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Richardson, Kevin John

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SUBMILLIMETRE MOLECULAR LINE
OBSERVATIONS AND MODELLING
OF MOLECULAR CLOUDS

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A thesis submitted in accordance with the regulations for the degree of Doctor of Philosophy in the University of London.

1985
Submillimetre molecular line observations of molecular clouds in our galaxy are presented, and the data analysed using various alternative cloud models.

A critical review is given of the methods commonly used to interpret molecular line data, including both theoretical considerations and issues relating to calibration and comparability of results obtained with different telescopes. A detailed comparison is made between results predicted from large velocity gradient (LVG) models, including the generalisation to non-monotonic velocity flows, and those given by "microturbulent" clouds.

An LVG model is employed in an investigation of conditions in the molecular outflows frequently found in star formation regions, for which observations in the CO J=3-2 rotational transition at 345 GHz are presented. These are combined with lower frequency data from the literature to derive various properties of the outflows for a sample of 13 sources. The most important result is that local H$_2$ densities exist in the outflows which are higher, typically by an order of magnitude, than previously derived average values obtained using only lower frequency data.

Observations are presented of the S255 and DR21 clouds in the transitions CO J=2-1, CO J=3-2, CS J=7-6, HCN J=4-3, HCO$^+$ J=4-3 and
$^{13}$CO$^+$ J=4–3 and are supplemented by continuum data at 350 μm and (for DR21) at 20 μm. It is shown that, although some features of the data can be understood in terms of an LVG model, there is compelling evidence for fragmentation of the clouds on length scales much smaller than the cloud sizes. The data are used to constrain the local H$_2$ densities and relative molecular abundances in the clumpy cloud cores, and compared with lower frequency results from the literature.

The implications of these results for the star formation environment are discussed, and an assessment made of possible strategies for their further investigation.
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ACKNOWLEDGEMENTS

I should like to express my thanks to the following colleagues:

Glenn White, for his help, support and encouragement throughout this work;

Lorne Avery, for much encouragement and useful advice on cloud modelling; also for permission to make use of his Monte Carlo transfer program, which plays an important part in the discussions of Chapter 3;

Graham Gee, for reducing the 350μm continuum data presented in Chapters 6 and 7, and for many useful insights;

Tania Monteiro, for information and guidance on the use of collisional rates;

Peter Phillips, for numerous helpful discussions;

all members of the QMC astrophysics group who have helped at various times in acquiring the data presented here, and provided a stimulating working environment;

UKIRT staff, for support at the telescope; and also for giving me the opportunity of working with them over a period of several months, during which I was able to obtain the 2.12 μm and 20 μm data presented in Chapters 6 and 7.

I am grateful to Tina Blah for her fast and efficient typing of the manuscript.
Molecular clouds are relatively dense (> $10^2$ hydrogen molecules per cm$^{-3}$) regions of gas and dust in the interstellar medium in which the hydrogen exists predominantly in molecular form. This is because at such gas densities the rate of H$_2$ formation on the dust grains is sufficiently great to build up a self-shielding layer of molecules against the dissociating interstellar ultraviolet radiation field (e.g. Solomon 1978). Their importance lies in the fact that they provide the environment for star formation, and a knowledge of their dynamical states, structures and chemical constitutions is therefore essential to any detailed investigation of this process.

The term "molecular cloud" embraces objects with a very wide range of properties, including diameters from ~ 1-100 pc, local molecular hydrogen (+ helium) densities, $n_{H2}$, of ~ $10^2$ to $\times 10^6$ cm$^{-3}$ and gas temperatures from ~ 10K to 100K or more. (For a more extensive summary, see e.g. the recent review by Elmegreen 1984). Neither is the term totally well defined, since the more extended regions usually contain smaller subcondensations of comparatively high density and/or temperature which may be interacting with each other in a complex way.

Often associated with the clouds are particular phenomena which have come to be identified with the mechanisms of star formation, or with the presence of stars newly formed. These include HII
regions (observed either directly from their optical radiation or indirectly from their associated radio continuum flux), maser emission, shock fronts, evidence for high dynamical activity such as outflowing gas (drawn from observations of high velocity wings on molecular spectral lines), and local enhancements of temperature as inferred from the detection of compact infrared sources.

A number of schemes has been used for categorising the clouds. These have included classification according to the presence or absence of one of the characteristic features mentioned above, or alternatively on some quantitative criterion such as size, visual extinction or temperature. The last of these has proved particularly useful because the distinction between hot and cold clouds, according to whether they contain any regions of temperature greater than ~ 20K, has some objective physical basis. The heating of the molecular cloud gas by cosmic rays is, as a rule, adequate to maintain its kinetic temperature at ~ 10-15K without any additional internal sources of heating. The occurrence of any embedded stellar or protostellar objects in the cloud, however, will generally give rise to temperature enhancements to > 20K over at least part of its volume.

