses time-dependent perturbation theory, and it is here applied to describe scattering of light.

Time-dependent perturbation theory for scattering of one electron ions is explained in Trulsen (2011) (and eg. Sakurai & Napolitano (2011)). Denoting the wave function of an one-electron atom $|\psi\rangle$, which may be expanded in terms of the eigenkets of the eigenvalue problem

$$H_0|\psi\rangle = E_0|\psi\rangle = \sum_i E_{0i}c_i|\phi_i\rangle$$

(C.1)

where $|\phi_j\rangle$ is the $j$-th excited state of the ion which may be obtained by using the ladder operator $a^\dagger$, weighted by the expansion coefficient $c_i$, with $\sum_i c_i E_{0i} = E_0$. $H_0$ is the zeroth-order (or unperturbed) Hamiltonian operator.

The states $|\phi_j\rangle$ are orthogonal, ie. $\langle \phi_j | \phi_k \rangle = \delta_{jk}$ where $\delta_{jk}$ is the Kronecker delta.
C. Understanding the density matrix elements: relation to time-dependent perturbation theory

However, in the presence of an external (position- and time-dependent) monochromatic electric field (Trulsen 2011)

\[
E(x, t) = \frac{E_0}{2} (\varepsilon \exp [i k \cdot x - i \omega t] + \varepsilon^* \exp [-i k \cdot x + i \omega t])
\]  

(C.2)

where \( \varepsilon \) is the polarisation vector of the field, \( x \) is the position of the electron the field affects, \( k \) is the wave vector, \( \omega \) is the frequency and \( t \) is the time, the Hamiltonian of the system is no longer given by its unperturbed component \( H_0 \).

The external field will interact with the electron. This interaction can be expressed in terms of the classical dipole moment

\[
m = -e x
\]  

(C.3)

of the electron with charge \(-e\) and position (relative to the center of the mass of the system) \( x \).

A non-zero dipole moment will affect the Hamiltonian of the system and provide a potential term,

\[
H' = -m \cdot E(x, t)
\]  

(C.4)

\[
= \frac{e E_0}{2} (x \cdot \varepsilon \, e^{ikx - i\omega t} + x \cdot \varepsilon^* \, e^{-ikx + i\omega t})
\]  

(C.5)

so that the total, now time-dependent, Hamiltonian is

\[
H = H_0 + H'.
\]  

(C.6)

This time-dependence infers that the wave equation no longer may be considered stationary, which the time-dependent Schrödinger equation displays,

\[
i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle
\]  

(C.7)

and an expansion of \(|\Psi(t)\rangle\) in terms of a set of eigenkets to the zeroth order eigenvalue problem is needed,

\[
|\Psi(t)\rangle = \sum_i c_i(t) \exp \left[ -\frac{i}{\hbar} E_{0i} t \right] |\phi_i\rangle
\]  

(C.8)

where the time-dependence resides in the coefficients \( \{c_i(t)\} \) and the phase factor, whereas the eigenkets still are the same as in Eq. (C.1), see Trulsen (2011) and Sakurai & Napolitano (2011).

The physical interpretation of the coefficients and their time dependence is displayed if the system is considered to be prepared in the
ground state, such that \( c_0(t = t_0) = 1 \), and consequently must the others \( c_j(t = t_0) = 0 \). An incident wave may excite the system into the various eigenstates \( |\phi_j \rangle \), giving them a non-zero \( c_j(t > t_0) \), and the ground state

\[
c_0(t > t_0) = c_0(t = t_0) - \sum_{j > 0} c_j(t > t_0)
\]  

\[
< 1
\]

only considering radiative excitation and not induced de-excitation. The latter may provide positive contributions from the higher levels \( (j > 0) \) to the ground level \( (j = 0) \).

Trulsen (2011) defines the transition rate of going from the state \( j = i \) to \( j = f \) as

\[
w_{f \rightarrow i} = \frac{d}{dt} |c_f|^2
\]

Transition rate

where the transition probability is defined (Griffiths 2005; Sakurai & Napolitano 2011) as

\[
P_{i \rightarrow f} = |c_f|^2.
\]

Transition probability

Trulsen (2011) proceeds to plug the time-dependent wave-function (Eq. (C.8) into the Schrödinger equation, Eq. (C.7), which yields

\[
i\hbar \frac{d}{dt} (c_j(t)e^{-iE_0jt/\hbar}) |\phi_j \rangle = \sum_i Hc_i(t) \exp \left[ -\frac{iE_0t}{\hbar} \right] |\psi_i \rangle
\]

\[
i\hbar c_j = \sum_i c_i(t) \exp [i\omega_{ji}t] \langle \psi_j | H | \psi_i \rangle - E_0c_j(t)
\]

\[
= \sum_i c_i(t) \exp [i\omega_{ji}t] \langle \psi_j | H' | \psi_i \rangle
\]

(C.13)

note the perturbed \( H' \), which arose from \( \langle \psi_j | H_0 + H'| \psi_i \rangle = \langle \psi_j | H' | \psi_i \rangle + E_{0j} \) due to the orthogonality of the basis wave-functions, \( \langle \psi_j | \psi_i \rangle = \delta_{ji} \).

