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<th>Star formation in extreme environments</th>
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<tr>
<td>Author(s)</td>
<td>Mullins, Aonghus</td>
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<tr>
<td>Publication Date</td>
<td>2015-12-22</td>
</tr>
<tr>
<td>Item record</td>
<td><a href="http://hdl.handle.net/10379/5424">http://hdl.handle.net/10379/5424</a></td>
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Star Formation in Extreme Environments

by

Aonghus Mullins

A thesis submitted in partial fulfillment for the degree of Doctor of Philosophy

in the
Centre for Astronomy
School of Physics
under the supervision of Dr. M.P. Redman.

December 2015
Abstract

The study of star formation bridges many vastly disparate scales. From the small, nearby, quiescent cores of low mass star formation, to the highly turbulent conditions in which the most massive stars form, to the extreme gravitational potential of the inner Galaxy, where clouds pass close to the supermassive black-hole Sgr A*.

Low mass cores are far more common than their massive counterparts, and so far more are observed nearby. The molecular line data from these nearby sources is of extremely high spectral resolution. In order for accurate modelling to take place, the molecular physics needs to understood to the finest detail. In this work we have shown that for HCN, an anomaly in the observed relative line-strengths of the hyperfine lines in the $J=(1\rightarrow0)$ transition emerges naturally when the radiative transfer is carried out over each hyperfine line separately, using a proportional method to calculate scaled collisional rate coefficients for these transitions. A parameter sweep is carried out over a range of parameters typical of low mass star forming regions, and the $J=(1\rightarrow0)$ line is found to be highly unstable to the optical depth of the cloud, thus making it a poor choice of tracer for dynamical processes. Model fits are also presented for the prototypical low mass core TMC-1, in which these anomalies were first noted in the early 80’s.

High mass star formation is less simple than its low mass counterpart. High mass star forming cores accrete enough matter to ignite nuclear fusion before they are finished accreting. The feedback from the protostar is a source of turbulent energy to its surroundings, and the absorption and reemission by dust grains of their photon flux, leads them to shine brightly in the infrared. The ionising flux from the newly formed massive star leads to the formation of an expanding shock front, surrounding a region of highly ionised hot gas known as a H II region. These shocks can compress gas in the surrounding interstellar medium, leading to second generation “triggered” star formation. Radiative transfer modelling of the swept up gas surrounding these regions can place limits on the expansion velocity thorough analysis of the shape of spectral line emission. For the bubble H II region RCW120, an upper limit of 1 km s$^{-1}$ is found. A model for the object RCW36 is then, through fitting of the HCO$^+$ $(1\rightarrow0)$ line, shown to be consistent with triggered star formation in the gas surrounding a H II region.

Finally, the clouds near the Galactic centre are subject to some of the most extreme conditions in the Galaxy. The tidal gravitational field can disrupt them, the intense local star formation bombards them with ionising radiation, and the turbulent feedback from the high supernova rate leads to clouds which are far removed from the quiescent cores of low mass star formation. In this work we study one such cloud, G0.253+0.016, “the Brick”, which is unusual in its apparent lack of star
formation. We model the observed molecular lines for the dense gas tracers HCN, HNC, HCO$^+$ and N$_2$H$^+$, finding a good fit to the observed data for a model in which the Brick is treated as a recent cloud-cloud collision. The observed position of a water maser [an early indicator of massive star formation] consistent with the cloud overlap region of our model strengthens our claim, while widespread SiO [a shock tracer] emission from recent surveys further supports this hypothesis.

A comparison is then made to previous modelling work on another galactic centre cloud, Sgr B2, which is rich in ongoing star formation. The Brick is found to be much colder and more chemically depleted than Sgr B2, indicative of widespread freeze-out of molecular ices onto interstellar grains. The turbulent velocities of the two clouds are found to be comparable, which would suggest that similar support against gravitational collapse exists in each. The precise mechanism by which the Brick is currently resisting star-formation remains an open question. How does $10^5$ M$_\odot$ of gas accumulate without any star formation? Our model for cloud-cloud collision modelling alleviates that requirement, by having two smaller turbulently supported clouds.

Overall, this thesis shows that over a large range of scales, the radiative transfer modelling of molecular line data can be used to investigate a number of extreme cases, in chemistry, turbulence, and density. From the thin, highly resolved lines of low mass star formation in the Solar neighbourhood, to the broad, velocity shaped lines of high mass star formation, and the Galactic Centre.
Publications

The work contained in this thesis has contributed to the following peer-reviewed publications.


Where any of the work done by co-authors on these papers is used in this thesis, credit is given in either the figure caption, or in the text.
Acknowledgements

Throughout the course of this thesis I have had the privilege of working with some exceptional people. My supervisor Dr. Matt Redman, who has guided me to this point, from being a complete novice in practically everything to do with this thesis. My main collaborators Dr. Eric Keto, and Dr. Robert Loughnane, and Nevenoe Guegan who’s contributions were invaluable to this project, the HCN chapter in particular. Dr. Nadia Lo and Dr. Paul Jones who obtained the observations upon which this modelling work was based, and last but not least the inimitable Dr. Brandon Wiles, the language guru, be it C, FORTRAN, Classical Greek, he was always there and willing to help.

To my family, my parents Mary and Padraig, my brothers Darragh and Fergal, my uncles, aunts and cousins, without who’s unerring support and encouragement from a very young age, I absolutely would not be where I am today.

People often say that doing a PhD can be a lonely time, I have been extremely fortunate to able to say that was not the case. The Physics group of 2011 (plus a few stragglers) who had nothing better to do than be friends with me: Shane, Mike "Schan", John "Pancakes", Ronan E, Ronan R, Mags, Steph, Leah, Collins, Aedan, and the optics trio of Colm "arah you’ll have one" Lynch, Conor "The Mackerel" Sheil, and Niamh.

To the guys in 38: Ross, Jodi John, Steve, Clora, Wez and Aran, thanks for putting up with me!

In the Centre for Astronomy, there has always been a great sense of camaraderie, right from day one. I’ve shared a corridor with a great number of people, from Leon, Ronan, Sean Andrea, Brandon, Diarmaid, Paul, Niall and Alan, through to the new(ish) generation, Lisa, Laura, Deirdre, Eamonn, Gordon, Ana, Majed, Nevenoe Karol and James. The academic staff Andy, Mark, Gary and Ray. The technical staff, Gary, Ollie, Conor, PJ, Stuart, Padraig and Bridget, and finally Tess Mahoney, without whom the whole thing would fall apart.

From open nights, to Sea2Sky, it’s been a great place to work, and I have thoroughly enjoyed my time here.

Thank you all so much.

[If you think I’ve forgotten you, I’m really sorry, deadlines eh? ______________
Just imagine your name here , and I’ll owe you a pint.]
“The two most common things in the Universe are Hydrogen and Stupidity”

- Harlan Ellison

“Nothing in the universe can travel at the speed of light they say, forgetful of the shadow’s speed.”

- Howard Nemerov
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Declaration of Authorship

I, Aonghus Mullins, declare that this thesis titled, ‘Star Formation in Extreme Environments’ and the work presented in it are my own. I confirm that:

■ This work was done wholly or mainly while in candidature for a research degree at this University.

■ Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.

■ Where I have consulted the published work of others, this is always clearly attributed.

■ Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.

■ I have acknowledged all main sources of help.

■ Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Signed:

Date:
To my parents, to whom I owe so much.
Chapter 1

A Review of the Theory of Star Formation

“We will never know how to study by any means the chemical composition (of stars), or their mineralogical composition”

- Auguste Comte (1835)

Stars have undoubtedly piqued the curiosity of mankind since its earliest days. Massive, burning sources of energy, they are responsible for almost all of what we observe when we look at the night sky. They are the birthplace for heavy elements, elements such as iron, central to the haemoglobin molecule responsible for transporting oxygen around our bodies. The rarity of the precious metals, such as platinum and gold, can be attributed to the rarity of the supernova explosions required to form them. Such is the importance of stars to life on Earth, via the Sun, the question of the nature and origin of stars is one that has existed for as long as man looked at the night sky. The Sun governed the harvest, and the ancient civilisations of the world could predict its motions with incredible precision. Places such as Stonehenge and Newgrange stand testament to this. Ptolemy constructed an Earth-centric model of the solar system using complex deferents and epicycles,
as early as the 2nd century A.D, while Chinese, Hindu and Arabic astronomers noted the appearance of guest stars - what we now know to be supernovae - in their otherwise constant celestial sphere. These observations give us timings for particular supernovae such as the Crab, which was observed in 1054. As scientific techniques advanced, so did our understanding; Kepler’s laws of elliptical orbits could predict planetary motions with new precision, while Copernicus’ heliocentric solar system was making waves with the powers of the time. Through sheer dedication, Tycho Brahe mapped the sky to arcminute precision, while Galileo was the first to use telescopes extensively, observing craters on the Moon, sunspots, and most importantly discovering the moons of Jupiter, which was the first observation of anything in the universe conclusively orbiting something other than Earth.

The real birth of modern astrophysics however, came with Isaac Newton and his Law of Universal Gravitation. Combined with Kepler’s previous work, celestial motion could be explained by a single underlying force, gravity. We will see in the coming review, that gravity is the force which governs the formation of stars, both low mass and high mass, and it is through the differing forces opposing gravity, that we see different regimes of star formation.

1.1 Introduction

It has been long accepted that stars form via gravitational condensation of diffuse matter in space, even suggested as far back as 1692 by Sir Isaac Newton (though it would take much longer for these ideas to take hold). However, the above quote by Auguste Comte was indicative of the general consensus of the time. This pessimism was borne on the back of the first parallax estimates of the distances to the stars, which made it blatantly obvious that travelling to the stars was, for all intents and purposes, impossible. Unbeknownst to Comte, however, Joseph von Fraunhofer had already begun to take the first steps towards studying the composition of stars, by analysing light from our closest star, the Sun. Using a prism,
he diffracted a beam of sunlight onto a white wall, where he noticed something peculiar. The rainbow he expected to see was there, but as well as that, were a multitude of dark lines. Fraunhofer also observed the spectrum of the red giant star Betelgeuse in a similar manner, and found a different set of dark lines. He came to the conclusion that the lines somehow represented the composition of the objects he was looking at, but he did not know how. It would not be until almost 100 years later, with the advent of quantum mechanics, that the information contained in these spectra could be fully characterised.

What exactly can we glean from studying the spectra of astronomical objects? At low resolution we can infer colour (wavelength). We see most objects in the night sky as white, being a mixture of all colours, however, some we can see to be tinged with a particular colour, Betelgeuse or the planet Mars appear to be red, while Rigel appears to be blue. Colour can tell us about temperature, we know blue objects to be hotter than red objects. Objects emitting X-rays are very hot, whereas cold sources may only emit in the radio spectrum. High resolution studies can not only observe the colour, but also the central wavelength of the transition,
Fraunhofer’s work is a prime example of this. While more recently, very high resolution studies can now observe the line-shape of a transition, which can reveal much more detail about the physical conditions in the region of interest.

- The **composition** of an object can be inferred by knowing which atoms or molecules produce the observed spectrum.

- The **abundance** of a species can be inferred provided the intrinsic line strength of the transition is known, and the conditions are optically thin.

- The **velocity** relative to the observer can lead to a Doppler shift in the wavelength of the transition. Objects moving towards us are seen to be “blue shifted” while objects moving away from us are seen to be “red shifted”.

  \[
  \frac{\nu}{\lambda} = \frac{\delta \lambda}{\lambda}
  \]

  where \(\nu\) is the velocity relative to the observer, \(\lambda\) is the intrinsic wavelength, and \(\delta \lambda\) is the change in wavelength due to the Doppler effect.

- The **pressure** can be found through high resolution analysis of the lineshapes of transitions. In situations of high pressure, collisions lead to a broadening of the intrinsic lineshape.

- The **temperature** and **density** can be deduced from a knowledge of the transitions being observed, and the energy separation between the levels, which gives an estimate of the degree of excitation of the system. Also through Doppler broadening, whereby the hotter species move faster that the cooler species, and so their lineshapes are broadened by more.

- Any **magnetic field** present can be deduced because certain spectral lines are subject to Zeeman splitting where the degree of splitting is indicative of the strength of the local magnetic field.
Using these properties, the scientific community has attempted to trace the evolution of gas in the Universe, from its tenuous beginnings, all the way through to the formation of stars. It has only been in the past half century, through major advances in observation technology, and the move from optical to IR and radio astronomy that evidence has emerged of ongoing star formation, and even more recently that we have begun to glean a physical understanding of the processes involved. This has been achieved through ever more advanced computational techniques; multi-wavelength high resolution observational studies from the *Spitzer* (Benjamin et al., 2003a) and *Herschel* (Molinari et al., 2010) telescopes amongst others, and high powered numerical simulations, alongside extensive theoretical work. This review will aim to collate the results of these various methods of investigation, and outline the journey of gas from the cool, rarefied interstellar medium, into the stars we are familiar with.

### 1.2 The Interstellar Medium

The space between the stars is not a void, as it would appear to be to the naked eye. In the Milky Way, 99% of the mass of the ISM is gas, with the remaining 1% being made up of graphite and silicate dust particulates (Goldsmith et al., 1997). Table 1.1 outlines the main phases which constitute the gas content of the ISM. 90% of this interstellar gas is hydrogen, the fundamental building block of stars. This hydrogen is further subdivided into three main constituent parts, ionised hydrogen (H II), atomic hydrogen (H i), and molecular hydrogen (H$_2$). Table 1. outlines the properties of the various phases of the ISM. This review concerns star formation, and so we now delve into more detail on the cold neutral gas phase, molecular gas in particular, from which stars are born. This phase is more commonly referred to as *Molecular Clouds*. 
Table 1.1: Phases of the ISM

<table>
<thead>
<tr>
<th>ISM Component</th>
<th>Label</th>
<th>Temperature (K)</th>
<th>$n_H$ (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot ionised gas</td>
<td>Coronal gas</td>
<td>$10^6$</td>
<td>0.003</td>
</tr>
<tr>
<td>Warm ionised gas</td>
<td>Diffuse ionised gas</td>
<td>$10^4$</td>
<td>&gt;10</td>
</tr>
<tr>
<td>Warm neutral gas</td>
<td>Intercloud gas</td>
<td>$10^3 \rightarrow 10^4$</td>
<td>0.1</td>
</tr>
<tr>
<td>Cold neutral atomic gas</td>
<td>Diffuse clouds</td>
<td>100</td>
<td>10 $\rightarrow$ 100</td>
</tr>
<tr>
<td>Cold neutral molecular gas</td>
<td>Molecular /Dark clouds</td>
<td>0 $\rightarrow$ 50</td>
<td>$10^3 \rightarrow 10^5$</td>
</tr>
<tr>
<td>Hot molecular cores</td>
<td>Protostellar cores</td>
<td>100 $\rightarrow$ 300</td>
<td>$&gt;10^6$</td>
</tr>
</tbody>
</table>

1.2.1 Molecular Clouds

Molecular clouds are density enhancements in the ISM dominated by molecular H$_2$ rather than by atomic H typical of the rest of the ISM. Also contained within these clouds are other trace molecules such as CO, CH, HCO$^+$, NH$_3$ etc. They form the largest cohesive entities in the Galaxy. The dominance of molecular H$_2$ in these regions arises because they can self-shield against the destructive ambient ultraviolet (UV) radiation field. In such cold, protected environments the predominant form of matter, atomic hydrogen (HI), preferentially associates into molecular hydrogen (H$_2$) through interactions on the surfaces of dust grains. Table 1.2 outlines the general properties of molecular clouds on every length scale observed, from Giant Molecular Clouds (GMCs) all the way down to dense cores and Bok Globules. $A_V$ is the typical visual extinction along the line of sight through the cloud, $n_{\text{tot}}$, the number density, $L$, the characteristic length scale, $T$, the temperature, and $M$ is the mass.$^1$

But, how are these molecules observed? The temperatures of molecular clouds are far too low for electronic transitions, or even vibrational transitions in a lot of cases. Rotational transitions are the main source of information about interstellar molecules.

$^1$Table 1.2. is taken from Page 60 of The Formation of Stars by Stahler & Palla (2004).
Table 1.2: Properties of Molecular Clouds

<table>
<thead>
<tr>
<th>Cloud Type</th>
<th>$A_V$ (mag)</th>
<th>$n_{tot}$ ($cm^{-3}$)</th>
<th>$L$ (pc)</th>
<th>$T$ (K)</th>
<th>$M$ ($M_{\odot}$)</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffuse</td>
<td>1</td>
<td>500</td>
<td>3</td>
<td>50</td>
<td>50</td>
<td>ξ Ophuchi</td>
</tr>
<tr>
<td>Giant Molecular Clouds</td>
<td>2</td>
<td>100</td>
<td>50</td>
<td>15</td>
<td>$10^6$</td>
<td>Orion</td>
</tr>
<tr>
<td>Dark Clouds</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Complexes</td>
<td>5</td>
<td>500</td>
<td>10</td>
<td>10</td>
<td>$10^4$</td>
<td>Taurus-Auriga</td>
</tr>
<tr>
<td>Individual</td>
<td>10</td>
<td>$10^3$</td>
<td>2</td>
<td>10</td>
<td>30</td>
<td>B1</td>
</tr>
<tr>
<td>Dense Cores</td>
<td>10</td>
<td>$10^4$</td>
<td>0.1</td>
<td>10</td>
<td>10</td>
<td>TMC-1/B355</td>
</tr>
</tbody>
</table>

Figure 1.2: M20: The Triffid Nebula. This images shows the young OB stars, with their surrounding H II region and photodissociation regions (PDRs). The gas in the nebula is seen to glow as it re-radiates the energy absorbed from the stars radiation fields. Credit: Jim and Janet Castano/Adam Block/NOAO/AURA/NSF
In order for a molecule to undergo a rotational transition it must have a permanent dipole moment $\mu$. In the context of molecular clouds, we will only concern ourselves with the ground electronic state, and lowest vibrational state, since the band gap to the first excited states of both these types of transitions represents a temperature much higher than observed in the areas of interest, namely cold molecular gas ($T < 50 K$). In the rigid rotor approximation, the energy associated with a rotating molecule is given by

$$E_{\text{rot}} = \frac{L^2}{2I}$$

where $L = I\omega$, the angular momentum, and $I$ is the moment of inertia about the rotation axis. In quantum mechanics:

$$L^2 = J(J + 1) \left( \frac{\hbar}{2\pi} \right)^2$$

where $\hbar$ is Planck’s constant, and $J = 0, 1, 2, 3\ldots$ is the angular momentum quantum number. Hence:

$$E_{\text{rot}} = J(J + 1) \left( \frac{\hbar}{2\pi} \right)^2 \frac{1}{2I}$$

which is conventionally written

$$E_{\text{rot}} = hBJ(J + 1)$$

where $B$ is the rotational constant

$$B = \frac{\hbar}{(8\pi^2 I)}.$$ 

The selection rule for transitions in molecules where $\mu \neq 0$ is $\Delta J = +1$ or -1. These allowed values for $\Delta J$ represent the P and R branches in ro-vibrational spectroscopy. As we shall see in Chapter 3, certain molecules with hyperfine structure are not well represented by the rigid-rotor approximation, and can have
\[ \Delta J = 0 \] transitions, which are known as either, Q-branch or quasi-elastic transitions. If \( J'' \) is the rotational quantum number of the lower level of a transition, then the frequency of that transition is

\[
\nu = \frac{\Delta E}{h} = B \left( (J'' + 1)(J'' + 2) - J''(J'' + 1) \right) = 2B(J'' + 1)
\]

(1.6)

**Figure 1.3:** (Left) Sample rotational HCN spectrum. (Right) The evenly spaced rotational transitions of CO, the isotope shift from C\(^{17}\)O can be seen in the very slight offset of each C\(^{17}\)O from its corresponding C\(^{16}\)O line.

In order for a molecule to transition from one rotational state to another, a photon of energy \( h\nu = \Delta E \) must be emitted or absorbed. This photon flux is what we observe, and how we probe these clouds. [More detail on this in Chapter 2.]

**Formation of Giant Molecular Clouds**

Molecular clouds are, as the name suggests, clouds of gas and dust, where molecules dominate the chemistry. They consist primarily of molecular hydrogen (H\(_2\)) which forms via grain surface interactions on the surface of dust grains (Spitzer, 1978). Hollenbach et al. (1971) consider a recombination efficiency, \( \gamma(T) \), which is the fraction of adsorbed H atoms which form molecules before evaporating from the grain surface, for a particular temperature \( T \). They find the following relation,

\[
t_{\text{form}} = (1.5 \times 10^9 \text{ yr}) \left( \frac{n}{1 \text{ cm}^{-3}} \right)^{-1}
\]

(1.7)
where \( n \) is the number density of gas particles. GMCs are defined to have masses in excess of \( 10^4 \, M_\odot \), and consist of hierarchal structures from the scale of the cloud itself, down to the thermal Jeans mass representing the maximum stable mass for bound clouds, and smaller again for unbound structures (Langer et al., 1995; Heithausen et al., 1998). There are two contrasting models for the formation of molecular clouds, a top-down and a bottom up approach. The bottom up approach was proposed first. Field & Saslaw (1965) and Kwan (1979) suggested the idea of successive inelastic collisions of cold atomic hydrogen (HI) clouds would gradually increase the cloud size and mass, until a self-gravitating GMC is reached. There are problems with this however, in that it is a very slow process, where it would take up to \( 2 \times 10^8 \) years for a cloud of mass \( 10^5 \, M_\odot \) to form. With advances in simulation technology during the late 70s and early 80s, the focus shifted to top down mechanisms in order to try to alleviate the timescale problem. Mechanisms were suggested involving large scale instabilities in the diffuse ISM. Parker (1966) suggested differential vertical buoyancy of varying density regions along magnetic field lines parallel to the mid plane of the cloud. This is an instability that now bears his name, the Parker instability. Another mechanism is differential in-plane self-gravity of regions with varying surface density, a Jeans instability. The general consensus is now that GMCs form in the spiral arms of galaxies, downstream from the large scale shock fronts caused by these types of instabilities and are initially extremely turbulent. Once formed molecular clouds were originally thought to have lifetimes of the order 100 Myr (Scoville & Hersh, 1979), but subsequently Blitz & Shu (1980) found this estimate to depend too heavily on the conversion from CO intensity to \( H_2 \) mass. They downscaled the lifetime estimate to 30 Myr, based on the associations of clouds with spiral arms, apparent ages of the associated stars, and overall star formation rate in the Galaxy. Ballesteros-Paredes, Hartmann, & Vázquez-Semadeni (1999) argue that molecular clouds are transient entities with lifetimes of less than 10 Myr. This argument relies on the observation that there are suspiciously few 5→20 Myr old stars in molecular clouds. Leisawitz et al. (1989), Fukui et al. (1999) and Elmegreen (2000) make similar arguments.
based on the observation that only stellar clusters of ages less than approximately 10 Myr are associated with substantial amounts of molecular gas in the Milky Way and the Large Magellanic Cloud.

1.3 Core Formation and Support

It is well established that stars form through the collapse of gravitationally un-stable cores contained within molecular clouds, and more often than not, within filaments inside these clouds. However, just how these cores are formed, fragment and collapse remains an intense matter of debate in modern astrophysics. Young stars are associated with the high density regions of molecular clouds (Lada et al., 1993). What mechanisms could explain the hierarchical structure observed in molecular clouds?

1.3.1 Gravitational Instability

The seminal work of Jeans (1902) first described the conditions for the stability of a mass of gravitating gas, and how it was widely different from the previous analogies of incompressible fluids. Jeans studied the growth of plane wave instabilities in an infinite uniform medium, with no rotation, magnetic fields, or turbulence. A linear analysis leads to the dispersion relation in the gas

$$\omega^2 = c_s^2 k^2 - 4\pi G \rho_0,$$

(1.8)

where $c_s$ is the isothermal sound speed in the gas, $k$ is the wavenumber, $G$ is the gravitational constant, and $\rho_0$ is the central density. This shows that if the wavenumber, $k$, is smaller than $\sqrt{4\pi G \rho_0 / c_s}$, the waves cannot propagate and the
p perturbations are amplified. Short wavelength perturbations are pressure dominated and can propagate, whereas long wavelength perturbations are gravity dominated and do not propagate but grow exponentially. This leads to the Jeans length $\lambda_J$,

$$\lambda_J = \sqrt{\frac{\pi c_s^2}{G \rho_0}}$$  \hspace{1cm} (1.9)$$

Assuming the clumps formed by self gravity have similar dimensions to the Jeans length in all directions, a corresponding minimum mass for a gravitationally unstable density fluctuation can be calculated.

$$M_J = \rho \lambda_J^3 = \frac{5.57 c_s^3}{G^{3/2} \rho_0^{1/2}}$$  \hspace{1cm} (1.10)$$

There is one alarming aspect of the Jeans analysis however; it is mathematically inconsistent. Recall the fluid equations:

<table>
<thead>
<tr>
<th>Table 1.3: The fluid equations.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mass Continuity</strong></td>
</tr>
<tr>
<td><strong>Euler’s Equation</strong></td>
</tr>
<tr>
<td><strong>Poisson’s Equation</strong></td>
</tr>
</tbody>
</table>

where $\Phi$ is the gravitational potential, $P$ is pressure, $\rho$ is density, $\vec{v}$ is the velocity of a fluid element, and $G$ is the gravitational constant. A zeroth order analysis of these equations assumes a static medium, where $\rho_0 = const$, $P_0 = const$ and $\vec{v}_0 = 0$. The mass continuity equation is solved trivially, as both sides equal zero. Euler’s equation has the LHS go to zero, and since $\nabla P_0 = 0$, we get

$$\nabla \Phi_0 = 0.$$  \hspace{1cm} (1.11)$$
Poisson’s equation becomes

$$\nabla^2 \Phi = 4\pi G \rho_0 \quad \rightarrow \quad \nabla \Phi_0 = \frac{4\pi}{3} G \rho_0 \vec{r}$$  \hspace{1cm} (1.12)$$

If the previous 2 equations are to be believed, then this is where the inconsistency comes in. Assuming these to be true \( \rho_0 = 0 \), \textit{i.e.} an empty universe! Jeans continued on regardless, in what became known as the Jeans swindle. An analysis of these equations at first order, combining mass continuity with Euler’s equation gives

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \left( \frac{v_s}{\rho_0} \nabla^2 \rho_1 - \nabla^2 \Phi_1 \right) = 0$$  \hspace{1cm} (1.13)$$

which in turn leads to the dispersion relation given above.

Using Poisson’s equation to replace \( \nabla^2 \Phi_1 \),

$$\frac{\partial \rho_1}{\partial t} - v_s^2 \nabla^2 \rho_1 - 4\pi G \rho_0 \rho_1 = 0$$  \hspace{1cm} (1.14)$$

This is a wave equation with a driving term, with a solution of the form

$$\rho_1(\vec{r}, t) = \int d^3k c(k) \cdot e^{i(\vec{k} \cdot \vec{r} - \omega t)}$$  \hspace{1cm} (1.15)$$

This yields the dispersion relation mentioned above. Because of the uncertainty over the mathematical consistency of the Jeans analysis, a number of more rigorous stability analyses were carried out, using more realistic conditions. Spitzer (1978) investigated the behaviour of plane parallel layers, yielding a critical mass for instability of

$$M_{\text{crit}} = \frac{5.86 c_s^3}{G^{3/2} \rho_0^{1/2}}$$  \hspace{1cm} (1.16)$$
where $\rho_0$ is the central density of the layer. Chandrasekhar & Fermi (1953) began working on equilibrium cylinders as they gave a much better match to the observed filamentary structure of molecular clouds, and in more recent times, the results of high powered numerical simulations (McKee & Ostriker, 2007) have also matched these observations. By varying the adiabatic index, $\gamma$ which governs the critical behaviour of the Jeans mass as a function of density, they find that the results differ only by a numerical factor ranging from $3.32 \rightarrow 6.28$ as $\gamma$ goes from $1 \rightarrow \infty$. Larson (1985) performed stability analyses using spherical instabilities, where $M_J$ was taken to be the mass contained within the first minimum of the spherical eigenfunction $r^{-1} \sin kr$. This functional form was chosen as it has the same dispersion relation as Jean’s analysis did for plane parallel perturbations. The only difference was again simply a numerical factor of 8.53 as opposed to 5.86. Independently of one another Bonnor (1956) and Ebert (1955) derived analytical solutions for equilibrium structures of spherical density perturbations in self gravitating, isothermal, ideal gases, which now bear their names, (Bonnor-Ebert spheres) as well as a criterion for gravitational collapse. So even with much more rigorous analyses, the structures were found to also be unstable to perturbations of the order $\lambda_J$, making the Jeans analysis, in spite of its audacious assumptions, relatively accurate. Zuckerman & Evans (1974) pointed out that using the simplest assumption, namely that if all the molecular gas in the Galaxy was collapsing in a free-fall time, the observed star formation rate (SFR) would be a factor of 10-100 times higher than the $\simeq 3 \, M_\odot \, yr^{-1}$ observed in the Milky Way. Something must be slowing down the collapse of the gas. In order to address this, we must first understand what is causing the collapse in the first place.

1.3.2 Thermal Support

We consider the ratio between thermal energy and gravitational energy,

$$E_{\text{therm}} = \frac{M}{(\gamma - 1)m_p k_b T}$$

(1.17)
\[ E_{\text{grav}} = \frac{3}{5} \frac{M^2 G}{R} \]  

(1.18)

where \( M \) is the cloud mass, \( R \) is the radius, \( m_p \) is the mean particle mass, \( T \) the temperature, \( k_b \) and \( G \) are the Boltzmann and gravitational constants respectively, while \( \gamma \) is the adiabatic index, which depends of the degrees of freedom of the constituents. Comparing these two energies gives the relation

\[ \frac{E_{\text{therm}}}{E_{\text{grav}}} \propto R^{(4-3\Gamma)}, \]  

(1.19)

where \( \Gamma \) is the effective adiabatic exponent, which also depends on cooling processes. Clearly the critical case is given by \( \Gamma = 4/3 \), below which the thermal pressure can no longer prevent collapse. A physical interpretation of the Jeans length is that self-gravity tends to induce contractions in a time scale of the order \( 1/\sqrt{G \rho_0} \), whereas thermal pressure tends to return the cloud to uniform pressure in a sound crossing time \( R/c_s \). If the self-gravity timescale is shorter than the crossing time, then the waves cannot counterbalance the pressure variations induced by the gravitational contractions before the whole cloud collapses. It is possible to estimate the time for the collapse of an ideal cloud, (cold, spherical, uniform density) which gives a order of magnitude estimate for what is known as \( t_{\text{ff}} \) the free fall time (e.g. Prialnik, 2009).

\[ t_{\text{ff}} = \sqrt{\frac{3\pi}{32G \rho_0}} \]  

(1.20)

### 1.3.3 Rotational Support

Most star forming clouds have a rotational component to their motions (Goodman et al., 1993) as is to be expected due to the turbulence present in molecular clouds. However, the angular momentum contained in these clouds is orders of magnitude
Chapter 1. Star Formation

more than could be contained in any star. This is the classic "angular momentum problem" in astrophysics. Early thought on this issue was based on the cores getting their angular momentum from the galactic rotation (Mestel & Spitzer, 1956), which led to a disparity of many orders of magnitude. As observational techniques gained the required resolution the rates were much lower, with magnetic fields having carried away much of the angular momentum. In most cases collapse with rotation leads to the formation of binaries and clusters, whose orbital motions can account for the much of the initial angular momentum. When rotation is added to the singular isothermal sphere model of Shu (1977) the result is that most of the envelope matter does not fall directly onto the central protostar but resides in on a centrifugally supported disk around it.

1.3.4 Magnetic Support

Magnetic fields can also act as a barrier to gravitational collapse. Considering a spherical cloud of mass $M$, radius $R$, permeated by a uniform field $B$. The magnetic flux within the cloud is given by $\Phi = \pi R^2 B$. While the gas in the cloud remains well coupled to the magnetic field, the flux will remain constant, and the ratio of magnetic energy to gravitational energy can be expressed

$$\frac{E_{mag}}{E_{grav}} = \frac{B^2 V}{8\pi} \times \frac{2R}{5GM^2} \propto \frac{B^2 R^4}{M^2} \propto \left( \frac{\Phi}{M} \right)^2$$ (1.21)

Mouschovias (1978) calculated numerically the critical value for the mass-to-flux ratio, using the virial theorem. A cloud with a mass-to-flux ratio smaller than this value is termed as magnetically subcritical and cannot collapse. At a microscopic level the force on a charged particle due to a magnetic field is given by the Lorentz force $j \times B$. However, this force does not act upon any of the neutral particles in the cloud, meaning there are at least two fluids to be considered. (In reality there are several fluids cohabiting the ISM, including the neutral and charged dust fluids etc. For simplicity however, we only consider the neutral and ionised gas
Chapter 1. Star Formation

fluids.) The ions are subject to the Lorentz force, while the neutrals are not, meaning that the neutral particles can drift away from the ions. Considering an equilibrium between the Lorentz force and the drag force, a characteristic timescale for ambipolar diffusion can be obtained

$$\tau_{ad} \simeq \frac{4\pi \gamma \rho_i L^2}{B^2},$$  \hspace{1cm} (1.22)$$

where $\gamma \simeq 3.5 \times 10^{13}$ cm$^2$ g$^{-1}$ s$^{-1}$ is the drag coefficient, $\rho$ is the total density, $\rho_i$ is the ion density, $L$ is the characteristic spatial scale, and $B$ is the field strength. For the low ionisation fraction typical of dense molecular gas, this can be shown to approximate to

$$\tau_{ad} \approx (3 \times 10^6 \text{ yr}) \left( \frac{n_{H_2}}{10^4 \text{ cm}^{-3}} \right)^{-3/2} \left( \frac{B}{30 \mu G} \right)^{-2} \left( \frac{L}{0.1 \text{ pc}} \right)^2$$  \hspace{1cm} (1.23)$$

If we consider an initially magnetically subcritical core, after a few diffusion times the reduction in flux throughout the cloud will lead to it becoming supercritical and the field can no longer support it against collapse. Shu et al. (1987) compute the ratio of the diffusion and free-fall timescales for a typical isothermal sphere to be approximately 8.

This result implies that this ambipolar diffusion i.e. the relative drifting of the two fluids, can retard the SFR by an appreciable amount, bringing it closer to the observed value.

1.3.5 Turbulent Support

A turbulent fluid is defined as one “in which the velocity at any point fluctuates irregularly”. Much of the early theoretical work in the field of turbulent flows was done by Kolmogorov (1941), Chandrasekar (1949), and von Weizsäcker (1951), however this work considers what is known as incompressible turbulence, where
the root mean squared (rms) velocities are subsonic, and the density remains almost constant. Gas flows in the ISM deviate strongly from this idealised picture in three crucial ways. First, they are highly compressible, with Mach numbers $M$ ranging from order unity in the warm ($10^4$ K) diffuse ISM, up to as high as 50 in the cold (10 K) dense molecular clouds. Second, the gas has a very soft equation of state due to radiative cooling, so that $P \propto \rho^\gamma$ with the polytropic index $0.4 \leq \gamma \leq 1.2$. Third the driving of the turbulence is not uniform, but comes from blast waves and other inhomogeneous processes. For these reasons, supersonic turbulence is the preferred regime for astrophysical processes. Supersonic flows in compressible gas create strong density perturbations, and lead to rapid energy dissipation through shocks. Larson (1981) applied this model to star formation, where the complexity of the problem is exacerbated by the fact that the strong density enhancements observed can be caused, not only by compressible turbulence, but also by thermal phase transitions, (Field et al., 1969; McKee & Ostriker, 1977; Wolfire et al., 1995) or gravitational collapse (Kim & Ostriker, 2001).

In supersonic turbulence, shock waves offer additional possibilities for dissipation. Shockwaves can also transfer energy from vastly separated length scales, removing the local nature of turbulent cascade typical of incompressible turbulence. Porter et al. (1992) and (1994) found that shock waves do not however, dissipate all of the energy, as rotational motions continue to contain a substantial portion of the kinetic energy, which is then dissipated in small vortices. To try and characterise the overall effect of turbulence on the SFR is not trivial. Unlike in the case of thermal support and magnetic support, the exact functional form of the turbulence is not known, so numerical simulations provide the only means to investigate turbulence’s role. Its effects are twofold. On the one hand, the turbulent motions act to spread out the gas, thereby reducing the ability of the gas to collapse, while on the other hand, the turbulent motions can lead to density enhancements in regions of converging flows, thereby increasing the likelihood of collapse in those
regions.

The results of simulations both with and without magnetic fields suggest that in the case of turbulent motions a significant fraction of the initial turbulent energy is dissipated in about one crossing time, \( (L/V_{\text{rms}}) \), where \( L \) is the characteristic length scale of the system in question (Mac Low & Klessen, 2004). This leads to the conclusion that if the turbulence is not driven, then it cannot significantly delay the collapse of a self-gravitating cloud. Therefore, in order to explain the low SFR in the Galaxy, we must invoke a driving force which continuously replenishes the turbulent energy. Matzner (2002) and (2007) suggests models based on feedback from stars due to their winds, jets or HII regions.

### 1.4 Core Collapse and Star Formation

Once a core undergoes collapse, calculations imply that a central stellar object is formed with a very low mass. Stars acquire most of their mass via accretion processes following the initial collapse. Characterising this is a two stage process:

- modelling the accretion process and determining the accretion rate
- modelling the evolution of a protostar using the calculated accretion rate

For low to medium mass stars, the feedback from the central stellar object in the form of stellar wind is subsonic, however stars with \( M > 8M_\odot \) these feedback effects become supersonic, which dissipate large amounts of energy in the surrounding gas via shocks. This transition from sub-to-supersonic turbulence demarcates the boundary between the low mass and high mass star forming regimes.
Figure 1.4: The 4 stages of star formation. (a) Cores form within molecular clouds as magnetic and turbulent support is lost through ambipolar diffusion. (b) A protostar with a surrounding nebular disk forms at the centre of a cloud core which is collapsing (c) A stellar wind breaks out along the rotational axis of the system, creating a bipolar flow. (d) The infall terminates, revealing a newly formed star with a circumstellar disk. (Shu, 1977)

1.4.1 Low-Mass Star Formation

Low mass star formation is the most well studied regime as it is (a) the most common, and occurs in relatively nearby clouds, and (b) because it can occur sometimes in isolation from other forming stars, allowing high detail of study. As outlined above, pre-stellar cores form in an interplay between self-gravity and the numerous support mechanisms at work. These cores are centrally condensed and can be modelled as Bonnor-Ebert spheres, constant density cores with power law \([n(r) \propto r^{-2}]\) envelopes surrounding them. Collapse leads to a core which grows via continued infall from the outer layers, (Larson, 1969; Boss & Yorke, 1995) and is
still molecular. Once the temperature rises above 2000K, the molecular matter begins to dissociate collisionally, leading to the collapse to the true protostar. Rotation creates a centrifugally flattened disk (Terebey et al., 1984). Magnetic fields and rotation lead to winds and jets (Matt & Pudritz, 2007), which in turn lead to molecular outflows from young stars (Wu et al., 2004). These jets and outflows carry away a lot of the angular momentum. Fig. 1 shows the classic four-stage star formation process of Shu (1977).

The evolution of a star from its prestellar core, through to the main sequence, is characterised by 4 classifications of protostar, 0, I, II, and III. Classically, a star is characterised by its position on a Hertzsprung-Russell (colour-luminosity) diagram. Luminosity is determined from flux measurements and distance estimates, while colour is related to the peak wavelength of the emission spectrum which is itself related to the stellar surface temperature, if the star is thought of as a black body, where Wien’s Law states that \((\lambda T)_{\text{max}} = 2.97 \times 10^{-3} \text{ mK}\).

These protostars however, are deeply embedded and the light they emit is processed by the enveloping core in which they are forming. The radiation is absorbed and re-radiated at much longer wavelengths by dust grains. Furthermore, the radiation from the circumstellar material usually arises from a wide range of distances from the central object, which leads to an extended continuous spectrum which does not resemble a blackbody. However, the total luminosity escaping the envelope can be determined through broadband photometry, giving the bolometric luminosity. An appropriate substitute for the optical colour was suggested by Adams et al. (1987), involving a property of the spectral energy distribution (SED), which is the distribution of radiated power with wavelength. A spectral index \(\alpha\) is defined such that

\[
\alpha = \frac{d \log (\lambda F_\lambda)}{d \log (\lambda)}
\]

(1.24)
calculated for \(2.2 < \lambda < 20 \mu\text{m}\). The shape of the SED in this mid-IR region is used to classify the stage of protostellar evolution. Figure 1.5 shows some example
Figure 1.5: The characteristic SEDs for the four classes of protostars (Persson, 2014).

Table 1.4: My caption

<table>
<thead>
<tr>
<th>Classification</th>
<th>Spectral Index ($\alpha$)</th>
<th>$T_{bol}$ (K)</th>
<th>Mass Relations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Class 0</td>
<td>Undetectable at $\lambda &lt; 20 , \mu m$</td>
<td>$&lt; 70$ K</td>
<td>$M_* &lt; M_{envelope}$</td>
</tr>
<tr>
<td>Class I</td>
<td>$\alpha &gt; 0.3$</td>
<td>$\sim 70-650$ K</td>
<td>$M_* &gt; M_{envelope}$</td>
</tr>
<tr>
<td>Class II</td>
<td>-0.3 &gt; $\alpha &gt; -1.6$</td>
<td>$\sim 650-2880$ K</td>
<td>$M_{disk} &lt; 0.01 M_*$</td>
</tr>
<tr>
<td>Class III</td>
<td>$\alpha &lt; -1.6$</td>
<td>$&gt; 2880$ K</td>
<td>$M_{disk} &lt; M_{Jupiter}$</td>
</tr>
</tbody>
</table>

SEDs for each of the four classifications, while Table 1.4 outlines some of the key properties of each of the classes of protostar.

**Class 0** The "birth" of a protostar is generally taken to be the point when the gaseous sphere is thermally enclosed for the first time. Photons cannot directly escape the sphere but are instead radiated from a photo-sphere. Almost all of the bolometric luminosity is at wavelengths above 350 $\mu m$. They are distinguishable
observationally form prestellar cores by a central infrared point source and/or evidence of jets and outflows.

**Class I**  As accretion of mass onto the central body progresses, heating occurs and the spectrum shifts towards lower wavelengths. A black body spectrum with a very large excess in the IR region is observed, with increasing flux for increasing wavelength around $\lambda = 2 \mu m$. This corresponds to panel c in Figure 1.4.

**Class II & III - T-Tauri Stars**  Once the envelope has been depleted by accretion onto the central object all that remains is an accretion disc and often a jet. The disc is gradually destroyed (accreted and/or blown away and/or used in planet formation). The distinction between Classes II and III is in the shape of the SED which is determined by the amount of the remaining disc material.

### 1.4.2 High Mass Star Formation

High mass protostars are characterised by Kelvin Helmholtz timescales, which are smaller than the accretion timescale. The Kelvin-Helmholtz timescale is related to the conversion of gravitational potential energy into heat energy, which is the main source of energy for a protostar prior to the ignition of nuclear burning and it’s ascent to the main sequence. For this reason, it determines the lifetime of the protostar, and leads to massive stars undergo nuclear burning whilst still accreting. This creates two important feedback features which low mass star forming cores do not have to deal with, namely, radiation pressure and photoionisation. High mass protostars are rare and also tend to form in clusters, so the interaction with other protostars may be significant. The turbulent core model for high mass star formation first proposed by McKee & Tan (2003), follows the assumption that massive stars form in turbulent gravitationally bound cores. The key assumptions in this model are that stars form from pre-assembled cores; that the cores and
clumps in which they are embedded are in approximate virial equilibrium; and that they are magnetically supercritical, so the magnetic field does not significantly limit the rate of accretion. The model uses the micro-turbulent approximation to treat turbulence as a local pressure term. This model has been criticised on the grounds that these massive cores would fragment and form many low mass stars rather than a single massive star, however Krumholz et al. (2007) find that radiative heating by a rapidly accreting high mass protostar strongly suppresses fragmentation. The turbulent core model is consistent with the correspondence between the CMF and the IMF and it naturally allows for the disks and winds associated with high mass stars.

**Radiation Pressure**

There have been several mechanisms proposed to allow for the formation of massive stars in the presence of radiation pressure. The Eddington luminosity is defined as the point where the force due to radiation pressure balances gravity, demarcating the maximum stellar mass possible through accretion alone.

\[
L_{Ed} = \frac{4\pi G m_\ast}{\kappa_d} \tag{1.25}
\]

where \(\kappa_d\) is the dust opacity. The Eddington luminosity should place an upper limit on the accretion rate of a protostar, however the accretion luminosity of some systems can exceed this limit. This arises from a combination of numerous effects, such as inhomogeneity in the accreting medium, rotation and photoionisation feedback.

**3D effects** Early 2-D simulations with limited resolution initially suggested that radiation pressure can reverse accretion, however in later higher resolution 3D simulations, the accreting gas, in optically thick flows can reshape the radiation
field, beaming it away from the bulk of the oncoming matter Krumholz et al. (2005).

Rotation & Magnetic Field Effects  Nakano (1989) showed that the higher ram pressure associated with disk accretion allows escape of IR radiation. This permits accretion onto a $100M_\odot$ star even with a low accretion rate. While MHD simulations show complex accretion patterns consistent with “flux tube accretion” (Miller & Stone, 1997; Romanova et al., 2003; Calvet & Gullbring, 1998)

Photoionisation Feedback

The most massive stars radiate in the UV with photon energies high enough to ionise the surrounding gas. The regions ionised by the stellar photon flux of high mass protostellar objects (HMPOs) (known as $H_\alpha$ regions) provide strong feedback on infall and accretion. The ionisation fronts associated with them expand into a turbulent background medium with strong density fluctuations produced by
the supersonic turbulent flow. These fluctuations both shape the shell and seed instabilities in it. It is not yet clear whether these feedback processes determine the maximum stellar mass. However, it is known that the expansion of these regions into the ambient gas energises GMCs, contributing to the overall turbulent energy fuelling new generations of star formation.

1.5 Overview

The key physical processes at play in the formation of dense cores from diffuse interstellar gas can be probed only within the Galaxy, and much more progress is expected to be made in the upcoming years with the new observing technologies coming online recently, and more in the not too distant future. Tools such as the Galaxy Evolution Explorer (GALEX), Spitzer, Herschel, as well as new instruments on the Hubble Space telescope. The Atacama Large Millimeter Array (AMLA) has begun to give unprecedented resolution at millimetre and sub-millimetre wavelengths, which has been and will continue to be extremely beneficial for the observations of star forming regions. What can be said for certain at this moment in time is that the overall SFR in the Galaxy is determined by the interplay over a number of vastly different length scales, of a hierarchy of physical processes. The accretion of gas onto galactic discs from the IGM (Mpc); the cooling of this gas to form a cool neutral phase (kpc); the formation of molecular clouds ($\sim 10 \rightarrow 100$ pc); the fragmentation and accretion of these clouds into smaller denser objects such as clumps ($\sim 0.1$ pc); and the subsequent contraction of these clumps to form stars ($R_\odot$) and planets ($\sim$ AU).

1.6 This Thesis

This thesis will outline a number of extremes of star formation over many scales.
• Chapter 2 presents an outline of the tools used in this work to observe and model molecular line spectra from star forming regions. From single dish telescopes to long-baseline multi dish interferometry, and finally the radiative transfer code, MOLLIE.

• Chapter 3 presents the work which forms the basis for the paper Mullins et al. (2015, submitted to MNRAS). The anomalous hyperfine structure of the rotational spectrum of hydrogen cyanide (HCN) is investigated, and a parameter study over the parameter space of low mass star formation is undertaken. Model fits to the observed star-forming core TMC-1 are also outlined, and recommendations on the use of HCN as a dynamical tracer for observers and modellers are given.