The resonance (or core) frequency \( \omega_{ji} \) was introduced,

\[
\omega_{ji} = \frac{E_{0j} - E_{0i}}{\hbar}
\]

(C.14) Core frequency

which corresponds to the energy difference between two atomic levels \( i \) and \( j \).

The derivative in Eq. (C.13) has to be integrated, but two approximations are done by Trulsen (2011):
C. Understanding the density matrix elements: relation to time-dependent perturbation theory

Dipole approximation

1. **The electric dipole approximation**: the wavelength of the field is considered much larger than the size of the atom, see eg. Rybicki & Lightman (1979), and the electric field is considered constant across the atom: \( E(x, t) \approx E(0, t) \). This simplifies the exponentials in Eq. (C.5): \( e^{\pm ikx \mp i\omega t} \approx e^{\mp i\omega t} \).

2. Only transitions from the initial state \( i \) contributes significantly in the sum in Eq. (C.13), that is: the summation can be dropped. Furthermore, this makes \( c_i(t) \sim 1 \) whereas the other coefficients in the sum are negligible.

This leaves

\[
i\hbar \hat{c}_j(t) = \exp \left[ i\omega_{ji} t \right] \langle \psi_j | \frac{eE_0}{2} (\mathbf{x} \cdot \mathbf{e} e^{-i\omega t} - \mathbf{x} \cdot \mathbf{e}^* e^{i\omega t}) | \psi_i \rangle \tag{C.15}
\]

to be integrated, which yields

\[
c_j(t) = \frac{eE_0}{2\hbar} \left[ \langle \psi_j | \mathbf{x} \cdot \mathbf{e} | \psi_i \rangle \frac{1 - \exp \left[ i(\omega_{ji} - \omega) t \right]}{\omega_{ji} - \omega} + \langle \psi_j | \mathbf{x} \cdot \mathbf{e}^* | \psi_i \rangle \frac{1 - \exp \left[ i(\omega_{ji} + \omega) t \right]}{\omega_{ji} + \omega} \right]. \tag{C.16}
\]

It is important to note that the coefficients are dependent on the polarisation vectors.

Eq. (C.16) powerfully shows the effect of the resonance frequencies \( \pm \omega_{ji} \). The only significant contributions to the transition coefficient are those where the incoming frequency \( \omega = \pm \omega_{ji} \), and applying L'Hôpital’s rule to the 0/0 fractions when \( \omega \to \pm \omega_{ji} \) yields

\[
\lim_{\omega \to \pm \omega_{ji}} \frac{1 - \exp \left[ i(\omega_{ji} \mp \omega) t \right]}{\omega_{ji} \mp \omega} = \lim_{\omega \to \pm \omega_{ji}} \pm it e^{i(\omega_{ji} \mp \omega)t} = \pm it \tag{C.17}
\]

which shows a linearly increasing time dependence (for a transition to the level \( j \)). Trulsen (2011) shows that the transition probability is linear in \( t \), and hence must the transition rate be independent of time.

Furthermore, the two resonance frequencies \( \omega = \pm \omega_{ji} \) correspond to an excitation (where the excited level has a higher energy than the initial level, \( E_{0j} > E_{0i} \), hence \( \omega > 0 \)) and a de-excitation (where \( \omega < 0 \)).

An attempt to proceed to describe the system using the density matrix formalism will also shed light on another important feature.
density operator definition, Eq. (B.10), on the expansion of the wave function in terms of zeroth order states,

\[ \rho = |\Psi(t)\rangle\langle\Psi(t)| \]
\[ = \sum_i c_i(t) \exp \left[ -\frac{iE_{0i}t}{\hbar} \right] |\phi_i\rangle\langle\phi_i| \exp \left[ \frac{iE_{0i}t}{\hbar} \right] c^*_i(t) \]
\[ = \sum_i c_i(t) c^*_i(t) |\phi_i\rangle\langle\phi_i| \]
\[ = \sum_i c_i(t) c^*_i(t) \delta_{ii} \quad (C.18) \]

or, simply,

\[ \rho = \text{Diag} \left( |c_0(t)|^2, |c_1(t)|^2, \cdots \right) . \quad (C.19) \]

The interpretation of this becomes evident if a monochromatic wave with a frequency close to, but not exactly at the core frequency associated with eg. the Ly\(\alpha\) transition perturbs the system. While it is evident from Eq. (C.16) that the state where the resonance frequency \(\omega_{ji}\) coincides with that of the wave is the most likely state for a transition to occur to, there is also a non-zero probability of the system being perturbed into the other states. This probability increases the further away \(\omega\) comes from one resonance frequency \(\omega_{ji}\) and approaches another \(\omega_{ji}\).