• Chapter 4 will present models on two sources indicative of the effects of massive stars on their surroundings. A model placing bounds on the expansion velocity of the bubble H II region RCW120 is presented. This model forms part of the paper Anderson et al. (2015) which has been accepted and published in the Astrophysical Journal in 2015. A model of the star forming region RCW36 is then presented, which using Mopra observations of the HCO$^+$ (1→0) line, is shown to be consistent with a simplistic model of triggered star formation.

• Chapter 5 follows the trend of increasing size and complexity, dealing with the most extreme environment of star formation in the Milky Way, the Central Molecular Zone. In particular, this work focuses on the object G0.253+0.016, otherwise known as “The Brick", a massive molecular cloud in the CMZ, with a peculiarly low star formation rate. (SFR). A model is presented placing constraints on the physical parameters of this cloud, and offering a possible solution for this low SFR.

• Finally, Chapter 6 outlines the overall conclusions of the thesis and presents possible future work stemming from the work contained within.
Chapter 2

Tools for Submillimetre Astronomy

“The history of astronomy is a history of receding horizons.”

- Edwin Powell Hubble

2.1 Introduction

As mentioned in Chapter 1, man has been looking into the night sky for thousands of years. Up until the Middle Ages, the naked eye was the only observational tool we had. The invention of the telescope led to the first paradigm shift in astronomy, with the increased angular resolution allowing for much smaller features to be observed, such as the Gallilean moons of Jupiter, sunspots, and craters on the Moon. These telescopes were initially refractive in nature, and chromatic aberrations - arising from the wavelength dependence of the refractive index - were a problem. Broadband sources could not be brought to a sharp focus. This was solved via the invention of the reflective telescope. These had numerous advantages over their refractive counterparts: they were not affected by chromatic aberration, they were much lighter, with different focal configurations allowing for more stable mountings for instruments.
With these tools, people could see much finer details, however, they were still limited by the sensitivity of the human eye to brightness. The integration time of the eyes is $\approx 30$ ms, increasing to $\approx 200$ ms, if dark-adjusted. The number of photons hitting the eye in that time placed a limit on what could be seen. Astronomers would observe through their telescopes, and sketch what they saw, this was fraught with possible errors. The so-called *canals* of Mars, first observed by Giovanni Schiaparelli, have recently been proposed to have actually been secondary reflections of the observers retina. The advent of photography in the mid to late 1800’s allowed for much longer integrating times, and thus fainter detections. Photographic plates were the foremost optical detectors until the development of solid-state technology, which advanced hugely in the mid 20th century, from the photo-multiplier tube (PMT) to the charge-coupled device (CCD). As a result, finer and finer spectral and spatial resolution were achieved.

This technology was primarily concerned with optical/IR wavelengths, which the cold ISM is opaque to due to dust. In order to probe these regions, longer wavelengths would need to be observed. Heinrich Hertz had discovered electromagnetic radiation at radio wavelengths in 1888, and in 1931 Carl Jansky made the first discovery of these radio waves from the sky. This lead to the formation of a field of observation which would reveal the inner depths of the regions previously occluded from view, *radio astronomy*. Much of modern astronomy is based on complementary observations over many different wavelengths, from x-ray through optical and IR, out to radio waves. In order to fully characterise the target, multi-wavelength studies represent the best approach.

### 2.2 Astrophysical Signals

Light from very distant sources behaves like a point source. At these large distances, the rays are essentially parallel when they arrive at the telescope, *i.e.* a plane wave. Telescopes capture the portion of the radiation which is incident on
their apertures. The larger the aperture, the more photons per second captured. (see Figure 2.1 for the sizes of many modern telescopes.) At the focal points of these systems, various instruments and detectors can be used to extract information from the incoming flux of photons, such as (but not limited to);

- Rate of incoming photons (\( \vec{E} \) field amplitude for radio waves),
- Arrival direction - allows angular shape to be described,
- Photon energy - \( h\nu \) - gives spectral information about the source,
- Polarisation - direction of the \( \vec{E} \) - gives information about \( \vec{B} \) or level of dust scattering.
Figure 2.2: (Left) The 22 m Mopra Telescope located in Coonabarabran in north-west New South Wales, with a beam size of 36" at 3-mm wavelength. [Image credit: http://www.csiro.au/en/Research/Facilities/ATNF/Mopra-radio-telescope Date of access: 08/12/2015]

(Right) The radiation pattern of a parabolic antenna (such as Mopra), shown in polar co-ordinates on a logarithmic scale. The actual Mopra beam has been characterised by Ladd et al. (2005) and the beam efficiencies used are listed there. [Image credit: https://commons.wikimedia.org/wiki/File:Sidelobes_en.svg Date of access: 08/12/2015]

Depending on the frequency of interest, there are many possible systems for detection. Focusing systems are the most common for most fields, only at very high energies such as X-ray and gamma-ray are non-focusing systems required. As stated above, telescopes were initially refractive in nature, using lenses to focus light. The chromatic aberration associated with this was a problem, and when larger systems were sought, the weight of glass required for larger lenses became a structural issue.

2.2.1 The Beam

For the signals of interest to work in star formation, namely dust-emission at the µm scale, and rotational transition in interstellar molecules, at the mm and sub-mm scales, dish antennae are the most common telescope in use. From ground
based telescopes such as Mopra (Fig. 2.2) and the VLT, to space based ones such as Herschel. In receiving mode, the antenna of a radio telescope receives signals from the same light cone in which it would broadcast, were it in broadcast mode. Any source within this cone would be detected, with efficiency dependent on the position relative to the viewing axis. If two point sources lie within the beam, then they cannot be resolved. The angular size of the beam represents approximately the angular resolution of the telescope. Smaller beams can resolve more closely spaced sources, but larger beams have an advantage when trying to map a large part of the sky. Because of the limited diameter of the antenna, the beam is not perfectly parallel, diffraction shapes the beam into lobes. (see Fig. 2.2). The main lobe is effectively the observing beam, however, the side lobes can be sources of noise, and false detections due to extraneous radio signals, so extra caution must be taken to isolate radio telescopes from signals such as these.

### Beam Pattern

How can we work out where this lobe pattern comes from? It is referred to as the beam pattern, and is simply the power gain as a function of direction. For a parabolic dish diameter D, the aperture is simply the plane circle of the same diameter.

The concept of reciprocity in antenna theory is important. The weak reciprocity theorem states that "The power pattern of an antenna is the same for transmitting and receiving". This is because of the validity of the solutions to Maxwell’s equations under time reversal. We consider the example of a 1D aperture of width D (Fig. 2.3), and treat it as a transmitting antenna, and calculate the electric field pattern at a distant point (R ≫ D). The aperture is illuminated by the feed with a sine wave signal of frequency $\nu$ and electric field strength $g(x)$ that varies across the aperture. The illumination induces currents in the reflector. The current densities
J will vary with both position and time:

\[ J \propto g(x)e^{-i\omega t}. \]

Using Huygens’ Principle, the aperture can be treated as an ensemble of smaller elements which each act as small antennae. The electric field produced by the aperture at large distances is the vector sum of the fields due to each smaller aperture element. The field from each element of width \( dx \) from \( x \) to \( x + dx \) is:

\[ df \propto \frac{e^{-ikr}}{r} dx. \]

At the large distances we are considering, the Fraunhofer approximation holds,

\[ r \approx R + x \sin \theta = R + x l \]

where

\[ l = x \sin \theta. \]
We can also make the approximation \( \frac{1}{r} \approx \frac{1}{R} \). This quantity is nearly constant over the aperture, so can be absorbed into any constant of proportionality. We cannot discount the periodic contribution at any distance however:

\[
df \propto g(x)e^{-ikR}e^{-ikxl}
\]

\( e^{-ikR} \) is also constant so can drop out of the integration Remembering that \( k = \frac{2\pi}{\lambda} \) and defining \( u = \frac{x}{l} \) which expresses position along the aperture in units of wavelength, then

\[
f(l) = \int_{\text{aperture}} g(u)e^{-2\pi ilu} du \tag{2.1}
\]

This is a very important result. The far field beam pattern of an aperture antenna is the *Fourier Transform* of the illuminating field, \( g(u) \). The similarity theorem for Fourier transforms allows us to make some powerful statements about the behaviour of this pattern.

If \( f(l) \) is the Fourier transform of \( g(u) \), then

\[
\frac{1}{|a|}f\left(\frac{l}{a}\right)
\]

is the Fourier transform of \( g(au) \), where \( a \neq 0 \) is a constant.

Making the function \( g \) wider makes \( f(l) \) taller and narrower, while making \( g \) narrower makes \( f(l) \) shorter and wider. The area under the transform is maintained.

This implies that the *beamwidth* of the aperture is inversely proportional to the aperture size, and the voltage gain is directly proportional to the aperture size.

For a uniformly illuminated aperture (*i.e.* a square wave) the Fourier transform is the *sinc* function \( \text{sinc}(x) = \frac{\sin(x)}{x} \). Rotated about the centre of the aperture, this gives the famous *Airy Disk* diffraction pattern. The radiated power per unit area is proportional to the square of the electric field strength, so the power pattern \( P(l) \) is (for small angles)

\[
P(l) \propto \text{sinc}^2 \frac{\theta D}{\lambda}
\]
The full width between half-maximum points (FWHM) is the convention for the angular width of the beam. That is the angle between points where the power has dropped to half of the peak value. For a normalised power spectrum

\[ P\left(\frac{\theta_{\text{FWHM}}}{2}\right) = \frac{1}{2} = \sin^2\left(\frac{\theta_{\text{FWHM}} D}{2\lambda}\right) \]

\[ 0.443 \approx \frac{\theta_{\text{FWHM}} D}{2\lambda} \]

\[ \theta_{\text{FWHM}} \approx 0.89 \frac{\lambda}{D} \]

The similarity theorem allows us to state

\[ \theta_{\text{FWHM}} \propto \frac{\lambda}{D} \]  \hspace{1cm} (2.2)

with the scaling factor depending on the illumination.

The FWHM is sometimes called the resolving power of a telescope because two equal point sources separated by this angle can just be resolved by the Rayleigh criterion: the peak response to one source coincides with the first minimum response to the other (Fig. 2.5). This is the response of an antenna to two ideal point
Figure 2.5: Ideal point response of an antenna, with separation a) greater than, b) equal to, and c) less than the Rayleigh criterion.

sources, and represents the minimum resolvable angular separation of sources, sometimes known as the *diffraction limit*. For many reasons, this limit is rarely reached due to other effects, such as atmospheric turbulence, and aberrations in the optical system which can lead to blurring of the signal over a larger area than the diffraction pattern. The *Hubble Space Telescope* has a relatively small primary mirror in comparison to some ground based telescopes, but because it is in space, atmospheric turbulence is negated completely allowing for much sharper images to be taken than would be possible with a commensurate size mirror on Earth.

### 2.3 Interferometry: Beyond the diffraction limit

More recently, technology has been developed to detect the atmospheric turbulence during observation, and use a deformable mirror to correct the wavefronts
which have been altered by the turbulence. This is known as adaptive optics and can produce results similar to Hubble from ground based observations, minus the prohibitive cost of a space based mission. For optical and NIR observations, the improved resolution provided by adaptive optics is sufficient to make many meaningful discoveries. For radio astronomy however, even operating at the diffraction limit can be quite restrictive. Equation 2.2 shows that the angular resolution of a system scales directly with the wavelength of observation. Radio waves being the longest, have the largest diffraction limit. Astronomer have learned to overcome this limit through the use of multiple telescopes viewing the same source simultaneously, in what is known as interferometry.

In a telescope array, each dish can be thought of as a small element of a hypothetical larger dish comparable in size to the largest distance between two telescopes in the array, with much larger resolution than the individual components. This large separation is known as the baseline, B, and from equation 2.2 information can be extracted on the scale $\approx \frac{\lambda}{B}$. Arrays of telescopes spread out over 10’s of kilometres such as ALMA (Atacama Large Millimetre Array) can give angular resolution of less than 1 arcsecond, while arrays spread out over continents SKA (Square Kilometre Array) can probe down to milli-arcsecond scales.

Interferometry will never produce a perfect image (Fig. 2.6) since the point response of an array of telescopes is not a complete sampling of a full dish, however it can be shown that with multiple dishes, over multiple scans, alongside sophisticated analysis techniques, high quality images can be produced by interferometry.

### 2.3.1 Sampling the (\(u,v\)) plane - From Sky Brightness to Visibility

For two telescopes, the beam pattern on the sky is a set of interference fringes, and as the earth rotates, this pattern sweeps across the sky. If there is a source, the observation yields a time varying interference pattern when the two signals are
Figure 2.6: Single dish vs Interferometry "Eye Test". The single dish lacks the resolution to see the finer detail of the image. The interferometer image picks up this detail (high spatial frequencies), but at the expense of some of the power (low spatial frequencies). Many artefacts are also visible.

summed. This gives a single Fourier (spatial frequency) component of the source. The angle between the source and the telescope pair changes as the source moves through the sky, repeated observations add more Fourier components to the image. Furthermore, if there are N telescopes, they can combine to form N(N-1) unique baseline pairs, each generating another unique Fourier component for the image.

The interference pattern is directly related to the source brightness, the complex visibility $V(u, v)$ is the 2D Fourier Transform of the brightness on the sky $T(x, y)$, where $u$ and $v$ are the co-ordinates in the frequency domain, and $x$ and $y$ are the co-ordinates on the sky.

\[
V(u, v) = \int_y \int_x T(x, y) e^{2\pi i (ux + vy)} dxdy \tag{2.3}
\]

\[
T(x, y) = \int_v \int_u V(u, v) e^{-2\pi i (ux + vy)} dudv \tag{2.4}
\]
Figure 2.7 shows how the point response of one of these systems changes as more baselines and more observations are added. Provided that the Fourier plane is sufficiently sampled, the Fourier Transform of $V(u,v)$ can yield a reasonable approximation of the true sky brightness pattern, but at much increased resolution compared to a single dish observation. This process is known as aperture synthesis.

### 2.3.2 ALMA: Atacama Large Millimetre Array

Consisting of over sixty 12-meter, and 7-meter diameter radio telescopes, ALMA is the largest astronomical interferometer in operation today. Since a high and dry site is crucial to millimetre wavelength operations, the array has been constructed on the Chajnantor plateau at 5,000 meters altitude, near Llano de Chajnantor Observatory and Atacama Pathfinder Experiment.

ALMA’s main array has fifty 12 m antennas, arranged in configurations spread over distances from 150 metres to 16 km. Four additional 12 m dishes, along with twelve 7 m dishes form the Atacama Compact Array. These tighter arrays sample smaller regions in the Fourier plane more densely, and because of the similarity theorem, this array extracts information about the broad structure of the target, while the longer baselines of the main array extract the finer details of the higher spatial frequencies.

### 2.4 Radiative Transfer Theory

#### 2.4.1 Quantum states of molecules

The gas content of the interstellar medium is observable primarily through molecular and atomic transitions, commonly referred to as lines. These are bound-bound interactions between energy levels in the molecules or atoms. Suppose there exists a multi-level molecule, with energy levels $E_i$, where $i = 0 \rightarrow N_{\text{levels}}$, arranged in
Figure 2.7: Point responses for different arrays of dishes. [Images: Wilner (NRAO)]
ascending order, such that \( E_{i+1} > E_i \). Consider 1 cm\(^3\) of space containing these molecules, and count how many are in each state, \( i \).

\[
n_i = \frac{N_i}{N} \tag{2.5}
\]

subject to the conditions, (\(\Sigma N_i = N \& \Sigma n_i = 1\)). \(N_i\) and \(n_i\) are the occupancy number density, and fractional occupancy, respectively. Often atoms and molecules have states of equal energy, owing to rotational symmetry of the wavefunctions, so these states of equal energy are treated as a single state, with a statistical weight, or degeneracy \(g_i\). This is simply the number of states of equal energy which are combined to give the \(i\)th energy level. In dense environments, collisions between molecules occur so often that a thermal distribution can be assumed for the occupancies. Considering all of this, the relative occupancies of two levels \(i\) and \(j\) is given by the following formula:

\[
\frac{n_i}{n_j} = \frac{N_i}{N_j} = \frac{g_i}{g_j} e^{-(E_i-E_j)/k_B T} \tag{2.6}
\]

This is one of the conditions for what is known as Local Thermodynamic Equilibrium, or LTE. In order to calculate the actual occupancies, rather than the ratio \(n_i/n_j\), the partition function must be calculated. This is the normalisation constant

**Figure 2.8:** *(Left)* Artist representation of the baselines of ALMA. *(Right)* ALMA dishes. [Images: (NRAO)]
of the system, based on the fact that the probabilities must sum to 1.

\[ Z(T) = \sum_{i} g_i e^{-E_i/kT} \]  

(2.7)

The fractional occupancy of the \( i \)th state can now be written as

\[ n_i = \frac{1}{Z(T)} g_i e^{-E_i/kT}. \]  

(2.8)

One of the tasks for radiative transfer is to calculate these occupancies.

### 2.4.2 Collisional Transitions

The rate at which a molecule in state \( i \) is collisional changed to state \( j \) can be written as

\[ C_{ij} = N K_{ij}(T) \]  

(2.9)

where \( N \) is the number density of possibly colliding molecules, and \( K_{ij}(T) \) is the collision coefficient. These collisional coefficients come from complex calculations involving the potential energy surfaces of the molecule of interest, and all possible collisional partners. In the past, these coefficients were calculated using the conveniently simple spherical potential energy surface of the helium atom, which is the second most common collisional parter for any molecule. These helium rates would then be scaled to give rates for collisions with \( \text{H}_2 \). These approximate rates have worked reasonably well, however, with recent advances in computational resources, the much more complex system of a molecule colliding with the potential energy surface of the linear \( \text{H}_2 \) molecule has been modelled, and more realistic rates calculated (e.g. Ben Abdallah et al. (2012, for HCN with para-\( \text{H}_2 \))). InLTE situations, a restriction is placed such that the collisional transitions maintain the overall level populations.

\[ n_i C_{ij} = n_j C_{ji} \]  

(2.10)
Which when combined with Eq 2.6 gives

\[ C_{ji} = C_{ij} \frac{g_i}{g_j} e^{-\left(\epsilon_i - \epsilon_j/kT\right)} \]  

(2.11)

This allows a further simplification, the calculation of the downward collisional coefficients only. They are weakly temperature dependent, and the upward rates can be calculated from them using Eq 2.11.

### 2.4.3 Radiative Transitions

In the low density conditions typical of interstellar space, however, radiative transitions can occur more often than collisional transitions. These transitions involve changing state via the absorption or emission of a photon, leading to a non-LTE situation where the level populations no longer follow Eq 2.6. There is a critical density associated with this transition to non-LTE populations, and it is represented by the density at which the probability to decay radiatively or collisionally is equal. Above this density, certain forbidden radiative transitions become possible collisionally.

If radiation passes through a medium, energy can be gained or lost by emission, absorption or by scattering.

#### Emission

The change in energy due to emission along a beam per unit volume \((V)\), solid angle \((\omega)\), frequency \((\nu)\) and time, \((t)\) is given by

\[ dE = j_\nu dV d\omega dt \]  

(2.12)
where \( j_\nu \) is the monochromatic spontaneous emission coefficient. For an isotropic emitter, which an ensemble of randomly oriented molecules is,

\[
j_\nu = \frac{1}{4\pi} P_\nu
\]

(2.13)

Sometimes, it is convenient to consider \( dE \) in terms of an emissivity, \( \varepsilon_\nu \), which is the spontaneously emitted energy per unit mass, frequency and time.

\[
dE = \varepsilon_\nu \rho \, dV \, dt \, d\nu \, d\omega \frac{d\omega}{4\pi}
\]

(2.14)

which gives

\[
j_\nu = \frac{\varepsilon_\nu \rho}{4\pi}
\]

(2.15)

In going through a distance \( ds \) a beam \( dA \) sweeps out a volume \( dV = dA \, ds \)

\[
dI_\nu = j_\nu \, ds
\]

(2.16)

Where \( I_\nu \) is the specific intensity such that \( dE = I_\nu \, dA \, d\nu \, d\omega \, dt \). Another useful quantity to define is the mean intensity, averaged over the entire solid angle.

\[
J_\nu = \frac{1}{4\pi} \int I_\nu \, d\Omega
\]

(2.17)

**Absorption**

A similar expression can be arrived at for absorption. This process can be thought of as the absorption by individual particles of number density \( n \), and absorbing cross-section \( \sigma_\nu \), each with a random orientation. Fig 2.9 shows a beam traversing an area filled with these absorbers. The number of absorbers in the swept up volume \( dV \) is, \( n \, dV = n \, dA \, ds \), which gives a total absorbing cross section of \( \sigma_\nu \, n \, dA \, ds \). The total energy removed from the beam is

\[
dI_\nu = -n\sigma_\nu I_\nu \, ds
\]

(2.18)
Figure 2.9: Ray $dA$ passing through a medium of absorbers/emitters, with solid angle $d\omega$.

giving

$$dI_\nu = -\alpha_\nu I_\nu \, ds$$  \hspace{1cm} (2.19)

where

$$\alpha_\nu = n\sigma_\nu = \rho \kappa_\nu$$  \hspace{1cm} (2.20)

is the absorption coefficient, and $\kappa_\nu$ is the mass absorption coefficient, more commonly known as the opacity.

**Einstein Coefficients and Statistical Equilibrium**

In order to satisfy the laws of thermodynamics, the following condition must be satisfied

$$\frac{j_\nu}{\alpha_\nu} = B_\nu(T)$$  \hspace{1cm} (2.21)

This is *Kirchoff’s Law*. A medium in thermal equilibrium can have any emissivity and or absorptivity, so long as their ratio is the Planck function $B_\nu(T)$. The link between emission and absorption for a thermal emitter implies some microscopic relationship between the two processes. This relation was first discovered by Albert Einstein, through analysing the interaction of radiation with a discrete, two energy level, atomic system. The energy levels are $E$, and $E + h\nu_0$, with statistical weights $g_1$ and $g_2$ respectively. The system undergoes a transition from 1 to 2 via the
Figure 2.10: A diagram representing a simple two-level system, showing schematically the three main quantum processes identified by Einstein. Absorption, spontaneous emission, and stimulated/induced emission. [Credit: SEO Project, http://www.seos-project.eu/modules/laser-rs/laser-rs-c02-p06.html (Date: December 8th 2015)]

absorption of a photon of energy $h\nu_0$ and similarly, a transition from 2 to 1 occurs via the emission of an identical photon.

Einstein identified three processes, which are outlined visually in Figure 2.10:

1. **Spontaneous Emission**: This occurs when the system is in level 2 and drops to level 1 by emitting a photon, and occurs in the absence of a radiation field. The *Einstein A-coefficient* is defined as the transition probability per unit time for spontaneous emission, $A_{21}$ ($s^{-1}$).

2. **Absorption**: Occurs in the presence of a radiation field, so the transition probability is dependent on the density of photons *i.e.* mean intensity of the field as per Eq. 2.17. Due to Heisenberg’s Uncertainty principle ($\Delta E \Delta t > \hbar$) the transitions between energy levels are governed by a line-shape function $\phi(\nu)$ which outlines the relative effectiveness of photons with frequencies $\nu$. 

centred on $\nu_0$, in causing transitions.

$$\bar{J} \propto \text{transition probability per unit time}$$

where the constant of proportionality is $B_{12}$, the Einstein $B$-coefficient and $\bar{J}$ is the mean intensity averaged over the line-shape function.

$$\bar{J} = \int J(\nu) \phi(\nu) d\nu$$

(2.22)

3. **Stimulated Emission:** In order to derive Planck’s Law, Einstein found that a third process was necessary, directly opposite to absorption, wherein an atom in level 2, in the presence of a suitable photon, is stimulated to emit a photon of frequency $\nu_0$. This is the process behind astrophysical masers, and also lasers. It has another $B$-coefficient associated with it, $B_{21}$.

With these probability coefficients in hand, it is possible to define the equilibrium configurations for both a two-level and a multi-level system. In equilibrium, the number of transitions into a particular state, is balanced by the number of transitions out of that state. This is the principle of *detailed balance*. If the number densities of atoms in states 1 and 2, are $n_1$ and $n_2$ respectively, then,

$$n_1 B_{12} \bar{J} = n_2 A_{21} + n_2 B_{21} \bar{J}.$$  

Solving for $\bar{J}$

$$\bar{J} = \frac{A_{21}/B_{21}}{(n_1/n_2) (B_{12}/B_{21}) - 1}.$$ 

In thermodynamic equilibrium the ratio of $n_1/n_2$ is given by Eq. 2.6, such that

$$\bar{J} = \frac{A_{21}/B_{21}}{(g_1 B_{12}/g_2 B_{21}) \exp (h \nu_0/kT) - 1}.$$ 

Now we can say, for a particular transition from level $i$ to level $j$
\[ j_{ij}(\nu) = n_i A_{ij} \phi_{ij}(\nu) \quad (2.23) \]

\[ \alpha_{ij}(\nu) = (n_j B_{ji} - n_i B_{ij}) \phi_{ij}(\nu) \quad (2.24) \]

We can see that the Einstein A and B coefficients are related if we consider detailed balance at thermal equilibrium,

\[ A_{ij} = \frac{2h\nu^3}{c^2} B_{ij} \quad (2.25) \]

Finally, we can now show that the critical density for a transition can be written as

\[ (n_{\text{crit}})_{ij} = \frac{A_{ij}}{k_{ij}} \quad (2.26) \]

where \( A_{ij} \) is the Einstien A coefficient, representing the average time for a radiative transition to occur between states \( i \) and \( j \), and \( k_{ij} \) is the collisional rate coefficient between states \( i \) and \( j \). Above this density, a particular excited state is more likely to be collisionally de-excited than it is to be radiatively de-excited, the line is said to be quenched.

\[ C_{ij} = n k_{ij} > A_{ij} \quad \text{when } n > n_{\text{crit}} \quad (2.27) \]

So in order to probe the densest regions of molecular clouds, transitions with high critical densities must be sought.
2.4.4 Transfer Equation

These expressions for the change in intensity due to emission and absorption lead to the equation of radiative transfer.

\[
\frac{dI_\nu}{ds} = j_\nu - \alpha_\nu I_\nu \tag{2.28}
\]

This differential equation takes a convenient form if a new term, \( \tau_\nu \) - the optical depth, is considered.

\[
d\tau_\nu = \alpha_\nu ds \tag{2.29}
\]

\[
\tau_\nu(s) = \int_{s_0}^{s} \alpha_\nu(s') ds' \tag{2.30}
\]

If \( \tau_\nu > 1 \), a medium is said to be optically thick, or opaque. If on the other hand, \( \tau_\nu < 1 \) the medium is optically thin, or transparent. Typically, an optically thick medium is one which the average photon cannot pass through without being absorbed, an optically thin medium is one through which it can. Dividing the transfer equation by \( \alpha_\nu \)

\[
\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \tag{2.31}
\]

where \( S_\nu = \frac{j_\nu}{\alpha_\nu} \), is known as the source function. Comparing this to Eq. 2.21 we can see that this quantity has a physical significance, related to the Planck blackbody formula. For a particular transition

\[
S_{ij} = \frac{f_{ij}(\nu)}{\alpha_{ij}(\nu)} = \frac{n_i A_{ij}}{(n_j B_{ji} - n_i B_{ij})} \tag{2.32}
\]

A formal solution Eq. 2.31 can be sought, by using an integrating factor \( e^{\tau_\nu} \), [See Appendix A] giving the full solution of the equation of radiative transfer

\[
I_\nu = I_\nu(0)e^{-\tau_\nu} + \int_{0}^{\tau_\nu} S_\nu e^{(-\tau_\nu-\tau_{\nu}')}d\tau_{\nu}' \tag{2.33}
\]

This equation contains two terms, the initial intensity attenuated by absorption, plus the integrated source also attenuated. For a constant source function,
\[ S_{\nu}(\tau'_{\nu}) = S_{\nu} \]

\[ I_{\nu}(\tau_{\nu}) = S_{\nu} + (I_{\nu}(0) - S_{\nu}) e^{-\tau_{\nu}} \]

As \( \tau_{\nu} \to \infty \), \( I_{\nu} \to S_{\nu} \), a relaxation process. Optically thick clouds contain no information about the initial radiation field. They are opaque, and behave as purely emitting clouds.

As \( \tau_{\nu} \to 0 \), \( I_{\nu} \to I_{\nu 0} (1 - \tau_{\nu}) + S_{\nu} \tau_{\nu} \). Optically thin clouds contain information about the background radiation field, attenuated by the intervening gas, plus any source within the cloud itself, also attenuated.

### 2.5 Numerical Methods in Radiative Transfer

The challenge for a radiative transfer code is to consistently solve the equation of radiative transfer 2.33, in conjunction with the statistical equilibrium equations. For a more realistic multi-level system, these relations must be summed over all levels, giving the full equation for statistical equilibrium

\[
\sum_{j>i} \left[ n_j A_{ji} + (n_j B_{ji} - n_i B_{ij}) \tilde{J}_{ji} \right] - \sum_{j<i} \left[ n_i A_{ij} + (n_i B_{ij} - n_j B_{ji}) \tilde{J}_{ij} \right] + \sum_j \left[ n_i C_{ij} - n_j C_{ji} \right] = 0. \quad (2.34)
\]

Equations (2.22–2.24) and (2.32–2.34) form a coupled set of equations. The way in which the quantities depend on each other is depicted in Fig. 2.11. The intensities are found by integrating the source function (Eq.2.33) plus an attenuated background contribution. The source function and extinction coefficients depend on the level populations (Eqs. 2.23–2.24). These in turn depend on the intensities.
(Eqs. 2.34, 2.22). To solve this set of equations one must determine the radiation field and the level populations simultaneously. Since the radiation field couples the level populations at different spatial positions to each other through the transfer integral (Eq. 2.33), the only way of solving this system directly seems to be through complete linearisation and solving a huge matrix equation involving all level populations at all spatial positions. In practice, the evaluation of the matrix elements and the inversion of the problem consumes far too much CPU-time as well as memory and is therefore beyond current computing capabilities. An alternative and much simpler way is to iteratively evaluate all equations, following the arrows, as illustrated in Fig. 2.11. This method is called *Lambda Iteration*.

An initial background is chosen $I_{\nu 0}$ and a trivial first iteration takes place. The mean intensity is calculated, and used to solve Eq. 2.34 for the level populations, $n_j$, these are then used, along with the Einstein co-efficients, to generate a source function using Eq. 2.32. This process continues iteratively, until the code converges to a solution.
2.5.1 Accelerated Lambda Iteration

Through use of an approximate lambda operator, the ALI algorithm of Rybicki & Hummer (1991) reduces these coupled equations to a set of linear ones which can be solved quickly, even in optically thick conditions. The $\Lambda$ operator is a matrix operator which acts on the source function, in order to generate the mean intensity.

$$\bar{J}_{\mu\nu} = \Lambda_{\mu\nu} [S_{\mu\nu}]$$  \hspace{1cm} (2.35)

where $\nu$ is the frequency, and $\mu$ the directional cosine, making terms with the $\mu\nu$ subscript frequency and angle averages.

Approximate lambda operators are favoured for many-level problems due to their simple inversion and their subsequent iterative corrections. A single iteration can be likened to moving the contained photons approximately one free path in the medium. However, for strong line cores, the mean free path is characteristically small requiring many iterations to move them a comparable distance. Even if the line is not considered strong, the involved photon is still prone to being trapped requiring limitless number of random walks to exit a cyclic group of transitions.

The difficulties summarised above were overcome by Rybicki [1984], who explicitly treated only photons contained in the line wing. Accordingly, line core photons were considered quiescent and were removed from the process by a successful preconditioning of the statistical equilibrium (SE) equations. An essential feature of this so-called “core saturation” scheme is that the SE equations remain linear hence drastically improving the efficiency of the method over that of lambda iteration (LI). Two crucial prerequisites therefore form the principles of the majority of ALI methods. These are:

- The solution to the radiative transfer equation is sought with a simplified operator,
• Solving some form of the modified SE equations at every step of the iteration cycle.

The operator-splitting technique was initially proposed by Cannon (1973)

\[ J = (\Lambda - \Lambda^\ast)[S] + \Lambda[S] \]  (2.36)

In this equation, \( \Lambda \) and \( \Lambda^\ast \) are the exact and approximate operators, the latter with a simple inverse. \( S^\dagger \) is the source function from a previous iteration. This is passed through the equations of SE and solved for an updated source function, S. The form of solution given in Eq. 2.36 is only appropriate if the source function eventually converges, i.e. \( S = S^\dagger \), i.e. as long as convergence is achievable. The development of ALI schemes is hinged on an effective choice of the approximate operator. Rybicki (1984) tended to stick with diagonal or tridiagonal operators. (A tridiagonal matrix has zeros in all elements except for the main diagonal, and the first diagonal either side of it.) Olson et al. (1986) demonstrated that the diagonal part of the true lambda operator is the most efficient approximate operator and does not require the involvement of secondary arbitrary parameters.

The techniques highlighted above especially with regard to the requirement of linearisation at every step in the iteration process have been avoided in this formalism. Such a linearisation is far too computationally intense and instead a preconditioning of the SE equations is sought. Photon trapping is successfully eliminated by the preconditioning, especially for the cores of optically thick lines while maintaining linearity of the SE equations.

The multilevel problem is tackled by simultaneously solving both the SE equations for the level populations and the radiative transfer equation for the radiation field (Rybicki & Hummer, 1991). For frequencies near a line \( \nu_{ij} \),

\[ I_{\mu\nu} = \Lambda_{\mu\nu}^\ast S_{ij} + I_{\mu\nu}^{\text{eff}} \]  (2.37)
In this version of the Lambda Iteration the approximate lambda operator is local, so that it acts like a scalar multiplication of the source function. The mean integrated intensity is

$$\bar{J}_{ij} = \Lambda_{ij}^* S_{ij} + J_{ij}^{\text{eff}}$$  \hspace{1cm} (2.39a)

$$\Lambda_{ij}^* = \int d\Omega \int d\nu \phi_{ij} \Lambda_{\mu\nu}^*$$  \hspace{1cm} (2.39b)

$$J_{ij}^{\text{eff}} = \int d\Omega \int d\nu \phi_{ij} I_{ij}^{\text{eff}}$$

$$= J_{ij}^\dagger - \bar{\Lambda}_{ij}^* S_{ij}$$  \hspace{1cm} (2.39c)

The latter two expressions represent the angle and frequency averages of $\Lambda_{\mu\nu}^*$ and $I_{\mu\nu}^{\text{eff}}$ using the lineshape function $\phi_{ij}$ for weighting.

With the above results substituted into the SE equations (Eq. 2.34) along with the source function (Eq. 2.32) we arrive at a preconditioned form of the SE equations:

$$\sum_{j>i} \left[ n_j A_{ij} (1 - \Lambda_{ij}^*) + (n_j B_{ij} - n_i B_{ij}) J_{ij}^{\text{eff}} \right]$$

$$- \sum_{j<i} \left[ n_i A_{ij} (1 - \Lambda_{ij}^*) + (n_i B_{ij} - n_j B_{ij}) J_{ij}^{\text{eff}} \right] + \sum_j \left[ n_i C_{ij} - n_j C_{ji} \right] = 0.$$  \hspace{1cm} (2.40)

The Einstein A has now become $(1 - \Lambda_{ij}^*) A_{ij}$, and the mean integrated intensity replaced by the effective mean integrated intensity from Eq. 2.39c. The conditioning of Eq. 2.40 is apparent due to the omission of the transfer in the line core, which is primarily due to the choosing of the the diagonal of the full lambda operator as the approximate operator. This leaves an SE equation which is still linear in level populations.
Including an Active Continuum

With an active continuum the total emissivity and absorptance around a frequency \( \nu_{ij} \) are

\[
\begin{align*}
\dot{j}_{\mu\nu} &= \dot{j}_{ij} + \dot{j}_{c\nu} \\
\alpha_{\mu\nu} &= \alpha_{ij} + \alpha_{c\nu}
\end{align*}
\] (2.41a, b)

The continuum contributions to emission \( (\dot{j}_{c\nu}) \) and absorption \( (\alpha_{c\nu}) \), are evaluated at \( \nu_{ij} \). A modified source function now reads

\[
S_{\mu\nu} = r_{ij}S_{ij} + (1 - r_{ij})S_{c\nu}
\] (2.42)

where

\[
r_{ij} = \frac{\alpha_{ij}(\mu, \nu)}{\alpha_{ij}(\mu, \nu) + \alpha_{c\nu}}
\] (2.43)

As before \( r_{ij} \) is a local operator, however it is no longer a straightforward matter to linearise the equations of SE as before, since \( \alpha_{ij}(\nu, \nu) + \alpha_{c\nu} \) is not linearly proportional to the level populations. Rybicki & Hummer (1991) introduce an altered form of this operator, using “old” quantities from the previous iteration.

\[
r_{ij}^\dagger = \frac{\alpha_{ij}^\dagger(\mu, \nu)}{\alpha_{ij}^\dagger(\mu, \nu) + \alpha_{c\nu}}
\] (2.44)

This does not affect the final solution, since upon convergence, \( r_{ij}^\dagger = r_{ij} \). Note also that the continuum operator remains unchanged between Eqs. (2.43–2.44).

Expressing the source function in terms of this new operator, analogous to Eq. 2.37

\[
I_{\mu\nu} = \Lambda_{\mu\nu}^* r_{ij}^\dagger S_{ij} + \bar{I}_{\mu\nu}^{\text{eff}}
\] (2.45)
where

\[
\dot{I}_{\mu \nu}^{\text{eff}} = \Lambda^{*}_{\mu \nu} [S_{\mu \nu}^\dagger] - \Lambda^{*}_{\mu \nu} r_{ij}^\dagger S_{ij}^\dagger, \tag{2.46a}
\]

\[
\dot{I}_{\mu \nu}^{\dagger} - \Lambda^{*}_{\mu \nu} r_{ij}^\dagger S_{ij}^\dagger. \tag{2.46b}
\]

with continuum quantities cancelling due to an assumption of their constant nature. [Although \( S_{c,ij} \) does not appear explicitly in Eq. 2.46a, it is included implicitly in the term \( S_{\mu \nu}^\dagger \).

The mean integrated intensity now becomes

\[
\bar{J}_{ij} = \tilde{\Lambda}_{ij}^\dagger S_{ij} + \tilde{J}_{ij}^{\text{eff}} \tag{2.47}
\]

where,

\[
\tilde{\Lambda}_{ij}^* = \int d\Omega \int d\nu \phi_{ij} \Lambda^{*}_{\mu \nu} r_{ij}^\dagger, \tag{2.48a}
\]

\[
\tilde{J}_{ij}^{\text{eff}} = \int d\Omega \int d\nu \phi_{ij} I_{\mu \nu}^{\text{eff}} = \tilde{J}_{ij}^\dagger - \tilde{J}_{ij}^\dagger S_{ij}^\dagger, \tag{2.48b}
\]

\[
\bar{J}_{ij}^\dagger = \tilde{\Lambda}_{ij}^* S_{ij}^\dagger + \tilde{J}_{ij}^{\text{eff}} \text{ from Eq. 2.39c}
\]

2.6 Radiative Transfer Modelling Strategy

2.6.1 MOLLIE A 3D Molecular Line RT Code

The 3-D molecular line radiative transfer code used throughout this work was written and developed by Keto and collaborators (see Keto et al., 2004; Rawlings et al., 2004; Redman et al., 2006; Carolan et al., 2008; Lo et al., 2011, for examples of its use). The code, MOLLIE (MOLecular LIine Explorer), is used to generate synthetic line profiles to compare with observed molecular rotational transition lines. MOLLIE splits the overall structure of a cloud into a 3-D grid of distinct cells where density, abundance, temperature, velocity and turbulent velocity are defined as
described above. In order to calculate the level populations, the statistical equi-
librium equations are solved using an Accelerated Lambda Iteration as outlined in
the previous section. For an arbitrary viewing angle to the model cube, ray-tracing
is then used to calculate the molecular line intensity as a function of velocity, for
a set of positions that matches in number the fixed gridding of the model.

MOLLIE has been benchmarked against a suite of problems (van Zadelhoff et al.,
2002) and all the models were found to reproduce the test observations to within
a few per cent. We emphasise that this benchmarking plus the model description
presented in this work, means it should be possible to replicate the model line pro-
files with other 3-D line radiative transfer codes (e.g. LIME, Brinch & Hogerheijde,
2010) and that such line radiative transfer codes have been used successfully since
the mid 1990s (Rawlings et al., 1992; Choi et al., 1995; Hogerheijde & van der
Tak, 2000; Ward-Thompson & Buckley, 2001; van Zadelhoff et al., 2002).

2.6.2 Constraining a Model

Typically we have a base physical model in mind for an object, often taken from
literature, along with it’s observed size. There is then a choice of which molecular
line to model that is context dependent. It depends on the type of object, and the
data available. The most ideal tracer is not always feasible. From our model we
want to infer properties such as infall, rotation and turbulence, which are present
in the line data, but are not easily extracted. We want to constrain these as best
as possible, ideally using multiple molecular lines to reduce the number of free
parameters.

This section will outline the modelling process, as laid out in (Lo et al., 2015), in
adapted form. The procedure followed to constrain a model is:

• Define source geometry
• Pre-constrain density and temperatures from continuum observations
• Identify tightly constrained parameters from line observations

• Fit the few remaining parameters to match line profiles using a radiative transfer code

• Determine source physical properties from best fit models

Define source geometry

Properties such as cloud size and shape can be determined from spatially resolved maps of the target of interest, if available. The specific morphologies of any outflows, infalls, jets, etc can often be determined by the lineshapes themselves. Rawlings et al. (2013) find that several low mass star forming cores can be replicated using the same underlying model geometry, but viewed from different viewing angles. Often, relatively simple geometric functions such as spheres (cores), rings & tori (ridges), \( \text{tanh} \) functions (outflows) can give relatively good matches to the observations.

Constrained source properties from continuum observations

Dust continuum observations provide a measurement of the density and temperature in the core that is independent of the molecular line observations. This is achieved through spectral energy distribution (SED) fitting. Sometimes, more than one temperature component is required, however pressure balance can be maintained provided the term \( nT \) is kept constant. For example, if a two-component model is required to fit the observed SED, one at \( T=20 \) K and another at \( T=80 \) K, the density of the hot gas would need to be \( \approx 4 \) times lower, to maintain a constant \( nT \) throughout.

Similarly, the central densities are constrained by the SED fitting. The fall off in the density away from the central peak will follow a power law such that the cloud will be observed as a distinct feature. The Plummer sphere profile for the
density (Arreaga-García et al., 2010) is a useful approximation to the more rigorous Bonnor-Ebert sphere solution for a self-gravitating sphere in an environment with significant external pressure (Bonnor, 1956; Ebert, 1955; Chandrasekhar, 1967).

$$\rho_{\text{Plummer}}(r) = \rho_0 \frac{R_{\text{Plummer}}^2}{R_{\text{Plummer}}^2 + r^2}$$  \hspace{1cm} (2.49)

where $R_{\text{Plummer}}$ is a constant scaling factor. The Plummer profile gives an approximately constant central density which smoothly transitions into an inverse square law density drop.

**Tightly defined properties from line observations**

From a set of line observations of different species, transitions and offsets, it is possible to readily determine the minimum line width from either a rare isotope species such as $\text{H}^{13}\text{CO}^+$, by structure within a line profile shape or by a resolved hyperfine line such as HCN (though see Loughnane et al., 2012, for dealing with hyperfine line anomalies).

The minimum line width (in the absence of dynamics) is related to the temperature and degree of turbulence in the gas

$$\sigma_{\text{tot}}^2 = \sigma_{\text{turb}}^2 + \sigma_{\text{th}}^2,$$  \hspace{1cm} (2.50)

where $\sigma_{\text{tot}}$ is the total velocity dispersion and is calculated using $\sigma_{\text{tot}}^2 = \Delta v^2 / 8 \ln 2$ where $\Delta v$ is the observed FWHM of a representative molecular line profile. $\sigma_{\text{th}}$ is the thermal velocity dispersion given by $\sigma_{\text{th}}^2 = kT/\mu$, where $\mu$ is the molecular mass, $T$ is the gas temperature and $k$ is Boltzmann’s constant.

Molecular line emission can be strongly affected by freeze-out of molecules onto the surface of dust grains, which obviously prevents them from emitting rotational line radiation, with the CO isotopologues particularly affected. Estimates of the total gas column density implied by an optically thin molecular line and by the
dust continuum can be used to quantify the degree of depletion. This can also be readily seen in radiative transfer modelling where depletion is required to avoid line profile strengths that are far too large for affected species. Freeze out proceeds fastest in the warmer regions of the cloud (until the sublimation temperature is reached at which point the grain mantles are re-released back into the gas phase in the hot core phase of massive star formation) and this is modelled by adopting a characteristic freeze-out radius, inside which the gas is significantly depleted out of the gas phase.

**Velocity structure modelling with MOLLIE**

With the adoption of the source geometry, density and temperature structure, degree of turbulence and freeze-out, the cores are largely defined. To solve the equation of radiative transfer for each species, line and position requires two remaining parameters: the local velocity of the gas and the chemical abundance of the species.

To fix the chemical abundance, a full dark cloud chemical model should ideally be run and would be crucial across regions of changing temperature, density and desorption such as in the protostellar disk. However, again the most extreme chemical variations will be taking place at boundaries layers between regions, e.g. bipolar outflows. These boundary layers are not well resolved by the single dish observations contained in this work. Bizzocchi et al. (2013) find little difference between two completely different choices of $\text{N}_2\text{H}^+$ radial abundance profiles for the core L1544, so we consider it reasonable to adopt uniform chemical abundances here for simplicity.

The velocity structure is the key remaining quantity to be specified. Along a given line of sight, the velocity of any infalling gas will vary from approximately static in the outer regions of the cloud to very large values, with a significant rotational component, as the gas approaches the disk. From the line observations limited
constraints on the infall can be made based on the degree of Doppler splitting of red-shifted and blue-shifted components measured in the profiles of species such as HCO$^+$ which best trace the dense infalling gas. This can only be done for sources where the direction of any jets or outflows is such that they are not orientated along our line of sight. If this is the case, they will not interfere with the dynamical signature of the infalling gas. The fraction of the beam occupied by infalling gas must also be taken into account when calculating infall velocities. Splittings of approximately $5 - 10 \text{ km s}^{-1}$ are seen, corresponding to infall velocities of a few km s$^{-1}$.

2.7 Overview

In this chapter we have outlined the theory of observing astronomical targets, both with single aperture, and interferometry techniques. We have covered the different telescopes from which the observations in this work have come, namely MOPRA, SMA and ALMA. We have laid out the theory of radiative transfer, and how numerical codes such as MOLLIE can solve the coupled set of equations, radiative transfer and statistical equilibrium, through use of an approximate lambda iteration. Finally we present a strategy for matching the synthetic spectra produced by codes such as MOLLIE to observed spectra, constraining the physical parameters of a model.
Chapter 3

HCN Hyperfine Anomalies in Low Mass Star Forming Regions

“Not all chemicals are bad. Without chemicals such as hydrogen and oxygen, for example, there would be no way to make water, a vital ingredient in beer.”

- Dave Barry

3.1 Hydrogen Cyanide

Hydrogen Cyanide (HCN) is a linear molecule, containing a H-C single bond and a C≡N triple bond. It was first observed in the ISM by Snyder & Buhl (1971), via the J=1→0 rotational transition, of the ground (ν=0) vibrational state. Since then, HCN has emerged as an attractive choice of tracer species for molecular gas since it is chemically well behaved, has a high critical density, is less susceptible to freeze-out onto dust grains than CO, and is relatively abundant. It is routinely used in low mass star forming cores (Sohn et al., 2007; Daniel et al., 2013), disks (van der Plas et al., 2014) and high mass star formation (Rolffs et al., 2011; Jin et al., 2015). HCN has also been used to observe comets (Hogerheijde et al., 2009;
Friedel et al., 2005; Hirota et al., 1999), evolved stellar atmospheres (Schilke & Menten, 2003; Smith et al., 2014), active galaxies (Aalto et al., 2012; Salas et al., 2014) and high redshift molecular clouds (Gao & Solomon, 2004).