This wing-scattering effect is evident in Fig. (C.1) from Dijkstra (2014), where different approximations to the Ly\(\alpha\) cross section are plotted. A precise treatment is done by Lee (2013), who expand the Kramers-Heisenberg formula around the Ly\(\alpha\) transition for wing (Rayleigh) scattering and for Raman and Rayleigh scattering around Ly\(\beta\) and present discrepancies between his results and earlier approximations for the Ly\(\alpha\) cross section (ie. the Voigt profile whichs fits excellently only in the core regime), and conclude that these fail to describe the cross section. In particular, the approximation done by Peebles (1993) “fails to include the contributions from the infinitely many p states that participate in the electric dipole interaction” (Lee 2013).

Eq. (C.16) is on the same form as Eq. (2.1) in Lee et al. (1994), for a state \(|e\rangle\) excited from the state \(|g\rangle\);

\[ c_e = -\frac{i|e\rangle}{\hbar} \langle e| x \cdot \tilde{E}|g\rangle \quad (C.20) \]

where \(\tilde{E} = \hat{E}_g e_g\) is the Fourier transform of the electric field (efficiently picking out only the resonance frequency) along the basis vectors \(\{e_g\}\).
C. Understanding the density matrix elements: relation to time-dependent perturbation theory

Approximations to Lyα cross section

Figure C.1: Logarithmic plot of different approximations to the Lyα cross section taken from Dijkstra (2014) as a function of offset from the line center in km s\(^{-1}\). The Voigt function is a convolution of a Gaussian function (red dashed, fits best in the core) and a Lorentzian (blue dotted, fits better in the wings). The Rayleigh curve (grey) is a modified Voigt function that has an extra frequency dependence from Peebles (1993). The Lee curve (green dotted) accounts for contributions from the other possible Hydrogen transitions through an expansion of the Kramers-Heisenberg formula (Lee 2013). The lower plot shows the deviations from the Voigt profile.

From the preceding discussion, the coefficient of Eq. (C.20) is having the dipole operator (from the perturbed Hamiltonian) act on the ground state. Scattering is however a transition from the ground state to the ground state through an intermediate state.

Lee et al. (1994) describes the initial and final states in terms of density matrices, as well as the polarisation. However, before proceeding to do so, they transform from the scattering ion basis \( \{ f_e q \} \) to a photon basis \( \{ e_a \} \). They present the spontaneous transition rate to a solid angle element \( d\Omega \),

\[
d\tilde{P} = A |M_{eq}(e_a)|^2 \, d\Omega
\]  

(C.21)

from an excited state \( |e\rangle \), subscript \( e \), to a ground state \( |g\rangle \), subscript \( e \), where \( A \) is the total Einstein \( A \) coefficient. The matrix element \( M_{eq}(e_a) \) is composed of a rotation to the photon frame \( (S_{aq}) \) and the Clebsch-Gordan coefficient \( (R_{eg}^q) \) for the different ion basis vectors \( q \);

\[
M_{eg}(e_a) = S_{aq} R_{eg}^q
\]  

(C.22)
where the rotation operation to the photon basis (\( e_a \) with two components) is defined as
\[
e_a = S_{aq} e_q.
\] (C.23)

Whereas Ahn et al. (2002); Lee & Ahn (2002) applies the presented formalism to describe scattering events, does Lee (2013) calculate the matrix elements directly by integrating the radial and angular wave functions, noting that these can be found analytically as each combination of states can be treated as a two-level problem.

The density matrices introduced by Lee et al. (1994) are those of the ground state;
\[
\rho_{gg'} = \frac{c_g c_{g'}^*}{c_{g''}^* c_{g''}}
\] (C.24)
where \( g \rightarrow g' \) denotes the transition of the ground state, and \( c_{g''} \) is a normalisation coefficient, and the polarisation density matrix;
\[
P_{aa'}(\theta, \phi) = \frac{\tilde{E}_a \tilde{E}_{a'}^*}{\tilde{E}_{a''}^* \tilde{E}_{a''}}
\] (C.25)
where the subscripts \( a, a' \) and \( a'' \) now refer to the photon basis components, the incoming (unprimed), outgoing (primed) and normalisation-factor (double-primed). Lee et al. (1994) proceeds to derive expressions for the time-evolution of the coefficients using physical arguments and not the Liouville theorem, except for magnetic mixing.
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