**Formation & Destruction**

HCN forms in the gas phase by two main processes, neutral-neutral interactions,

\[ \text{CH}_2 + N \rightarrow \text{HCN} + \text{H} \]

or dissociative recombination.

\[ \text{NH}_3 + \text{C}^+ \rightarrow \text{HCNH}^+ + \text{H} \]

\[ \text{HCNH}^+ + \text{e}^- \rightarrow \text{HCN} + \text{H} \]

The neutral-neutral pathway is hindered by the necessity for intermediate carbon-hydrides CH and CH\(_2\), while the dissociative recombination relies on the availability of H\(_2\)CN. In dense regions with adequate UV shielding, grain surface interactions such as those mentioned in Section 1.2.1, can also lead to the formation of HCN. The increased amount of intact atomic nitrogen (N\(_2\)) leads, via cosmic ray driven interactions, to the formation of the nitrogen hydrides, NH and NH\(_2\), which can interact with a carbon atom undergoing hydrogenation towards CH\(_4\).

\[ \text{N}_2 + \text{p} \rightarrow \text{N} + \text{N} \]

\[ \text{N} + \text{p} \rightarrow \text{N}^+ + \text{e}^- \]

\[ \text{N}^+ + \text{H}_2 \rightarrow \text{NH} + \text{+H} \]

\[ \text{NH}^+ + \text{e}^- \rightarrow \text{NH} \]
Sequential reactions of N\(^+\) with H\(_2\), interrupted by electron recombination, lead to the formation of NH, NH\(_2\) and NH\(_3\).

Photodissociation, cosmic ray interactions, and ion-neutral interactions are the main destructive processes for HCN.

\[
\begin{align*}
\text{HCN} + \nu & \rightarrow \text{CN} + \text{H}^+ \quad \text{[photodissociation]} \\
\text{HCN} + p & \rightarrow \text{CN} + \text{H}^+ \quad \text{[cosmic-ray interaction]} \\
\text{HCN} + \text{HCO}^+ & \rightarrow \text{H}_2\text{CN}^+ + \text{CO} \quad \text{[ion-neutral (low density)]} \\
\text{HCN} + \text{H}^+ & \rightarrow \text{HCN}^+ + \text{H} \quad \text{[ion-neutral (high density)]}
\end{align*}
\]

Many of the products of the destruction processes are in turn reactants for the formation processes, allowing a chemical equilibrium to be reached, dependent on the energetics of the ambient medium.

**Critical Density**

One of the reasons mentioned above for the suitability of HCN as a dense gas tracer is its high critical density. Papadopoulos (2007) gives the relation \( n_{\text{crit}} \propto \mu^2\nu_{J\rightarrow J+1}^3 \), for the critical density of an optically thin line. This comes from considering the average power radiated by an electric dipole. Given its higher dipole moment (\( \mu = 2.98 \, \text{D vs 0.122 D} \)), this allows HCN to trace gas up to 500 times denser than CO.

**Resistance to Freeze-Out**

Carbon bearing species such as CO are highly susceptible to freeze-out (Redman et al., 2002), and cannot trace dense gas reliably. Hily-Blant et al. (2010) find that
HCN remains in the gas phase at densities well above that at which CO depletes onto grains.

### 3.1.1 Hyperfine Structure

The nitrogen atom in HCN is responsible for its distinct hyperfine structure. The large quadrupole moment leads to widely spaced hyperfine lines, especially for the lowest rotational transitions (Walmsley et al., 1982; Sohn et al., 2007; Loughnane et al., 2012). The effect of these hyperfine splittings is to spread out the emission over a wider bandwidth, effectively reducing the optical depth of the parent rotational transition. Furthermore, since the estimates of density temperature and molecular abundance depend on opacity, the hyperfine structure should be considered when analysing spectral line observations. One useful application of the hyperfine structure is the relative strengths of individual hyperfine components can be used to constrain the optical depth independently of the molecular abundance, and independently of the spatial correlation between the telescope beam and the cloud structure, otherwise known as the beam filling factor (Keto & Rybicki, 2010).

The cause of the hyperfine splitting comes mainly from the non-spherical charge distribution of nuclei with spins \( I > \frac{1}{2} \), such as \(^{14}\)N (\( I = 1 \)), and \(^{17}\)O (\( I = \frac{5}{2} \)). The non-spherical distribution of charge in the nucleus leads to a non-zero electric quadrupole moment, which couples with the gradient of the electric field at the nucleus, giving rise to a significant hyperfine structure. There is also a small contribution from the interaction of the nuclear magnetic dipole with the magnetic field generated by the moving charges of the molecule, however, this effect is small compared to the quadrupole interaction.

The hyperfine quantum number, \( F \) is defined as the total angular momentum, such that \( F = J + I \) where \( J \) is the rotational angular momentum quantum number, and \( I \) is the nuclear spin quantum number. \( F \) ranges in value from \(|J+I|...|J-I|\) in what
is known as the Clebsch-Gordon series. For HCN, electric dipole selection rules stipulate that $\Delta F = 0, \pm 1$, and $\Delta J \pm 1$, and since $I=1$, the energy level structure becomes evident. The $J=0$ level remains a singlet, since $F=1$ is the only possible hyperfine level. Each higher level is split into a triplet state, $(F=J-1, J, J+1)$. The number of transitions allowed is therefore, 3 into the $J=0$ level, and six into each higher $J$ level.

### 3.1.2 Hyperfine Anomalies

Observations of the HCN hyperfine lines have shown that for a given rotational level, particularly $J=1 \rightarrow 0$, they are commonly found in ratios that cannot be reproduced by a single excitation temperature, for any optical depth. In other words, they are prone to anomalous line strengths in their hyperfine spectra (Guilloteau & Baudry, 1981; Loughnane et al., 2012). Figure 3.1 shows this using two sets of synthetic line profiles generated using mollie, alongside observations of two anomalous sources, TMC-1 and L1622A2. The models used are extracted from the parameter sweep which will be outlined in Section 3.3.3. These we chosen on visual inspection in order to best show the difference between the expected LTE profiles, and the observed anomalous profiles.

The degree of anomaly in the $J=1-0$ transition of HCN can be characterised by the relative strengths of the individual hyperfine lines using the ratios $R_{02}$ and $R_{12}$ (Cernicharo et al., 1984; Loughnane et al., 2012) where:

$$R_{02} = \frac{F(0 \rightarrow 1)}{F(2 \rightarrow 1)}; \quad R_{12} = \frac{F(1 \rightarrow 1)}{F(2 \rightarrow 1)}$$

(3.1)

The variation in $R_{02}$ (marked $A$ in Figure 3.1) is particularly exaggerated in that the $F=0 \rightarrow 1$ can sometimes exceed the other lines in strength, which could never occur in a single excitation temperature model. HCN hyperfine anomalies are widespread among low-mass star forming molecular clouds and are also evident
Figure 3.1: The upper panels show example radiative transfer models of the lowest four rotational lines of HCN. The left-hand panel shows the expected LTE line strength ratios between the hyperfine components, while the right-hand panel shows anomalous line strengths. The labels A and B denote the JF=10→01, and JF=32→22 transitions, which are susceptible to anomalous hyperfine line strengths. (bottom left) Observation of TMC-1, with the JF = 10→01 transition anomalously boosted. (bottom right) JCMT observation of L1622A2 with the anomalously boosted transition JF=32→22 marked B.

in massive protostellar cores (Pirogov, 1999b; Sohn et al., 2007; Loughnane et al., 2012).

Many theories have been proposed to explain the anomalies, ranging from photon trapping caused by hyperfine components with differing optical depth (Kwan & Scoville, 1975), to scattering of radiation from the core in a moderately dense envelope (Cernicharo et al., 1984), to small scale clumpiness in low mass cores with thermal local line widths (Pirogov, 1999a). However, further investigation shows that the hyperfine lines can be found to vary in width within a single rotational line pattern, and for lines exhibiting dynamical effects such as asymmetric profiles (due
to doppler broadening in moderate opacity gas) the sense of the asymmetry can switch from red to blue within a single observation of a single rotational level (Sohn et al., 2007; Loughnane et al., 2012). These behaviours are all formally impossible to reproduce when HCN is analysed in terms of rotational levels only, and suggests that the radiative transfer of each single hyperfine line must be carried out.

An intriguing feature of the anomalous intensity problem is that C\textsuperscript{17}O, which also exhibits a hyperfine pattern, is not subject to anomalies and agrees with the LTE ratio irrespective of the brightness temperature of the observed medium. Redman et al. (2002) treat the hyperfine structure of C\textsuperscript{17}O as a modification of the rotational lineshape function $\phi(\nu)$, and perform the radiative transfer at the J level only. This will not work for HCN however, as an analysis of the selection rules for electric dipole transitions between J and F levels in HCN reveals that there is only a single pathway leading to the JF = 10→01 transition out of 36 total pathways to the J=0 level. This leaves the transition very susceptible to line overlap effects in the higher J levels, as any photons gained or lost are significant compared to the total photon flux into this transition. These overlap effects prevent a single lineshape function being used at the J-level, and force us to consider radiative transfer of each individual hyperfine F-level line.

Here we describe an F-level radiative transfer calculation that is then used to generate J-level emission line spectra for comparison with anomalous HCN line data. While the line frequencies are measured accurately, and radiative transition rates are well known analytically, determining collisional rate coefficients is a challenging numerical problem. There are different collisional rates available in the literature, involving different approximations. We carried out our radiative transfer calculations using three different sets of rates consisting either of a set of J-level rates (Green & Thaddeus (1974) as updated by Schöier et al. (2005), Vera et al. (2014)), or explicit calculations of the F-level rates (Ben Abdallah et al., 2012). For those rates with only J-levels (Green & Thaddeus, 1974; Vera et al.,
2014), we investigate different methods to calculate collisional rate coefficients for all possible F-level hyperfine transitions.

3.1.3 Molecular Physics of HCN

In order to describe the physical properties of the molecular cloud gas, we must fully take into account the motion of the gas at the microscopic level. We must also consider the relative populations for those levels that are being populated or depopulated as a consequence of the gas dynamics. There are three requirements for a complete treatment:

1. The frequencies of each individual hyperfine transition.
2. The radiative excitation/de-excitation coefficients, for both spontaneous and stimulated emission/absorption, namely the Einstein A and B coefficients.
3. The collisional rates with the two possible spin states ortho and para-H$_2$, He and electrons.

The evaluation of the frequencies of rotational energy levels and contained hyperfine levels of HCN uses the most precise set of spectroscopic constants to date (Ahrens et al., 2002). In that work, they improved on the values determined from molecular beam maser measurements by DeLucia & Gordy (1969), the previously accepted standard spectroscopic constants for HCN. The various constants were sought from both Saturation Lamb dip data as well as from the simultaneous fitting of a selected set of high precision measurements to the detailed hyperfine energy expression. For a Lamb (or saturation) dip measurement, a weak laser beam is sent through an absorption cell and to a detector while a strong laser beam of the same frequency is sent through in the opposite direction. Because these beams are sampling molecules traveling in different directions, they do not interact except in the center of the transition line where the molecules sampled
are traveling perpendicular to the laser beams. Here the detected light sees a dip in absorbance due to saturation of the molecular transition due to the strong counter-propagating beam. The results of these calculations are reproduced in Table 3.1.

In order to account for effects such as masering the Einstein B coefficients must also be known. These are related to the A coefficients by the equation,

$$ A_{ij} = \frac{2\hbar \nu^3}{c^2} B_{ij} \tag{3.2} $$

which arises from detailed balance at thermal equilibrium.

The fourth and fifth columns of Table 3.1 list, respectively, the Einstein A value, and the expected normalized relative intensity for each of the hyperfine transitions. These are given for the five lowest rotational transitions of HCN, the hyperfine lines become blended into one central line as the rotational level increases.

### 3.2 Investigating the choice of collisional rate coefficients.

Radiative rates are readily available and independent of the environment in which the particle is found. Collisional rates, however, are formed from the product of collisional rate coefficients and the population density of the collision partners. The rates are typically calculated for a discrete set of temperatures that can be interpolated between. Ideally, these should be calculated exactly for HCN’s hyperfine structure colliding with an appropriate mixture of ortho- and para-H$_2$, Helium gas, and perhaps electrons (electron rates have been calculated (Faure et al., 2007) but will be negligible for these cloud conditions). One complication is that the potential energy surface (PES) of H$_2$ is complex and must be approximated. HCN collisional rates with Helium have been calculated for transitions between rotational levels. These are then scaled to approximate the mixture of hydrogen and
Table 3.1: Spectroscopic values for hyperfine components of the lowest 5 downward J-level transitions, listed in ascending frequency. Here J is the upper and J’ the lower level and $R_{JF \rightarrow J'F'}$ is the relative intensity of the hyperfine transition compared to the parent rotational transition. Data from Ahrens et al. (2002).

<table>
<thead>
<tr>
<th>J F</th>
<th>J'F'</th>
<th>Frequency (GHz)</th>
<th>$A_{JF \rightarrow J'F'}$ ($10^{-5} \text{s}^{-1}$)</th>
<th>$R_{JF \rightarrow J'F'}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 1</td>
<td>0 1</td>
<td>88.630413</td>
<td>2.405060</td>
<td>0.3333</td>
</tr>
<tr>
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<td>0 1</td>
<td>88.631846</td>
<td>2.405177</td>
<td>0.5555</td>
</tr>
<tr>
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<td>0 1</td>
<td>88.633935</td>
<td>2.405347</td>
<td>0.1111</td>
</tr>
<tr>
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<td>1 2</td>
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<td>5.772518</td>
<td>0.0833</td>
</tr>
<tr>
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<td>12.826738</td>
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</tr>
<tr>
<td>2 3</td>
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</tr>
<tr>
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</tr>
<tr>
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</tr>
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</tr>
<tr>
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</tr>
<tr>
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<td>83.493759</td>
<td>0.4286</td>
</tr>
<tr>
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</tr>
<tr>
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<tr>
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<td>3 4</td>
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</tr>
<tr>
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</tr>
<tr>
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</tr>
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<td>100.195394</td>
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<tr>
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<td>4 5</td>
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<td>81.978097</td>
<td>0.3935</td>
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<td>443.116194</td>
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</tr>
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<td>5 4</td>
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<td>1.821738</td>
<td>0.0001</td>
</tr>
<tr>
<td>5 4</td>
<td>4 4</td>
<td>443.118063</td>
<td>20.039348</td>
<td>0.0133</td>
</tr>
</tbody>
</table>
helium (Green & Thaddeus, 1974; Monteiro & Stutzki, 1986), and more recently Dumouchel et al. (2010). Ben Abdallah et al. (2012), and more recently Vera et al. (2014) have directly calculated collisional rates for HCN with para-H\(_2\). The rates of Ben Abdallah et al. (2012) include explicitly calculated hyperfines, however the colliding partner is a structureless potential energy surface, which Vera et al. (2014) have improved upon, and shown to diverge by up to 50\% from their calculations, especially at low temperatures. Hyperfine rates using this new surface are in the process of being calculated. We will present an approximation to these rates, in which the J-level rates calculated by Vera et al. (2014) are scaled to the same ratios as the F-level rates of Ben Abdallah et al. (2012). We first outline the long-standing formalism to extract hyperfine rate coefficients from rotational rate coefficients using the proportional method.

### 3.2.1 The Proportional Method

For rates with only rotational J-levels given (Green & Thaddeus, 1974; Monteiro & Stutzki, 1986; Dumouchel et al., 2010; Vera et al., 2014), it is possible to use the ‘proportional method’ to calculate collisional rate coefficients for all possible F-level hyperfine transitions, as initially suggested by Guilloteau & Baudry (1981). In the proportional method, the rates between each of the individual hyperfine levels are approximated as fractions of the net rotational collisional rate, scaled to the statistical degeneracy of the final hyperfine level. As the degeneracies of the hyperfine lines for a given rotational transition are different, the corresponding collisional coefficients will also be different. Stutzki & Winnewisser (1985) suggested that this could be a possible underlying trait of the anomalies with the hyperfine lines excited selectively based on their collisional coefficients. Thus the average net rates \(R_{\text{J,J'}}\) between rotational states, \(J, J'\), are specified by way of a weighted sum over the hyperfine rate coefficients,

\[
C_{J\to J'} = \sum_{FF'} \frac{2F + 1}{3(2J + 1)} R_{JF\to J'F'},
\]

(3.3)
where we have implicitly assumed that the initial hyperfine states are occupied in proportion to their statistical weights. It follows that in the absence of the individual hyperfine collisional rate coefficients, the coefficients may be approximated assuming that each rate is proportional to the statistical weight of the final level (Keto & Rybicki, 2010). In the case of HCN, these approximations for the rate coefficients take the form,

$$C_{JF \rightarrow J'F'} = \frac{2F' + 1}{3(2J' + 1)} R_{JJ'}, \quad (3.4)$$

where the factor of 3 in the denominator comes from the statistical degeneracy of the nuclear spin quantum number (I = 1), giving (2I+1) = 3. We use rotational collisional rate coefficients C(J → J') from Green & Thaddeus (1974) extrapolated and updated, as presented in Schöier et al. (2005). These are HCN-He rates and so must be scaled by a factor of 1.37 for collisions with para-H$_2$.

The rates scaled in this way can be completed with the inclusion of quasi-elastic rates where the rotational level does not change: ΔJ = 0, ΔF ≠ 0. These quasi-elastic rates were acquired through an empirical approximation for the rotational rate coefficients made by de Jong et al. (Eq.(17) 1975),

$$C(J \rightarrow J') = a(\Delta J) \frac{2J' + 1}{2J + 1} \left(1 + \frac{\Delta E_{JJ'}}{kT}\right) \times \exp \left[-b(\Delta J) \left(\frac{\Delta E_{JJ'}}{kT}\right)^{1/2}\right]. \quad (3.5)$$

For each of the 14 temperatures analysed between T=5 and 1200 K inclusive, the fitting function, Eq. (3.5), was manipulated so that the fitting variables a(ΔJ) and b(ΔJ) could be evaluated:

$$\ln \left[C(J \rightarrow J') \frac{g_J}{g_{J'}} \frac{1}{1 + \Delta E_{JJ'}/kT}\right] = \ln [a(\Delta J)] - b(\Delta J) \left(\frac{\Delta E_{JJ'}}{kT}\right)^{1/2}. \quad (3.6)$$
The resultant equation, Eq. (3.6), is a straight line, $y=mx+c$. A set of plots was obtained for each value of $\Delta J$ by plotting the LHS of Eq. (3.6) against $(\Delta E/kT)^{1/2}$. (see Figure 3.2) A least squares linear fit was performed where the coefficients $b(\Delta J)$ and $\ln[a(\Delta J)]$ are given by the slope and y-intercept of this fit, respectively.

Once the list of $a$ and $b$ fitting coefficients were collected for a particular temperature and $\Delta J$, each was plotted versus $\Delta J$ so that an interpolation of the values present could be performed. The y-intercept following such an interpolation, as demonstrated in Figure 3.3, translates to the fitting coefficient corresponding to $\Delta J$. 

**Figure 3.2**: The linear plot of Eq.(12) for $\Delta J=5$ and $\Delta J=15$, respectively, at $T=40K$ (left) and $T=400K$ (right), where on the y-axis, $A(T) = (g_J/g_{J'} \times 1/[1 + (\Delta E_{J,J'}/kT)])$. Created by Robert Loughnane, as appears in Mullins et al. (2015).
3.2.2 Direct Scaling of Vera et al. (2014) rates

For the rates of Vera et al. (2014), although they are calculated at the J-level only, they use the same PES as the rates of Ben Abdallah et al. (2012), but consider also the structure of the H$_2$ colliding partner. This makes the calculation of exact F-level rates much more demanding. However, an approximation can be made by combining the two sets of rates together. Treating the F-level splitting as a perturbation on the J-level calculation, we generate a set of F-level rates based on

![Figure 3.3: Interpolation of fitting coefficients for ln[a(ΔJ)] at T=40K (left) and T=400K (right) (Eq. 3.6). The linear interpolation was carried out in order to calculate rates for ΔJ=0. There is a strong preference for even ΔJ-transitions reflecting the obvious propensity rule for such transitions with this particular species. Created by Robert Loughnane, as appears in Mullins et al. (2015).](image)
the rates of Vera et al. (2014) by taking the parent J-level coefficients and scaling them into the same proportions as the F-level rates calculated by Ben Abdallah et al. (2012), while maintaining the relation

$$\sum_{F'} k_{JF'\to J'F'}(T) = k_{J-J'}(T)$$

where \( k_{JF'\to J'F'}(T) \) are the hyperfine rate coefficients, and \( k_{J-J'}(T) \) are the rotational rate coefficients (Faure & Lique, 2012). Table 3.2 gives an example of this calculation.

**Table 3.2:** An example of the scaling of the Vera et al. (2014) rates, for the hyperfine states in the \( J = (2\to1) \) transition. \( i \) and \( j \) represent the initial and final hyperfine state respectively, and \( \text{bA Rates} \) are the rates of Ben Abdallah et al. (2012). All rates are in units of cm\(^3\) s\(^{-1}\).

<table>
<thead>
<tr>
<th>( i )</th>
<th>( j )</th>
<th>( \text{bA Rates} )</th>
<th>Proportions</th>
<th>( \text{Vera Rate} )</th>
<th>( \text{Scaled Rates} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>2</td>
<td>4.81E-12</td>
<td>0.683529</td>
<td>2.20E-11</td>
<td>1.50E-11</td>
</tr>
<tr>
<td>5</td>
<td>3</td>
<td>1.64E-12</td>
<td>0.233055</td>
<td>2.20E-11</td>
<td>5.13E-12</td>
</tr>
<tr>
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<td>0.083133</td>
<td>2.20E-11</td>
<td>1.83E-12</td>
</tr>
<tr>
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<td>0.461844</td>
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</tr>
<tr>
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</tr>
<tr>
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</tr>
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</tr>
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<td>1.77E-12</td>
<td>0.251529</td>
<td>2.20E-11</td>
<td>5.52E-12</td>
</tr>
</tbody>
</table>

We find that Vera et al. (2014) rates, both by the proportional method, and by the direct scaling method can readily reproduce the observed hyperfine anomalies of the low mass core TMC-1 as shown in Figure 3.4. We find similar results for the rates of Schöier et al. (2005), an update on Green & Thaddeus (1974), with the proportional method applied, and supplemented with our quasi-elastic rates. We find however, that the Ben Abdallah et al. (2012) rates on their own do not reproduce these observations as well as can be seen in Figure 3.4 where both sets of approximate rates are shown to better replicate the anomalies for the cloud TMC-1. This is noteworthy because Faure & Lique (2012) have argued, on the basis of the Ben Abdallah et al. (2012) calculations, that the proportional method may
be unsound because ‘statistical rates’ would lead to saturation in the hyperfine spectra at \( n(\text{H}_2) \sim 10^6\text{cm}^{-3} \). However, Vera et al. (2014, see Fig. 5) show a large difference in the coefficients between the Ben Abdallah et al. (2012) rates, and their rates, especially at the low temperatures typical of low mass star forming cores. We do note, however, that the results of our parameter sweep are largely unaffected by the choice of rates, which supports our assertion that carrying out radiative transfer over each F-level individually is essential.

We note also that the proportional method approach has been applied to the linear radical \( \text{N}_2\text{H}^+ \) by Keto & Rybicki (2010), and in that work they verify the validity of the proportional method in its ability to reproduce the non-LTE hyperfine intensities in the Taurus dark cloud, L1512. Keto & Rybicki (2010) simulated observational data towards the L1512 starless core using hyperfine collisional rate coefficients derived using the theoretically-based study of Daniel et al. (2005) and contrasted the results with simulations using the statistically weighted coefficients. Both methods produced results that were similar to the accuracy expected from observations.

While acknowledging that forthcoming rates based on the PES presented in Vera et al. (2014) will represent the foremost rates for the HCN molecule when published, we use the scaled version of their J-level rates in all the presented calculations below, alongside the proportional method applied rates of Green & Thaddeus (1974). We note however, that the proportional method applied to Vera et al. (2014) give very similar results, while converging slightly faster than the direct scaled rates. The central finding however, irrespective of the choice of collisional rate coefficients, is that the individual F-levels must be treated separately in a radiative transfer code, in order to reproduce the anomalous HCN spectra.
3.3 Radiative Transfer Modeling of HCN anomalies

We use the above radiative and collisional rates for the hyperfine lines of HCN to modify the fully parallelised 3D radiative transfer code MOLLIE (Keto et al., 2004), (outlined in the previous chapter), to calculate the strength and shape of each individual hyperfine line, including the effects of line overlap. MOLLIE is fully benchmarked against the test problems described in van Zadelhoff et al. (2002). Note that an alternative 1D or 2D non-LTE radiative transfer code (Brinch & Hogerheijde, 2010; Juvela, 1997), using the collisional and radiative rates above, should be able to reproduce the spherically symmetric model results we present here.

3.3.1 Model of the prototypical low mass source TMC-1

TMC-1 is a low mass star forming source in the Taurus Molecular Cloud, in which Walmsley et al. (1982) first observed the hyperfine anomalies in HCN. We have fitted a simple model of the J=1→0 transition of HCN in TMC-1, using data obtained from Sohn et al. (2007) observations. In Figure 3.4, we show first order fits to the observed spectrum for different sets of collisional rates. In this model, we use as a starting point the densities, temperatures and abundances as measured by Pratap et al. (1997). Our model is a sphere of constant density, and temperature, with a low turbulent width, which is slowly infalling. Table 3.3 outlines the parameter values used. It is notable straight away that the anomaly can be reproduced to first order, in a manner which is formally impossible in a radiative transfer treatment which considers only the rotational energy structure. We do not attempt a more detailed model of TMC-1 here, and note that more complex and realistic cloud dynamics can be implemented in low mass cores including rotation, outflows and freeze-out (Carolan et al., 2008). The simple model here is
Figure 3.4: Model (dashed line) of J=1→0 line of HCN for the cloud TMC-1 for each of the different sets of rate coefficients listed in the legends. These are overlaid onto observed data (solid line) from Sohn et al. (2007). The rates of Vera et al. (2014) (bottom panel) give the best fits to the observed data, with either method of hyperfine rates.

shown to illustrate that it should be readily possible to model the HCN line ratios in similar low mass sources, such as those seen in the data sets of Sohn et al. (2007); Loughnane et al. (2012). We once again note the poorest fit is given by the rates of (Ben Abdallah et al., 2012), while the choice of method for extracting hyperfine rates from the data of (Vera et al., 2014) is shown to be insignificant in this case, as both produce adequate fits. We find that a good approximation for the hyperfine rates, is superior to a poor direct calculation.
Table 3.3: Physical Parameters for TMC-1 model. Errors indicate flexibility in choice of model parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Model Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (cm$^{-3}$)</td>
<td>$6 \pm 0.5 \times 10^4$</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>$8 \pm 0.5$</td>
</tr>
<tr>
<td>Turbulent Velocity(cm s$^{-1}$)</td>
<td>$1.2 \pm 0.2 \times 10^3$</td>
</tr>
<tr>
<td>Infall Velocity (cm s$^{-1}$)</td>
<td>$1 \pm 0.2 \times 10^3$</td>
</tr>
<tr>
<td>Abundance (n(HCN)/n(H$_2$)) - (Green&amp;Thaddeus)</td>
<td>$2.75 \pm 0.25 \times 10^{-9}$</td>
</tr>
<tr>
<td>Abundance (n(HCN)/n(H$_2$)) - (Vera)</td>
<td>$2.75 \pm 0.25 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

3.3.2 Red-blue asymmetry switching in double-peaked line profiles

Doppler shifting of gas components in a molecular cloud that is undergoing dynamical processes such as collapse, expansion or rotation can lead to double-peaked line profiles. In optically thick clouds, there can be an asymmetry in the strength of the peaks. In particular, for a collapsing cloud the blue wing of the line profile can be stronger than the red wing (Evans, 1999). However, as another manifestation of the HCN anomalies concerns the red-blue asymmetry of some hyperfine lines such as those seen in Fig. 3.5, and in L234E-S by Schnee et al. (2013, see their Fig. 1). The asymmetries are observed to switch across the hyperfine lines within the $J = 1 \rightarrow 0$ level, with one line having the opposite asymmetry to the other two lines. Again, this is formally impossible to reproduce in an analysis of the HCN spectrum by rotational level only.

Using the MOLLIE HCN hyperfine treatment, an exploration of the parameter space reveals that this effect is due to an interplay between self-absorption and infall. For a model of constant parameters (velocity, density, turbulence, temperature, and abundance) and with a high optical thickness, even a slight infall velocity begins to present asymmetry switching which is only strengthened as the infall velocity is raised. The asymmetry switching can also be strengthened or weakened by increasing or reducing the degree of self-absorption (respectively) by
altering the density or abundance of the model. With further work this could be developed into a sensitive diagnostic tool. The model used to produce Fig. 3.5 is that of a simple sphere of radius 0.04 pc with constant temperature (7 K), density $5.5 \times 10^5$ cm$^{-3}$, abundance of $7.5 \times 10^{-10}$ HCN:H$_2$ and turbulence (2.5 km s$^{-1}$). The velocity goes as $v(r) = v_0(r/0.4R)^{-0.5}$ with $v_0$ of -5 km s$^{-1}$. This temperature regime, velocity gradient, and radius are taken from modelling papers looking at low mass pre-stellar cores such as Park et al. (2004) and Lee et al. (2004), while the abundance was chosen to generate the strongly self-absorbed profiles typically seen in observations such as those in Figure 3.5.
The effect on the asymmetry switching of including quasi-elastic rates was also investigated, with Figure 3.6 showing that their inclusion is crucial in order to reproduce the effect.

As can be seen in Fig. 3.6, the anomaly cannot be seen in the non-quasi-elastic dotted line models. It appears in the solid line model which includes the quasi-elastic rates. It can also be seen that in the J=(2→1) line, the F= 1→2 hyperfine (the small peak between the left and centre peaks), which should normally be of the order 1000 times smaller than the central peak (see Table 3.1), is anomalously boosted in the same conditions as produce this red-blue asymmetry switching.
Table 3.4: Sampling of Parameter Space for Green & Thaddeus (1974).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
<th>No. of Steps</th>
<th>Typical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density ($n_{H_2}$)</td>
<td>$1 \times 10^3 - 8 \times 10^6$ cm$^{-3}$</td>
<td>12</td>
<td>$1 \times 10^4$ cm$^{-3}$</td>
</tr>
<tr>
<td>Temperature ($T_{\text{kin}}$)</td>
<td>6, 8, 10, 12, 15, 25, 40 K</td>
<td>7</td>
<td>12 K</td>
</tr>
<tr>
<td>Abundance ($\chi_{\text{HCN}}$)</td>
<td>$1 \times 10^{-11} - 7 \times 10^{-9}$</td>
<td>12</td>
<td>$1 \times 10^{-11}$</td>
</tr>
<tr>
<td>Infall velocity ($v_{\text{inf}}$)</td>
<td>0, 0.3, 0.6, 0.9 kms$^{-1}$</td>
<td>4</td>
<td>0.3 kms$^{-1}$</td>
</tr>
<tr>
<td>Turbulent width ($\Delta v_{NT}$)</td>
<td>0.1, 0.2, 0.3 kms$^{-1}$</td>
<td>3</td>
<td>0.3 kms$^{-1}$</td>
</tr>
</tbody>
</table>

Table 3.5: Sampling of Parameter Space for Vera et al. (2014).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Range</th>
<th>No. of Steps</th>
<th>Typical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density ($n_{H_2}$)</td>
<td>$1 \times 10^4 - 7 \times 10^6$ cm$^{-3}$</td>
<td>9</td>
<td>$1 \times 10^4$ cm$^{-3}$</td>
</tr>
<tr>
<td>Temperature ($T_{\text{kin}}$)</td>
<td>6, 10, 15, 25, 40 K</td>
<td>5</td>
<td>12 K</td>
</tr>
<tr>
<td>Abundance ($\chi_{\text{HCN}}$)</td>
<td>$1 \times 10^{-11} - 7 \times 10^{-9}$</td>
<td>9</td>
<td>$1 \times 10^{-11}$</td>
</tr>
<tr>
<td>Infall velocity ($v_{\text{inf}}$)</td>
<td>0, 0.1, 0.5, 1.0 $\times$ $\Delta v$</td>
<td>4</td>
<td>0.3 kms$^{-1}$</td>
</tr>
<tr>
<td>Turbulent width ($\Delta v_{NT}$)</td>
<td>0.1, 0.15, 0.2 kms$^{-1}$</td>
<td>3</td>
<td>0.2 kms$^{-1}$</td>
</tr>
</tbody>
</table>

3.3.3 Parameter sweep across low-mass star forming conditions

The MOLLIE HCN hyperfine implementation seems to readily reproduce individual sources and be able to account for effects such as asymmetry switching. To use this treatment to widen the investigation of the anomalies, a parameter sweep through the 5 free parameters of the code was performed, for both the proportional method rates of Green & Thaddeus (1974) and the direct scaling rates of Vera et al. (2014), to investigate the physical conditions which cause the anomalies to be present. Table 3.4 below outlines this parameter space, and the sampling associated with each of the parameters for the proportional method applied to the rates of Green & Thaddeus (1974), while Table 3.5 does the same for the direct scaling of the rates of Vera et al. (2014).

For each unique set of parameters, a simple model of a spherical cloud was run, with density, temperature and velocity profiles as outlined in Table 3.6.
### Table 3.6: Functional Form of Physical Parameters for TMC-1 model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>$T(r) = \frac{T_0}{2} \left(\frac{r+1}{r}\right)$</td>
</tr>
<tr>
<td>Density</td>
<td>$n(r) = \frac{n_0}{5} \left(\frac{3r+2}{r}\right)$</td>
</tr>
<tr>
<td>Velocity</td>
<td>$v(r) = v(x,y,z) = \sqrt{\frac{T_0}{r}}$</td>
</tr>
</tbody>
</table>

Once the parameter sweep was completed, we investigated the effect on the anomalous ratios, $R_{02}$ and $R_{12}$ when each parameter was varied. Fig. 3.7 shows the variation of $R_{02}$ as a function of each free parameter. There is a clear trend in the density plots showing that for a range of densities from $10^5$ to $10^6$ cm$^{-3}$ any value of $R_{02}$ is possible, depending on the other parameters. Low densities tend towards the LTE optically thin case of $0.2$, with some variation, while high densities tend towards the optically thick LTE value of $1$, again with some variation. A bimodal distribution becomes clear at the high abundances for the proportional method rates, where the values tend towards the two LTE cases. This is less clear with the scaled rates, however, but shows that the amount of HCN along the line of sight is the crucial factor, as expected, and also that the distribution tends towards the two LTE regimes, depending on the combination of the other parameters. The infall and temperature showed little effect in restricting the anomalous ratio, there was a slight preference towards lower temperatures for the most anomalous profiles in the proportional method, and a much more pronounced effect was seen using the scaled rates. This trend can be shown more clearly by the plot in Figure 3.9.

Two of the variables in the plots in Figure 3.7 were density and abundance. Conveniently, the product of these two variables is of major physical significance, it is the density of HCN in the cloud, which we will refer to as the HCN density ($\chi_{mol} n_{H_2}$). We can use this parameter to constrain the optical depth of the cloud and see how the anomalous ratios vary with it. The optical depth is given by $\tau \propto \chi_{mol} n_{H_2} \Delta s \kappa_\nu$, where $\Delta s$ is the distance along the line of sight, $\chi n_{H_2}$ is the density of the molecule of interest, and $\kappa_\nu$ is the opacity of a transition of frequency...
Figure 3.7: Variation of $R_{02}$ with Density (top), Abundance (middle) and Temperature (bottom) for the rates of Green & Thaddeus (1974) on the left, and Vera et al. (2014) on the right. Each small cross represents an individual model run.
\( \nu \). Since we have adopted a spherically symmetric model, with a constant line of sight for each run - and provided that the infall velocity is held constant, fixing the transition frequency, and thus the opacity - the value of HCN density can then be used as a direct proxy for the optical depth.

The plots in Figure 3.8 show the possible values of \( R_{02} \) and \( R_{12} \) as a function of HCN density for a fixed value of the infall velocity in each parameter sweep. What we see, is that for low values of the HCN abundance density, the values of \( R_{02} \) and \( R_{12} \) are in line with the expected LTE values of 0.2 and 0.6 respectively. As the density (and thereby the optical depth) increases, we begin to see a range of possible values emerge. Similar trends can be seen for \( R_{12} \). Also worth noting is the sharp transition at \( \rho_{\text{hcn}} = 1 \times 10^{-4} \) which is visible in all plots. This shows the transition from optically thin to optically thick, above which the anomalies...
tend towards the LTE value of 1. These plots clearly highlight the importance of the optical depth on the observed ratios.

In Figure 3.7 we showed there was a temperature dependence for the anomaly. This can be shown much more readily in a 3D scatter plot, where the cumulative effect of three parameters can be plotted. Figure 3.9 shows the values of $R_{02}$ for a constant infall velocity of $0.3 \text{ km s}^{-1}$ and two values for abundance, $1 \times 10^{-11}$ (left) and $1 \times 10^{-10}$ (right). The colour of each point on the plot represents the $R_{02}$ value for that point as indicated on the colour bar to the right. It can clearly be seen in these plots that the anomalies show a propensity towards low temperature, high density gas, typical of low mass star forming cores. With the increase in the abundance of the left-hand plots, and thereby the optical depth, by a factor of ten, there is a clear shift of the same pattern towards lower densities, with the “anomalous zone” spreading outwards.

### 3.4 Conclusions

We have demonstrated the anomalous behaviour of the $J= 1 \rightarrow 0$ line of HCN, and replicated both the observed anomalies in TMC-1, and the red-blue asymmetry switching typical of sources such as L1512B2, L234E-S and L204C-2. These effects have emerged from simple first order models, through applying radiative transfer using the proportional method, and including quasi-elastic ($\Delta F=0$) collisional rates as calculated in §3. Through a wide ranging parameter sweep we have demonstrated that the satellite lines of the $J=1 \rightarrow 0$ transition are highly unstable to changes in optical depth, and cannot be relied on to infer physical properties.

Based on our investigations, we suggest the following guidelines for interpreting HCN observations and for including HCN in radiative transfer codes.

- The radiative transfer of HCN must be carried out over each F level individually.
Figure 3.9: 3D scatter plots of Density, Temperature and Infall Velocity, with two different abundance values, $1 \times 10^{-11}$ (left), and $1 \times 10^{-10}$ (right), for each set of rates, Vera et al. (2014) (top) and Green & Thaddeus (1974) (bottom). The colour-bar represents the value of the anomalous ratio $R_{02}$. The “anomalous zone” represented by the lighter coloured points is seen to be in the low temperature, high density corner of the cube, and is larger in the lower abundance cases. The “super-anomalous” cases ($R_{02} > 1$) are much more common with the new rates.

- The choice of collisional rates is significant. Good approximations to lower resolution calculations such as the proportional method, are shown to be consistent with both observed data and each other. The high resolution calculations of Ben Abdallah et al. (2012) are shown to be flawed in their assumption of a structureless colliding partner.

- For now, we recommend the use of the new rates of Vera et al. (2014), scaled to the same proportions as the rates of Ben Abdallah et al. (2012). They have been shown to generate good matches to observations, readily reproducing the spectrum of TMC1, and also replicating the observed “super-anomalous”
ratios seen in sources such as L1197 (Loughnane et al., 2012). We anticipate the forthcoming exact rates based on their PES to supersede these rates when they are released, and become the standard for HCN collisional rates.

• In the J= 1→0 transition, the F=(0→1) line is unreliable as a diagnostic of infall or dynamics. The central (F=2→1) line however is more robust and when it is resolved, it should be reliable as a dynamical tracer.

• The J=2→1 line is not usually observed due to its frequency location. However, it has been previously detected using IRAM (Daniel et al., 2013) and will be detectable with ALMA band 5 observations. The hyperfine components of this line are neither widely separated enough or centrally concentrated enough to be easily interpreted, and the line pattern will then be distorted further by the anomalies. The example model line in Figure 3.1 can be compared with the observation of the B1b low mass core carried out by Daniel et al. (2013, see Fig. 13), to illustrate this point. It may be useful for some calculations to compare the integrated intensity of this line with other transitions.

• In the J=3→2 line, the central component is actually four overlapping hyperfine components, and these can sometimes present as overly large infall signatures, particularly if interpreted as a single peak. The expected insignificant F=2→3 component is boosted into detectability by the anomaly, as can be seen by its intrinsic line strength in Table 3.1. This contributes to the distorted line shape of the central component. This can be seen by comparing the line width of the central components in the J=1→0 and J=3→2 transitions in the top left panel of Fig. 3.1.

• For massive star forming regions the problem is worse as the central component of the J=3→2 line may be partially blended with the satellite line marked B in Fig. 3.1. This can also present as a double peaked profile, which not only should not be used as a measure of the infall velocity, but also has a misplaced centroid velocity [see Figure 15 from Carolan et al. (2009)].
For the above reasons we strongly advise against the use of the $J=3\rightarrow 2$ line of HCN as a dynamical tracer, and advise that caution be used with $J=1\rightarrow 0$, using only the central component.

Finally, Keto & Rybicki (2010) have shown that a similar F-level radiative transfer treatment is required for $\text{N}_2\text{H}^+$, so we expect that all end N-bearing species such as HC$_3$N and the cyanopolynes, NO and NH$_3$ could be susceptible to hyperfine anomalies, and these represent a target for future work. The central positive conclusion is that it is readily possible to reproduce the anomalous HCN spectrum, if the radiative transfer is carried out over individual hyperfine lines.
Chapter 4

Effects of Massive Stars: The Swept Up Shell RCW120 & The Vela Molecular Ridge RCW36.

“Discover the force of the skies O Men: once recognised it can be put to use.”

- Johannes Kepler,

Epitome of Copernican Astronomy and Harmonies of the World.

4.1 Introduction

The effects of massive stars ( $M > 8 \, M_\odot$) on their surroundings are significant. Through their stellar winds and ionising photons, they can shape the gas around them. This occurs from very early in their life cycles since hydrogen burning ignites while massive stars are still deeply embedded in their nascent clouds. The ionising radiation sweeps out a shock bounded area of ionised gas known as a H II region, while the stellar wind applies an additional radiation pressure to the gas. Furthermore, at the end of a massive star’s life cycle, the resulting Type II
supernova explosion adds further energy to the surroundings in times much shorter than the sound crossing time.

In this chapter we will consider the effects of massive stars on their surroundings, and how this can lead to triggered star formation. Examples of possible triggered star forming regions will be presented, RCW120 and RCW36.

### 4.2 Effects of Massive Stars

Consider a massive star contained within the cloud from which it formed. For simplicity, assume a cloud of pure molecular hydrogen. The UV flux emanating from the star can both dissociate the molecular gas, and ionise the subsequent atomic gas. At the same time, the created protons and electrons are recombining upon impact with each other, creating two conflicting processes, ionisation and recombination, each with its own associated rate.

\[
H_2 + 3\gamma \rightarrow H^+ + e^-
\]

Each ionisation event removes photons from the beam, meaning that for a star of a fixed UV output, only a limited volume may be ionised. For a medium of uniform density, the ionisation spreads isotropically into the simplest case for a H II region, the Strömgren sphere. Noting that ionisation balance holds at each location with the region, this allows us to say that the volumetric rate of recombination of free electrons and protons in a particular parcel of gas, is just offset by the rate of ionisation. Integrating over the whole sphere, the total rate of recombinations must equal the total rate of ionising events, which by definition must be the ionising flux emitted by the star, i.e. the rate of emission of photons with energy greater than 13.6 eV (\(\lambda < 91.2\) nm), the ionisation potential of H gas.
Consider a recombination coefficient $\alpha_{\text{rec}}(T)$, the recombination rate per unit volume is given by

$$R = n_e n_p \alpha_{\text{rec}}(T) = n_e^2 \alpha_{\text{rec}}(T)$$

(4.1)

Here we have assumed total charge neutrality in the ionised plasma ($n_e = n_p$). The total rate of recombinations in the sphere is simply this volumetric rate, integrated over the total volume, again for simplicity uniform densities and temperatures are assumed. Ionisation balance dictates that

$$N_s = \frac{4\pi}{3} n_e^2 \alpha_{\text{rec}}'(T) R_s^3$$

$$R_s = \left[ \frac{3N_s}{4\pi \alpha_{\text{rec}}'(T)n_e^2} \right]^{1/3}$$

(4.2)

$R_s$ is called the Strömgren radius, and $\alpha_{\text{rec}}'(T)$ is a recombination coefficient which discounts recombinations to the $n=1$ state of atomic hydrogen, which produces another ionising photon and thus no net recombination occurs. Since inside the H II region the probability per unit time of recombination is much less than that of ionisation, the neutral density must be far less than the ionised density in order for the volumetric rates to be equal. This leaves a hot, almost totally ionised interior, surrounded by the neutral material.

We treat the ionisation front as being a sharp discontinuity, since the transition from totally ionised to totally neutral occurs over a multiple of the mean free path of the ionising photons in the neutral medium (Dyson & Williams, 1980). This is much less than $R_s$. The Strömgren sphere is not a static entity, initially there is no H II region, once the massive star begins to emit its ionising photons, there is a quick expansion to $R_s$, followed by a slower expansion beyond this.

This expansion happens quickly, since for $R < R_s$ the total recombinations within the H II region cannot balance the total ionising output of the star. Ionising photons will therefore reach the edge of the H II regions, the ionisation front. These photons further ionise the gas at the front, and so the front expands.
Figure 4.1: Spreading of the ionisation front from R to R+dR, into a cloud of hydrogen density $n^0_H$. For every three photons which cross the front, two ionisations occur. The photodissociation requires $E_{\gamma} > 14.7 \text{ eV}$, while each ionisation requires $E_{\gamma} > 13.6 \text{ eV}$.

Considering the set up in Figure 4.1, where $F_*(t)$ is the photon flux reaching R with $E_{\gamma} > 14.7 \text{ eV}$, which we assume is practically the same as the flux with energies greater than 13.6 eV. Over a time $\Delta t$ the front advances by $\Delta R$, engulfing $n^0_H \Delta R$ hydrogen molecules per unit area, thus creating $2n^0_H \Delta R$. $F_\ast \Delta t$ photons pass R, with 3 photons for every two ionisations.

$$\frac{F_\ast \Delta t}{2n^0_H \Delta R} = \frac{3}{2} \tag{4.3}$$

$$\frac{dR}{dt} = \frac{F_\ast}{3n^0_H} = \frac{2F_\ast}{3n^0_H} \tag{4.4}$$

Considering now the rate of recombinations within the spreading H II region, this also represents the rate at which photons are lost to ionisation, and since $4\pi R^2 F_\ast$ is the rate of photons crossing the boundary, we can say

$$\mathcal{N}_\ast = 4\pi R^2 F_\ast - \frac{4\pi}{3} n_e^2 a'_{rec} R^3 \tag{4.5}$$
which gives

\[
\frac{dR}{dt} = \frac{N_s}{6n_0^6\pi R^2} - \frac{2}{9}n_0^6\alpha_{rec}'R \tag{4.6}
\]

Changing to dimensionless variables \(\lambda = R/R_s\) and \(\tau \equiv t/t_{rec}\), where

\[
t_{rec} \equiv \frac{1}{n_0^6\alpha_{rec}'} \simeq 61 \text{ yr} \left( \frac{n_{H_2}}{10^3 \text{ cm}^2} \right)^{-1}
\]

gives,

\[
\frac{d\lambda}{dt} = \frac{2}{9\lambda^2} - \frac{2\lambda}{9} \tag{4.7}
\]

Using \(\lambda(0) = 0\) as a boundary condition, gives the solution

\[
\lambda = \left[ 1 - e^{-2/\tau} \right]^{\frac{1}{2}} \tag{4.8}
\]

which is known as an \(R\)-type ionisation front.

Using the example case of \(\tau=3/2\), gives \(\lambda=0.86\), in \(\sim 10^2\) years. The average expansion speed here is extremely fast (\(\sim 10^3\) km s\(^{-1}\)). In this early phase, the sound speed in the ionised gas (\(T\sim 10^4\) K) is \(~10\) km s\(^{-1}\), which is the speed at which pressure disturbances can travel, so the density has no chance to re-adjust as the ionisation front speeds past.

As \(R \rightarrow R_s\) the expansion slows following Eq. 4.6, the pressure difference is able to drive a second, slower phase of expansion, which manifests as a shock front preceding the ionisation front in the molecular gas, this time known as a \(D\)-type ionisation front. A thin shell of neutral material exists between the two fronts, whose emission is dominated by the photodissociation of its molecules by the ionisation front. This area is known in observations as the PDR, which can stand for either, \textit{photodissociation region} or the \textit{photon dominated region}. Such structures when observed are known as rings or bubbles, and the next section will outline these observations.
Figure 4.2: Second expansion phase of a H II region. Ionised gas surrounded by a shell of neutral material. The shell advances supersonically, creating an expanding shock front.

4.3 Bubbles/Rings around H II Regions

Observations of the Galactic plane at 8.0 $\mu$m by Spitzer-GLIMPSE (Benjamin et al., 2003b) revealed in the region of 600 infrared (IR) rings/bubbles (Churchwell et al., 2006, 2007). This number was increased to almost 6000 by the work of Simpson et al. (2012), and further extended to over 8000 by Anderson et al. (2014) through use of the Widefield Infrared Survey Explorer (WISE; Wright et al., 2010). Deharveng et al. (2010) find that nearly all bubbles enclose H II regions, while Anderson et al. (2011) find that nearly half of all H II regions are bubbles. This common, symmetric shape for observed H II regions indicates almost uniform expansion, at least in the later stages of their evolution. Peters et al. (2010) and Roth et al. (2014), through hydrodynamical simulations and analytical methods respectively, show that at the very earliest stages the expansion of these regions, and their morphologies are far from uniform. These ultra-compact, and hyper-compact H II regions are the precursors to the ridges, rings and bubbles we will discuss.

The 8.0 $\mu$m emission from the Spitzer observations traces the PDR of a HII region and surrounds the ionised gas. It is commonly assumed that the 8.0 $\mu$m emission is in part due to polycyclic aromatic hydrocarbons (PAHs), which are organic
molecules containing multiple aromatic rings - where electrons are delocalised - such as benzene. These molecules are destroyed within the harsh radiation field of the HII region itself (Povich et al., 2007; Pavlyuchenkov et al., 2013), but fluoresce when hit with ultra-violet photons in a weaker radiation field. It is this emission that forms the observed bubble structure. The PDR surrounds the ionised gas of the HII region, but it is frequently patchy, which allows some radiation to escape.

In spite of their commonness, the three-dimensional structure of bubbles is still a point of contention. Beaumont & Williams (2010) found no evidence of expansion for 43 bubbles, using $^{12}$CO ($3\rightarrow2$) observations. One would expect the associated molecular gas from the near- and far-side of an expanding HII region to be blue- and red-shifted, respectively. This placed a limit on bubble thickness of $\lesssim 20\%$ of the bubble radius [see their Fig. 2]. There were many bubbles for which even a thin three-dimensional shell does not agree with their data, leading them to the conclusion that bubbles are two-dimensional structures, i.e rings, formed in flat molecular clouds. Anderson et al. (2012) however, find that up to 20\% of the emission in Herschel observations is found to emanate from the shell interior, suggesting that there is a three-dimensional structure. They find that the percentage of far-infrared (FIR) emission coming from the bubble is inversely proportional to the wavelength, decreasing from 26\%±0.7\% at 100 $\mu m$, to 12\%±7\% at 500 $\mu m$.

In the following sections we will outline this thesis’ contribution to the understanding of rings and bubbles, with two models. The first, a constraint on the expansion of RCW120 through analysis of the lineshapes of CO. The second, a morpho-kinematic model of the swept up ridge RCW36, with model fits to HCO$^+$ ($2\rightarrow1$) spectra in two embedded cores.
Chapter 4. Effects of Massive Stars

4.4 RCW120: "The Perfect Bubble"

4.4.1 Introduction

With Galactic co-ordinates $l = 348.249^\circ$, $B = 0.469^\circ$ RCW120 is one of the closest H II regions to the Sun, at 1.3 kpc (Zavagno et al., 2007). The ionised gas is 7.5' in diameter, giving a physical diameter of 3.8 pc. The exciting star is an O8V star, LSS 3959, which is visible in the Hα emission.

4.4.2 Observations

The data were taken by Anderson et al. (2015) from 15 July 2011 to 18 July 2011 with the Australian National Telescope Facility (ATNF) Mopra 22 m radio telescope near Coonabarabran in New South Wales, Australia. The 3-mm receiver was used in wideband mode, providing simultaneous spectra coverage of 8.3 GHz.
in four spectral windows of 2.2 GHz, each with 8192 channels and dual linear polarisations. These settings allowed for the observation of the $fJ = 1 \rightarrow 0$ transition in the four CO isotopologues, $^{12}$CO, $^{13}$CO, $^{17}$O and $^{18}$O at 115.2712 GHz, 110.2013 GHz, 112.3590 GHz, and 109.7822 GHz, respectively. The Mopra beam was $\sim 30''$ for all tunings, which is 0.19 pc at the distance of RCW 120. Data reduction was performed using the ATNF GRIDZILLA (Sault et al., 1995) and LIVEDATA (Barnes et al., 2001) packages.

### 4.4.3 Tests for expansion of the molecular gas

The goal of the Mopra CO observations outlined above was to test for any expansion of the RCW120 bubble. The most obvious sign of expansion would be the detection of two velocity components in the centre of the bubble, one blue-shifted and one red-shifted with respect to the velocity of the PDR gas. If the expansion speed is slower than the turbulent velocity, the expansion signal may appear as enhancements in the line wings.

As outlined in Anderson et al. (2015) the dark absorption features across the face of RCW120 provide an opportunity to test for expansion. This gas is expected to be blue-shifted relative to the PDR, since it is on the near side of the bubble. Four apertures are chosen, and average spectra taken across each.

- The first aperture visually approximates the extent of the absorbing foreground material, using what is known as the “jagged approximation”, where an aperture is carefully selected to pick out the structure of absorbing gas.
- The second encloses the entire interior of the bubble.
- The third is space between the first two. Locations inside the bubble where no absorption is seen.
- The fourth is the PDR itself.
These apertures are shown visually in Figure 4.4

By comparing the spectra from the absorbing aperture, which should be co-moving with the ionisation front, with spectra from the PDR, an indication of the expansion speed of the bubble can be found. These spectra are shown in Figure 4.5.

### 4.4.4 Modelling with MOLLIE

The data in the upper panel of Figure 4.5 shows that there is no detectable expansion signature. Therefore, what modelling can do is find an upper limit for the expansion velocity. Using the MOLLIE code outlined in Section 2.6.1 we modelled the expansion of a molecular shell of radius 1.9 pc and thickness 0.4 pc (≈20% of the radius). Two expansion velocities are considered, 1.0 and 1.5 km s\(^{-1}\). We use a value of 1.5 km s\(^{-1}\) for the turbulent velocity of the model, approximated...
Chapter 4. Effects of Massive Stars

Table 4.1: Physical Parameters for RCW120 model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Model Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (cm$^{-3}$)</td>
<td>$1 \times 10^4$</td>
<td>(Anderson et al., 2012)</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>30</td>
<td>(Anderson et al., 2012)</td>
</tr>
<tr>
<td>Turbulent Velocity (cm s$^{-1}$)</td>
<td>$1.5 \times 10^5$</td>
<td></td>
</tr>
<tr>
<td>Abundance [n($^{13}$CO)/n(H$_2$)]</td>
<td>$5 \times 10^{-7}$</td>
<td>(Stahl et al., 2008; Lee et al., 1996)</td>
</tr>
</tbody>
</table>

from visual inspection of the individual $^{13}$CO spectra. The volume density of $1 \times 10^4$ cm$^{-3}$, and temperature of 30 K, are derived from column density and dust temperature values from Anderson et al. (2012), while the abundance of $5 \times 10^{-7}$ is consistent with $^{12}$CO abundances and ($^{12}$C/$^{13}$C) ratios from Stahl et al. (2008) and Lee et al. (1996).

From this model, synthetic spectra are generated, one from the centre of the model, and one from the edge. The bottom panel of Figure 4.5 shows these spectra for both locations, and both expansion velocities. We find that the observed data is more consistent with the 1.0 km s$^{-1}$ expansion. A turbulent velocity which exceeds the bulk velocity of the gas, will always mask an expansion signature. Since the turbulent velocity of the model is well constrained by the line width of the observed lines, we conclude that RCW120 is expanding slower than 1.5 km s$^{-1}$. 
**Figure 4.5:** (Top): Spectra from the four apertures defined in the text and in Figure 4.4, for both $^{13}$CO and C$^{18}$O. (Bottom): MOLLIE $^{13}$CO spectra from the centre and edge of an expanding shell for expansion velocities of 1.0 and 1.5 km s$^{-1}$. The profiles for 1.0 km s$^{-1}$ are consistent with the data in the top panel, while the profiles for 1.5 km s$^{-1}$ expansion are not.
4.5 Triggered Star Formation: Vela Molecular Ridge: RCW 36

As mentioned in Chapter 1, many stars form in converging flows of molecular gas. Triggering is generally associated with an increase in the star formation rate, or star formation efficiency in a region. Surveys by Snider et al. (2009) and Thompson et al. (2012) suggest that 25-50% of young stellar objects (YSOs) are triggered. We have seen above how the expansion of H II regions can lead to a swept up shell of neutral material, such as RCW120. Depending on the initial morphology of the parent molecular cloud, the expansion of H II regions can take on many different observed morphologies, from champagne flows, to ridges.

The “collect and collapse" model for triggered star formation was first proposed by Elmegreen & Lada (1977), and Figure 4.6 outlines its main stages. The neutral material is accumulated in a swept-up shell surrounding the H II region. Density perturbations seed gravitational instabilities in the swept up material, leading to a second generation of star formation. The spatial segregation of age groups within some OB associations is often cited as supporting evidence for this mechanism.

4.5.1 Observations

The molecular line data modelled in this section is taken from a survey carried out on the Mopra telescope by Nadia Lo and the group at the University of New South Wales. HCO+ (1→0) lines were observed towards RCW 36, and an integrated intensity (or Moment 0) map generated, along with spectral lines from a 53×35 grid.
4.5.2 MOLLIE Model

A model for RCW36 was devised following the procedures outlined in Section 2.6.2, and a synthetic moment 0 map (see Fig. 4.8), and HCO+ J = (1→0) spectra (see Fig. 4.9) were generated using the MOLLIE code. The co-ordinate space of the model (x,y,z) will be expressed in relative terms to the radius of the model. (e.g. x=0.4 refers to an x-coordinate of 0.4 times the radius of the model.) The x-coordinate is the depth and is positive inwards, the y-coordinate is the height and is positive upwards, and the z-coordinate is the width and is positive to the right.

The model consists of two dense cores within an expanding shell of gas. The radius of the shell was set to be 0.6 pc, and the thickness 0.2 pc (~35% of the radius). In order to best match the morphology observed, the density of the model was set to zero for all values of x-coordinate greater than 45% of the absolute value of the
Figure 4.7: Vela C, as observed by Hill et al. (2011) using Herschel. Results from the 70, 160 and 250 µm wavebands are shown. At shorter wavelengths only the warmer objects are seen, such as protostars and H II regions, while deeply embedded filaments and possible high-mass progenitors are seen at the longer wavelengths. The black star marks the location (RA = 8 hr 59" 20', DEC = -43° 45" 21') where the molecular line data for HCO+ (J=1→0) was taken using the Mopra telescope.
radius, and for all positive values of the z-coordinate. The result is the lower half of an expanding ring of gas. The parameters for this model are listed in Table 4.2

Density Enhancements & Profiles  Within this shell of gas, two density enhancements were placed at co-ordinates (0,0.3,-0.6) and (-0.1,-0.4,-0.5), with densities of 12 and 4 times the background density, respectively. These clumps are modelled with Plummer profiles (Arreaga-García et al., 2010; Whitworth & Ward-Thompson, 2001) for their densities, following the functional form

\[
n(r) = n_0 \left( \frac{R_{\text{Plummer}}^2}{R_{\text{Plummer}}^2 + r^2} \right)
\]

where \(n_0\) is the central density, and \(R_{\text{Plummer}}\) is the characteristic radius at which the central flat density profile transitions into the \(r^{-2}\) drop-off. We note that there are more suitable density profiles available, but these differ from the Plummer model in the central unresolved regions, and so would be indistinguishable at this resolution.

Temperature Profiles  The background gas temperature of the model is 30 K, with a temperature profile in the clumps following a relation,

\[
T(r) = T_{\text{clump}} + T_{\text{background}} \left( 1 - \frac{r}{R_{\text{clump}}} \right)
\]

Temperature increases towards the centre of the core in a Plummer-like profile, with \(T(r) = T_{\text{clump}} = 10 K\) at \(r = R_{\text{clump}}\). While not the most realistic boundary condition, it fits to the resolution of the data, and any more sophisticated profiles do not lead to more constraints, without further assumptions.

Velocity  The shell of gas was given an infalling velocity relative to the centre of the model. (This is not to suggest that this is an infalling shell, merely that relative to the observer the line profiles are well matched by gas moving in this
direction. We make no claims about the physical significance of the centre point of the model sphere.] Within the clumps the velocity is in an outwards direction, from the centre in order to match the observed line-shapes. This may be indicative of the expansion stage of triggered star formation, however further data is needed to constrain this.

Relative to the spherical co-ordinates \((r, \theta, \phi)\) a uniform infall velocity field is given in Cartesian coordinates by

\[
\begin{align*}
v_x &= v_r \cos \theta \sin \phi \\
v_y &= v_r \sin \theta \sin \phi \\
v_z &= v_r \cos \phi
\end{align*}
\]  
(4.11)

where \(v_r\) is the velocity parameter set in MOLLIE. This profile can equally be applied within the clumps, by defining coordinates relative to the clump centres, and adding these components to the bulk velocities in each direction.

Rotation is included, in order to match the observed line shapes. This is achieved by replacing the \(\theta\) and \(\phi\) arguments to the trigonometric functions with arguments which vary in \(r\). A characteristic velocity of the same order as the outwards expansion velocity is used, with a \(1/r\) variation within each clump.

**Turbulence** The turbulent velocity values used come from visual best fit matching to the observed line widths of the data.

All other parameters are uniform within the regions to which they are attributed in Table 4.2.
4.5.3 Results

Using the model outlined above, a synthetic moment 0 map was generated for the model, along with HCO$^+$ (1→0) spectra for two pointings towards the centres of the density enhancements, the left hand of which is referred to as "the Ridge", while the right-hand enhancement is referred to as the "Main Clump". These synthetic observations are compared to the Mopra data in Figures 4.8 and 4.9. These data are shown to be in good agreement with the observations, and show that the observed line profiles in this ridge are consistent with those from a dense core, with some expanding/outflowing gas.

4.6 Conclusions

We have outlined the processes by which massive stars accumulate shells and ridges of gas around them. We have shown that through MOLLIE models, we can constrain the expansion velocity of bubble H II regions such as RCW120, which we find to be expanding slower than 1.5 km s$^{-1}$.

In RCW36 we have shown that a simple model of rotating expanding clumps in a receding molecular shell, which is consistent with the collect and collapse model of triggered star formation, generates synthetic line profiles which are an excellent
Chapter 4. Effects of Massive Stars

Figure 4.8: (Top): Moment 0 map of RCW36 taken with MOPRA. (Bottom): Moment 0 map of the MOLLIE model. Both produced using kVIS (Gooch, 1996).

Figure 4.9: Synthetic HCO$^+$ (1-0) spectra (solid line), mapped at the centre of each of the density enhancements, compared to line observations taken by the Mopra telescope (dashed line).
match to the observed ones. This simplistic model is not constrained enough to
be a definitive description of the properties of RCW36, and further observations
with other molecular tracers are required to constrain the observed parameters.

For the \(~30\) K gas typical of these types of clouds, the sound speed is \(~0.5\) km s\(^{-1}\),
which is comparable to the turbulent velocities quoted in Table 4.2. We saw in
Chapter 1, that turbulence can provide a means of support in a cloud against
global collapse; this is the crucial distinction between the high mass and low mass
star formation regimes. In high mass star formation, coherent structures shaped
by higher sound speeds are possible, and with transonic to supersonic turbulence,
the velocities and densities in high mass star formation begin to display the highly
filamentary and non-linear distributions characteristic of gas shaped by shocks.
The cold quiescent cores we saw in the previous chapter are not possible at these
turbulent velocities, and as we will now see as we head towards the Galactic centre,
things become even more turbulent.
Chapter 5

Star Formation in the Galactic Centre

"An rud is annamh, is iontach."

- Anonymous (Old Irish Proverb),

5.1 Introduction

The final region of star formation to be investigated in this thesis is the Central Molecular Zone (CMZ) of the Milky Way [see Figure 5.1]. The local environment in which this region is located is the most extreme possible within our Galaxy, with the influence of the supermassive black hole Sagittarius A* dominating the local gravitational field. The clouds contained in the CMZ are highly dense, under large thermal pressures and extreme tidal gravitational fields. Interestingly however, the star formation rate (SFR) in the CMZ is a factor of $\geq 10$ times lower than would be expected for similar amounts of dense gas in the Solar neighbourhood. Kruijssen et al. (2014) outline a number of global and local mechanisms in the CMZ which could impede star formation and explain this marked difference in the observed
SFRs. From global mechanisms such as disk stability and episodic/localised star formation, to local mechanisms such as Galactic tides, turbulence, magnetic fields, and both radiation pressure and cosmic ray pressure support. They suggest, using canonical parameters for the CMZ, that turbulent support is the dominant mechanism, and is associated with a critical density which scales with $M^2$, where $M$ is the Mach number of the turbulence. For the $\sim 30-60$ K gas in the CMZ, $M \approx 30$. This gives a critical density for star formation to take place of $\sim 10^7$ cm$^{-3}$. A similar analysis for the Solar neighbourhood gives a critical density of $\sim 10^4$ cm$^{-3}$. We can see that for the CMZ, a much higher density of gas is required to accumulate before star formation can theoretically begin. In this chapter, we will model one of these CMZ clouds, G0.253+0.016 (hereafter ‘The Brick’) using the radiative transfer code MOLLIE in order to probe the physical parameters, investigate its peculiarly low star formation rate, and compare the results with the ideas above.

5.2 G0.253+0.016 - A Possible YMC Progenitor

The Brick (Lis & Carlstrom, 1994; Lis & Menten, 1998; Rathborne et al., 2014; Johnston et al., 2014) is a very massive, ($M \sim 1.3 \times 10^5 M_\odot$, within $\sim 3$ pc, Longmore et al., 2012), dense (average $n \sim 3 \times 10^4$ cm$^{-3}$, Kauffmann et al., 2013) cloud located on the 100 pc elliptical ring around Sgr A* (Molinari et al., 2011). However, despite its high mass and average density there is remarkably little ongoing star formation within the Brick, as evidenced by recent dust continuum observations (Immer et al., 2012) and maser surveys (Yusef-Zadeh et al., 2013; Mills et al., 2015, find many CH$_3$OH masers, but no strong evidence of star formation). Kauffmann et al. (2013) argue that there is no immediate expectation of star formation commencing. The only indication of any star formation is a single weak water maser as seen in Figure 5.2.

The Brick is an interesting target of study, as it represents a possible progenitor cloud for the formation of a young massive cluster (YMC) on the scale of the
Figure 5.1: Figure 1 from Koepferl et al. (2015) showing IRAC 8 μm, MIPS 24 μm and PACS 70 and 160 μm. The dark circles refer to the object G0.253+0.016, "The Brick" which will be modelled later in this chapter.

Arches. Rodríguez & Zapata (2013) find a total cloud IR luminosity of $3 \times 10^5 \text{ L}_\odot$ which they suggest is due to the presence of at least five embedded stars at evolutionary stages earlier than B0.

5.3 Observations

The observations used in this work were taken in July 2010 by the Millimetre Astronomy Legacy Team 90 GHz (MALT90). This survey utilised the Mopra 22 m telescope, and the full description of the survey strategy is outlined in Rathborne
Figure 5.2: Three colour image of the Brick from Rathborne et al. (2014). *Spitzer* 3.6 $\mu$m emission (stars) is in blue, 8.0 $\mu$m emission (Galactic background) in green, and ALMA 3 mm emission (dust) in red. The Brick is very cold and dense, making it appear as an absorption feature against the bright IR emission of the Galaxy. The position of a water maser is marked, which is evidence of active star formation.

et al. (2014). The molecules and transitions of interest, the ($J=1 \rightarrow 0$) lines in N$_2$H$^+$, HNC, HNC and HCO$^+$, and the ($2\rightarrow1$) lines in $^{13}$CS and SiO, represent a useful range in excitation energies, critical densities, and chemical evolution as shown in Table 5.1. The data was acquired from the Australia Telescope Online Archive (ATOA) in the form of a PPV (*position-position-velocity*) cube for each molecular transition. The cubes were read using kvis (Gooch, 1996), and synthetic line profiles extracted.

**Hanning Smoothing** These profiles were subject to a Hanning smoothing, which is achieved by a running mean across the spectral axis with a triangle as a smoothing kernel. The central channel is weighted by 0.5 and the two adjacent channels by 0.25 to preserve the flux.
Local Regression Smoothing - LOESS  Even after Hanning smoothing the noise levels were still quite significant, and so the spectra were further smoothed through by local regression method in OCTAVE (Eaton et al., 2015) to arrive at the data presented for comparison in Figure 5.6. At each point in the data set a low-degree polynomial is fitted to a subset of the data. The polynomial is fitted using weighted least squares, giving more weight to points near the point whose response is being estimated and less weight to points further away. The subsets of data used for each weighted least squares fit in LOESS are determined by a nearest neighbours algorithm. A user-specified input to the procedure called the “bandwidth” or “smoothing parameter” determines how much of the data is used to fit each local polynomial. The LOESS fit is complete after regression function values have been computed for each of the data points. Care must be taken to not over-smooth, and this is achieved through visual inspection of the profiles for differing values of the smoothing parameter.

5.3.1 Molecules Modelled

HCO$^+$  A good dense gas tracer, especially for molecular outflows, where shock enhanced radiation fields are present that can lead to local enhancement of the species (Rawlings et al., 2000, 2004).

HNC  Also a good tracer of dense gas, and its relative abundance compared to its isotopologue HCN is an excellent probe of temperature, with HCN being more common in hotter
gas. It also lacks the hyperfine anomalies of HCN, with it’s line pattern spread over only 0.4 km s\(^{-1}\).

**HCN**  As investigated in Chapter 3, HCN has a very broad hyperfine line pattern, with anomalous line strengths in low mass star forming regions, and anomalous integrated intensities or linewidths in high mass star forming regions. Provided the radiative transfer is dealt with at the hyperfine level, we can use HCN lines as a morphological test for our models. However, care must be taken when using HCN as a tracer of infall, as this anomaly in the line widths, coupled with infall may lead to displaced centroids, and false infall signatures (Redman et al., 2008; Carolan et al., 2009).

**N\(_2\)H\(^+\)**  A selective tracer of quiescent gas, N\(_2\)H\(^+\) is what is known as a “late depleter”, making is less susceptible to freeze out compared to C-bearing species. This causes it to become anti-correlated with CO, and makes it an excellent choice of tracer for the inner regions of dense clouds.

**SiO**  A shock tracer, SiO can trace the gas potentially associated with young outflows. Lo et al. (2007) show that the (2\(\rightarrow\)1) line can trace ongoing star formation even in cores which have not yet presented in the IR.

**\(^{13}\)CS**  An excellent dense gas tracer due to its high dipole moment, however, it is still subject to substantial freeze out, and so is often used as a diagnostic for the outer layers of clouds and cores.
Table 5.1: A summary of the excitation energies and critical densities of the tracers used in this work. Data taken from the Leiden Atomic and Molecular Database (Schöier et al., 2005).

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Frequency (Hz)</th>
<th>$E_u/k$ (K)</th>
<th>$n_{\text{crit}}$ (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCO$^+$</td>
<td>(1→0)</td>
<td>89.188526</td>
<td>4.28</td>
<td>$2 \times 10^5$</td>
</tr>
<tr>
<td>HCN</td>
<td>(1→0)</td>
<td>88.631847</td>
<td>4.25</td>
<td>$3 \times 10^6$</td>
</tr>
<tr>
<td>HNC</td>
<td>(1→0)</td>
<td>90.663572</td>
<td>4.35</td>
<td>$2 \times 10^5$</td>
</tr>
<tr>
<td>N$_2$H$^+$</td>
<td>(1→0)</td>
<td>93.173772</td>
<td>4.47</td>
<td>$2 \times 10^5$</td>
</tr>
<tr>
<td>SiO</td>
<td>(2→1)</td>
<td>86.847010</td>
<td>6.25</td>
<td>$3 \times 10^5$</td>
</tr>
<tr>
<td>$^{13}$CS</td>
<td>(2→1)</td>
<td>92.494303</td>
<td>6.66</td>
<td>$3 \times 10^5$</td>
</tr>
</tbody>
</table>

5.4 MOLLIE Model

We first constrain the morphology of the model. The Brick appears to be a curved body of gas of approximately 3 pc in scale. The underlying structure chosen for this model was the ring torus, which has circular cross-section but also a radius of curvature, making a decent approximation to a filament. The equation describing the surface of a torus is

$$\left[(x^2 + y^2 + z^2) + (a^2 + b^2)\right] = 4ab(b^2 - x^2). \quad (5.1)$$

By offsetting the co-ordinate system, and through conditional statements, a segment of the torus becomes the starting point for the model. [It can be noted that it is somewhat cumbersome to generate a complex morphology in MOLLIE. This will be discussed in the Conclusions chapter.] The parameters $a$ and $b$ define the size of the torus, and are selected as 3.1 and 0.8 times the radius of the model respectively, to match the observed aspect ratio. The radius of the model cube is chosen to be 4 pc, in order to approximate the size of the torus model, to the size of the observed source.
Figure 5.4: A ring torus, with the red circle describing the outer radius, $a$ and the blue circle describes the circular cross section (Jantzen, 2012).

Within this torus, two ellipsoidal density enhancements (clumps) are defined, one in the lower half, and one in the upper half. This density structure matches the dust and line observations of Rathborne et al. (2015). The major and minor axes of the lower clump are 0.7 and 0.28 times the model radius respectively, with the major axis aligned with the torus. For the upper clump, the values are 0.7 and 0.31 respectively. Figure 5.5 shows both observed and synthetic integrated intensity maps for HCO$^+$ and N$_2$H$^+$, which are shown to be in good agreement.
5.4.1 Model Parameters

Density Using the mass of $\sim 1.3 \times 10^5 \, M_\odot$ as a constraint, a torus $H_2$ density of $1.75 \times 10^5 \, cm^{-3}$ was chosen, with the upper and lower clump densities being 1.1 and 2.0 times this background value respectively. Recently the density profile of the Brick has been observed to be very flat, with an $r^{-1.2}$ dependence (Jens Kauffmann, private correspondence), and this profile was applied to our model, where $r$ in this case is the radial distance from the centre of the circular cross-section of the torus. Using these parameters, we get a mass for the Brick of $1.33 \times 10^5 \, M_\odot$ which is in good agreement with observations.

Turbulent Velocity The observed linewidths of molecular transitions provide a constraint for the level of turbulence in the Brick. We find values of 8 km s$^{-1}$ for the background, 10 km s$^{-1}$ for the enhancements, and 12 km s$^{-1}$ in the region of overlap, which when combined with the bulk velocities described below, give good agreements to the observed lines in Figure 5.6.

Temperature The temperature of the Brick has been modelled by Clark et al. (2013), who suggest a widespread, almost constant central temperature of 21 K rising gradually to 27 K in a thin shell at the edge. We take a constant value of 22 K, as the width of this "hot envelope" is small compared to the overall size of the cloud. We acknowledge a more realistic temperature profile would be preferred, however at the resolution of these data, we think the difference would be insignificant. Dust temperature measurements by Longmore et al. (2012) also suggest a temperature of $\approx 20$ K.

Abundances With all the other model parameters relatively well constrained, the only free parameter remaining to match the observed lines is the chemical
abundances. Table 5.2 gives a summary of the required abundances in the background material, the clumps, and in the cases of freeze-out, a radius and level of freeze out is given.

**Velocity** The observations of the Brick show a large systematic velocity gradient, the upper half is heavily blue shifted, while the lower half is heavily redshifted. A two component model was used, constant with a cloud collision model first suggested by Lis & Menten (1998). Each of the clumps were given a velocity compared to the bulk velocity of the cloud. The upper was given a velocity of $-14 \text{ km s}^{-1}$, while the lower was given a velocity of $+15 \text{ km s}^{-1}$. These values were chosen to best match the observed lineshapes of the chosen molecules, however a post-processing $V_{lsr}$ adjustment is required to match the data. This offset is done by inspection in the plotting process. These offsets are indicative of the overall velocity gradient of the cloud, which appears to be highly non-linear, and was unable to be fit using a global velocity gradient over the entire model.

These results indicate that the Brick may have formed from a cloud collision where the gradient is an effect of the two original velocity components of the colliding clouds. In support of this, the very limited star formation in the Brick, indicated by the maser in Fig 5.2, occurs in the overlap region of the model clumps, as opposed to the clump centres, which one might expect. Higuchi et al. (2014) have cited the ubiquity of SiO emission throughout the Brick as evidence of the presence of widespread shocked gas, consistent with a cloud-cloud collision model.
Table 5.2: Modelled abundance parameters for the Brick. A comparison to the CMZ cloud Sagittarius B2 is made using the modelled abundances from Wiles (2015).

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Abundance $(n/\text{n}_{\text{H}_2}) \times 10^{-11}$</th>
<th>Upper Clump</th>
<th>Lower Clump</th>
<th>$r_{\text{freeze}}$</th>
<th>Freeze Out Factor</th>
<th>Sgr B2 Abundances (Wiles, 2015)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCO$^+$</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>0.4</td>
<td>0.5</td>
<td>20</td>
</tr>
<tr>
<td>HCN</td>
<td>3.7</td>
<td>3.3</td>
<td>5.6</td>
<td>0.22</td>
<td>0.5</td>
<td>100</td>
</tr>
<tr>
<td>HNC</td>
<td>3.9</td>
<td>3.9</td>
<td>3.9</td>
<td>0.2</td>
<td>0.42</td>
<td>40</td>
</tr>
<tr>
<td>N$_2$H$^+$</td>
<td>0.66</td>
<td>0.66</td>
<td>1.1</td>
<td>0.45</td>
<td>2.0</td>
<td>-</td>
</tr>
<tr>
<td>$^{13}$CS</td>
<td>1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.4</td>
<td>0.5</td>
<td>-</td>
</tr>
<tr>
<td>SiO</td>
<td>0.16</td>
<td>0.08</td>
<td>0.54</td>
<td>0.4</td>
<td>0.5</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 5.3: $v_{\text{lsr}}$ offsets for each of the molecular lines shown in Figure 5.6

<table>
<thead>
<tr>
<th>Molecule</th>
<th>P2 (km s$^{-1}$)</th>
<th>P3 (km s$^{-1}$)</th>
<th>P4 (km s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCO$^+$</td>
<td>35</td>
<td>43</td>
<td>43</td>
</tr>
<tr>
<td>HCN</td>
<td>37</td>
<td>45.5</td>
<td>46.5</td>
</tr>
<tr>
<td>HNC</td>
<td>32</td>
<td>40</td>
<td>41</td>
</tr>
<tr>
<td>N$_2$H$^+$</td>
<td>35</td>
<td>41</td>
<td>43</td>
</tr>
<tr>
<td>$^{13}$CS</td>
<td>-</td>
<td>-</td>
<td>38.5</td>
</tr>
<tr>
<td>SiO</td>
<td>-</td>
<td>-</td>
<td>35</td>
</tr>
</tbody>
</table>
5.5 Results

Figure 5.6: Top to bottom: Synthetic line profiles overlaid on observed data for the dense gas tracers HCO$^+$, HCN, HNC and N$_2$H$^+$. The left column is at P2, the centre at P3 and the right-hand column is at P4. The pointings P2, P3, and P4 refer to the positions outlined in Rathborne et al. (2014), as shown in Fig. 5.3.

Figure 5.6 shows the final best fit model profiles for the four main dense gas tracers, HCO$^+$, HCN, HNC and N$_2$H$^+$, at the points P2, P3 and P4, as shown in Fig. 5.5. The synthetic and observed lines are found to be in good agreement, in both line width, and line strength for all three pointings using the parameters...
Chapter 5. Star Formation in the Galactic Centre

Figure 5.7: Synthetic line profiles for the dense gas tracer $^{13}$CS, and shocked gas tracer SiO, both at P4 as outlined in Figure 5.5

outlined above. However, the N$_2$H$^+$ lines are lacking the extended blue-shifted emission seen in the data. We feel that this could be caused from clumpy foreground dense gas, which is traced well by the late-depleting N$_2$H$^+$, but not by the other molecules which are more susceptible to grain surface freeze-out. A similar situation seen in the SiO (2→1) profile in Figure 5.7 - a known shock tracer - lends support to this explanation. Overall though, for a relatively uncomplicated model, the line profiles are a good fit to the observed data.

The $v_{lsr}$ offsets outlined in Table 5.3 show that P3 and P4 are very close together in velocity, which is in fitting with the latest velocity maps by (Rathborne et al., 2015).

5.6 Comparisons with Sagittarius B2

Wiles (2015) conducted a similar study on the Galactic centre cloud Sgr B2. In addition to an extensive, dense molecular cloud, a large number of compact and ultra-compact HII regions and masers indicate that this region is young with many embedded sources. This makes a contrast to the Brick which has almost no ongoing star formation. Through comparison of the modelled parameters for these two contrasting sources [Table 5.4] we find that Sgr B2 is hotter, rarer and more chemically rich. The high temperature desorbs much of the molecular material from ices on grain surfaces, back into the gas phase (Johnson et al., 1991; Roberts et al.,
The significantly lower abundances of molecules in the Brick is indicative of significant grain freeze-out, for all molecules bar $\text{N}_2\text{H}^+$, which is actually requires enhancement in the dense central regions. This fits nicely with the strong anti-correlation of CO and $\text{N}_2\text{H}^+$ seen by Qi et al. (2013) in protostellar discs. Table 5.4 compares the modelled properties of the two regions, and comments on the similarities and the differences.
### Table 5.4: A comparison of the modelled parameters of the Brick and Sgr B2.

<table>
<thead>
<tr>
<th></th>
<th>Brick (This Work)</th>
<th>Sgr B2 (Wiles, 2015)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass ($M_\odot$)</td>
<td>$10^5$</td>
<td>$10^6$</td>
<td>Sgr B2 is a far larger reservoir of gas than the Brick.</td>
</tr>
<tr>
<td>Radius (pc)</td>
<td>4</td>
<td>45</td>
<td>The Brick is much smaller in size, $\sim10%$ of the radius, so $\sim0.1%$ of the volume.</td>
</tr>
<tr>
<td>Mean density (cm$^{-3}$)</td>
<td>$10^5$</td>
<td>$10^4$</td>
<td>The Brick contains an order of magnitude denser gas on average than Sgr B2. However the very flat density profile $r^{-1.2}$ means that the peak densities may be lower in the Brick than Sgr B2.</td>
</tr>
<tr>
<td>Temperature</td>
<td>30</td>
<td>150</td>
<td>The much higher temperature in Sgr B2 can account for its much higher abundances, as shown in Table 5.2, due to the lower rate of grain surface freeze-out.</td>
</tr>
<tr>
<td>Line widths (km s$^{-1}$)</td>
<td>20</td>
<td>100</td>
<td>The line widths in Sgr B2 are much higher than those in the Brick. If this is a purely turbulent line width then Sgr B2 should have even less star formation than the Brick, if turbulent support is the limiting factor for star formation, as suggested by Kruijssen et al. (2014). However, it does not, which leaves an open question as to what the limiting factor is.</td>
</tr>
<tr>
<td>Velocity (km s$^{-1}$)</td>
<td>15</td>
<td>60-100</td>
<td>The large infall velocities present in Sgr B2 are indicative of the ongoing star formation in the region, and contribute largely to the observed line widths</td>
</tr>
<tr>
<td>Turbulence (km s$^{-1}$)</td>
<td>10</td>
<td>10</td>
<td>Interestingly the turbulent velocity required in both models is approximately the same.</td>
</tr>
<tr>
<td>Abundances</td>
<td>see Table 5.2.</td>
<td></td>
<td>As mentioned above the high temperatures of Sgr B2 release much of the frozen out molecules back into the gas phase.</td>
</tr>
</tbody>
</table>
5.7 Conclusions

Cloud collision has been suggested as a possible explanation for the lack of star formation in the Brick as far back as Lis & Menten (1998). We have shown through radiative transfer modelling that the observed line profiles in the Brick are consistent with a model of ongoing cloud-cloud collision. Recent observations by Rathborne et al. (2015) with their ALMA Moment 1 maps, reveal two distinct velocity components, merging towards the south of the cloud. This supports our values for the $v_{\text{lsr}}$ offsets from Table 5.3, which show the central and lower pointings P3 and P4 share almost common velocities.
Chapter 6

Conclusions and Future Work

In this thesis it has been shown that turbulence drives the characteristic properties of star formation. Beginning with the small quiescent cores such as TMC-1, where hyperfine anomalies of HCN persist with line widths of $\sim 0.5 \text{ km s}^{-1}$. Followed by the triggered massive star formation seen in RCW36 and the expanding H II region RCW120 where stellar feedback drives linewidths up to $\sim 5 \text{ km s}^{-1}$. Finally, showing the extreme conditions in the Galactic centre, where gravitational tides from orbiting the central supermassive black hole, drive linewidths even further up to $\sim 20 \text{ km s}^{-1}$ in the Brick, and almost $100 \text{ km s}^{-1}$ in Sgr B2. The differing strengths of the gravitational force on these clouds, cause them to expand and contract on their passage around the Galactic Centre. It is these increasing scales of turbulence which drive the different paradigms of star formation.

6.1 HCN Hyperfine Anomalies

The hyperfine anomalies of the HCN molecule have been shown to be readily reproducible using the radiative transfer code MOLLIE. Through consideration of the radiative transfer at the F-level, as opposed to the J-level used for other hyperfine structures such as C$^{17}$O, the anomalies emerge naturally.

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Table 6.1: Orders of magnitude comparison of properties of star forming regions from this work and related studies. Values for TMC-1, RCW36, RCW120, and The Brick come from this thesis, while values for G333 and Sgr B2 are from Wiles (2015).

<table>
<thead>
<tr>
<th></th>
<th>TMC-1</th>
<th>RCW36</th>
<th>RCW120</th>
<th>G-333</th>
<th>The Brick</th>
<th>Sgr B2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass ($M_\odot$)</td>
<td>10</td>
<td></td>
<td></td>
<td>$10^5$</td>
<td></td>
<td>$10^6$</td>
</tr>
<tr>
<td>Size (pc)</td>
<td>0.1 pc</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>50</td>
</tr>
<tr>
<td>Density (cm$^{-3}$)</td>
<td>$10^4$</td>
<td>$10^5$</td>
<td>$10^4$</td>
<td>$10^5-10^6$</td>
<td>$10^5$</td>
<td>$10^4$</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>10</td>
<td>30</td>
<td>30</td>
<td>25</td>
<td>25</td>
<td>150</td>
</tr>
<tr>
<td>Velocity (km s$^{-1}$)</td>
<td>0.1</td>
<td>5</td>
<td>1</td>
<td>5-10</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Turbulence (km s$^{-1}$)</td>
<td>0.1</td>
<td>5</td>
<td>1</td>
<td>5-10</td>
<td>10</td>
<td>10</td>
</tr>
</tbody>
</table>

The parameter sweep over typical conditions for low mass star formation found some general trends in the anomalies, towards cold quiescent gas, possibly indicating the anomalies as a good tracer for pre-stellar cores. Using ALMA, a high resolution study of HCN line profiles towards known prestellar cores, combined with the data from our parameter sweep could investigate this possibility.

The choice of collisional rates was investigated, and comparisons made between the proportional method as used by Keto & Rybicki (2010) applied to the J-level rates of Green & Thaddeus (1974); Schöier et al. (2005), and the explicitly calculate rates of Ben Abdallah et al. (2012, F-level) and Vera et al. (2014, J-level). We found the proportional method to give a good match to observed line profiles in TMC-1, for both Green & Thaddeus (1974) and Vera et al. (2014), while the explicitly calculated rates of Ben Abdallah et al. (2012) did not.

For now, we recommend the use of the new rates of Vera et al. (2014), scaled to the same proportions as the rates of Ben Abdallah et al. (2012). They have been shown to generate good matches to observations, readily reproducing the spectrum of TMC1, and also replicating the observed “super-anomalous” ratios seen in sources such as L1197 (Loughnane et al., 2012). We anticipate the forthcoming exact rates based on their potential energy surface to supersede these rates when they are released, and become the standard for HCN collisional rates.
In the J= 1→0 transition, the F=(0→1) line is unreliable as a diagnostic of infall or dynamics. The central (F=2→1) line however is more robust and when it is resolved, it should be reliable as a dynamical tracer.

### 6.1.1 Future Work

A natural follow up to this work would be to investigate these two sets of rates in the case of high mass star forming cores, where the higher temperatures and turbulent widths lead to a different manifestation of the anomalies. The proportional method is predicted to fail at the high optical depths associated with high mass star forming regions, and a further study could investigate this possibility, whilst also performing validation on the new rate coefficients as they are published.

Possible other future work regarding the anomalies include predicting HCN (2→1) spectra, which should be observable with ALMA Band 5. There is an anomaly in the JF = 21→12 transition, which sees it boosted to up to 100 times its expected line strength [see Figure 3.6, top right panel]. Wiles (2015) find that this anomaly may link to the observed red-blue asymmetries present in HCN, and this new radiative transfer scheme can be used to study this in more detail.

### 6.2 High Mass Star Formation

Through radiative transfer modelling of two expanding H II regions, RCW120 and RCW36, we have demonstrated the suitability of MOLLIE for placing constraints on the expansion velocities, through analysis of the observed line widths and line shapes. We have also shown that a model consistent with triggered star formation was capable of providing a good match to the observed line profiles of RCW36. More molecular line observations of this target would provide a better constraint on the physical properties, however the fits generated from this first order model are good, and suggest ongoing star formation in the Vela ridge.
6.3 Star formation in the CMZ

It has been shown that the highly turbulent clouds of the CMZ have peculiarly low star formation rates (Longmore et al., 2012; Kruijssen et al., 2014; Kauffmann et al., 2013). Through molecular line modelling of many molecular species over a wide range of excitation energies and critical densities, a model of a cloud-cloud collision in a turbulent medium is shown to be a good fit to observations. The comparison to Sgr B2 reveals that the Brick is more dense but less turbulent.

6.3.1 Future Work

We have seen in the previous two chapters how cumbersome the current implementation of MOLLIE is for modelling complex geometries. Suitable functional forms must be found and perturbed to suit the needs of the object being modelled, which is far from ideal for the highly turbulent structures typical of high mass star formation and the CMZ. With the advent of ALMA, increasingly higher resolution maps are available; more complex and higher resolution structures will need to be incorporated into MOLLIE models. For planetary nebulae, Clyne et al. (2015) have shown the capabilities of the morpho-kinematical modelling code SHAPE (Steffen et al., 2011). Figure 6.1 shows a model of the planetary nebula Mz 3, highlighting SHAPE’s capabilities for modelling complex structure.

Recently, Santander-García et al. (2015) have developed a molecular radiative transfer implementation for SHAPE called SHAPEMOL. They use it to generate synthetic CO line profiles, using the Large Velocity Gradient approximation. This assumes that the energy density at any point depends only on the local source function, and local optical depth. Remote points are radiatively decoupled by Doppler shifting due to the large velocity gradient. This vastly simplifies the radiative transfer calculation.
They can generate some good matches to observed CO profiles, however, the LVG approximation is not a good one for the optically thick conditions of the CMZ, and many cold dense clouds, since it ignores the contribution of radiation trapping to the problem of radiative transfer. It does however, generate an arbitrary parameter space with the same model parameters as MOLLIE. At each point in the model, values are assigned for density, temperature and velocity by SHAPE, and then molecular abundance and turbulent width are defined by SHAPEMOL. Outputting these values to a text file, and inputting them into MOLLIE would allow a full radiative transfer treatment to carried out over the modelled region, at high optical depths, and with other more complex molecules such as HCN, which require a more robust treatment than SHAPEMOL can provide.

Figure 6.2 outlines a modelling pipeline which would link the arbitrary morphokinematic modelling capabilities of SHAPE with the full non-LTE radiative transfer capabilities of MOLLIE to generate synthetic ALMA observations using the package SIMALMA. This pipeline could theoretically be used for any telescope system (e.g. Mopra, JCMT), provided the beam properties are known, using the inbuilt convolution routines already in MOLLIE.
Finally, with use of this pipeline, we plan to investigate further the observed depletion of molecular material in the CMZ. Jens Kauffmann (private communication) has initial results which suggest that depletion onto grain surfaces may not be a function of the gas temperature, but purely the dust temperature. Using the CMZ survey of Jones et al. (2012), this new MOLLIE pipeline could be used to produce a global model of molecular abundances for the CMZ. Kruijssen et al. (2015) find star-forming potential of dense molecular clouds in the CMZ is intimately linked to their orbital dynamics, potentially giving rise to an absolute-time sequence of star-forming clouds. Combining these results with the derived abundances could further investigate the differences in star formation rates both as a function of space and time.
Appendix A

Appendix A: Derivations

A.1 Derivation of the full transfer equation

\[
\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu
\]

\[
\frac{dI_\nu}{d\tau_\nu} + I_\nu = S_\nu
\]

\[
\left[ \frac{dI_\nu e^{\tau_\nu}}{d\tau_\nu} + I_\nu e^{\tau_\nu} \right] = S_\nu e^{\tau_\nu}
\]

The product rule states that

\[
\frac{d}{dx} [u(x)v(x)] = u(x) \frac{dv}{dx} + v(x) \frac{du}{dx}
\]

\[
\frac{d}{d\tau_\nu} [I_\nu e^{\tau_\nu}] = S_\nu e^{\tau_\nu}
\]

If we allow \( \mathcal{I}(\tau_\nu) = I_\nu e^{\tau_\nu} \) and \( \mathcal{G}(\tau_\nu) = S_\nu e^{\tau_\nu} \) then

\[
\int_0^{\tau_\nu} \frac{d}{d\tau_\nu} \mathcal{I}(\tau_\nu)d\tau_\nu = \int_0^{\tau_\nu} \mathcal{G}(\tau_\nu)d\tau_\nu
\]

\[
\mathcal{I}(\tau_\nu) = \mathcal{I}(0) + \int_0^{\tau_\nu} \mathcal{G}(\tau_\nu)d\tau_\nu
\]

\[
\mathcal{I}(\tau_\nu) = \mathcal{I}(0) + \int_0^{\tau_\nu} \mathcal{G}(\tau_\nu)d\tau_\nu
\]

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Appendix A. Derivations

\[ I_\nu e^{\tau_\nu} = I_\nu(0) + \int_0^{\tau_\nu} S_\nu e^{\tau_\nu'} d\tau_\nu' \]

giving the full solution of the equation of radiative transfer

\[ I_\nu = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu e^{-(\tau_\nu - \tau_\nu')} d\tau_\nu' \quad (A.1) \]

For a constant source function, \([S_\nu(\tau'_\nu) = S_\nu]\)

\[ I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + S_\nu \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau_\nu')} d\tau_\nu' \]

\[ I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + S_\nu \left[ e^{-(\tau_\nu - \tau_\nu)} - e^{-(\tau_\nu - 0)} \right] \]

\[ I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + S_\nu \left( 1 - e^{-\tau_\nu} \right) \]

\[ I_\nu(\tau_\nu) = S_\nu + (I_\nu(0) - S_\nu) e^{-\tau_\nu} \]


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