This led Evans (1978) to propose a division between Group A (cold) and Group B (warm, or hot-centred) clouds. Members of the former group, which includes the isolated dark globules (Bok and Reilly 1947) are often relatively small (< 10 pc diameter) and show no evidence of massive star formation, although the IRAS catalogue reveals that low mass star formation is occurring in some of them. They have typical masses < 1000 M_☉ and molecular linewidths of < 3 kms⁻¹. For Group B, the above approximate inequalities are reversed; these clouds are larger but less numerous, and include the so-called
"giant molecular clouds" (GMCs). They generally show distinct signs of massive star formation, such as the presence of molecular outflows, the proximity of OB clusters, or evidence for embedded stars such as infrared hot spots. They also often have very dense cores ($n_{\text{H}_2} \gtrsim 10^5 \text{ cm}^{-3}$ as compared with more typical cloud densities of $\sim 10^2 - 10^4 \text{ cm}^{-3}$). It is with these Group B clouds, especially their dense cores, that we are principally concerned in this thesis.

The observational problems which attend the investigation of star formation are well known. The process takes place cocooned in a cloud of gas and dust, which absorbs optical and near infrared radiation and re-emits it at far infrared, submillimetre and longer wavelengths. One must therefore observe in such spectral ranges in order to penetrate to the cloud cores. However, these wavelengths are appreciably absorbed (and also emitted) by the Earth's atmosphere. This problem can be partially overcome by observing from a high altitude site, such as Mauna Kea on the island of Hawaii (altitude 14000 ft), which is above most of the atmospheric water vapour. Here, the atmosphere is tolerably transparent over a significant proportion of the wavelength range longward of 300 $\mu$m (Ade et al. 1984). A more complete solution has recently been achieved by the IRAS satellite, which has conducted a continuum survey of the sky in broad bands centred near 12, 25, 60 and 100 $\mu$m.

From high altitude sites, broad band data can be taken in the atmospheric windows around 350 $\mu$m, 800 $\mu$m and 1100 $\mu$m (Cunningham 1982; Griffin 1985). These essentially measure the thermal emission from dust, and can be used to deduce, for example, dust temperatures and optical depths. An advantage of submillimetre continuum observations is that the emission is almost invariably optically thin, and its intensity can consequently be used to estimate dust...
column densities. Further assumptions about the ratio of \( \text{H}_2 \) molecules to dust grains and of the cloud dimensions can lead to estimates of the average \( \text{H}_2 \) densities and cloud masses. The reliability of these methods has been reviewed by Hildebrand (1983). Although they are subject to a number of uncertainties, the fact that the radiation is optically thin avoids the radiative transfer complications which can beset molecular line modelling. Continuum data are therefore used in Chapters 6 and 7 to derive average (as distinct from local) \( \text{H}_2 \) densities.

This thesis, however, is devoted mainly to molecular line observations and their interpretation. Although the dominant component of the gas in molecular clouds is \( \text{H}_2 \) (together with \( \sim 10\% \), by number, of \( \text{He} \) atoms), the symmetry of this molecule prevents its radiating under normal cloud conditions. However, the \( \text{H}_2 \) molecule can be detected indirectly through its ability to collisionally excite other molecular species which are present in much smaller abundances, and whose rotational transitions thus become observable. Over 50 molecules have been identified in this way, the vast majority of them in the last 15 years. (For a recent list, see Williams and Millar 1985).

The ease with which the transitions of a particular molecule become excited depends on its electrical dipole moment. (We shall however need to qualify this statement later). Broadly speaking, a more polar molecule requires higher local \( \text{H}_2 \) densities to excite it to an observable intensity. Molecules such as HCN and CS (especially in their millimetre and submillimetre transitions) are therefore regarded as good probes of the highest density condensations within cloud cores (\( n_{\text{H}_2} \gg 10^5 \text{ cm}^{-3} \)), whereas CO, which has a relatively low dipole moment, is observed towards regions of much
lower density ($\gtrsim 10^2$ cm$^{-3}$).

The observed intensity of a molecular line can be an extremely complex function of many variables. As well as the local gas density, these include its kinetic temperature, the abundance, $X$, of the molecule relative to H$_2$, and the overall density structure and dynamical state of the cloud. Over different physical regimes, the line intensities and profile shapes can serve as effective probes of these various properties; and such data can in principle be used to extract information on the cloud's state. Unfortunately, many (especially Group B) clouds are asymmetrical and inhomogeneous objects, and attempts to model them from observed data are apt to suffer from a surfeit of unknown free parameters, because all the above variables are initially unknown and may also vary over a variety of length scales through a cloud.

 Nonetheless, it is important that such modelling be attempted, for the evaluation of rival theories of star formation depends crucially on knowledge of the actual cloud structures and dynamical states, especially of the clumpy structures within cloud cores (Myers 1984; Silk 1985; Larson 1985; Turner 1984). Local gas densities have a determining influence on many of the physical processes associated with star formation, such as heating and cooling mechanisms, the initiation and growth of instabilities, and chemical evolution. The chemical structure of clouds is also potentially directly ascertainable from line observations, which thus provide a potential discriminant between alternative reaction schemes. (Even so, the wide disparity between derived relative molecular abundances that have appeared in the literature attest to the high model dependence of the analysis.)

The various mass, length and time scales associated with star
formation have widespread astrophysical ramifications. In the first instance, they determine the initial conditions for stellar evolution, such as the angular momentum and magnetic configuration of stars (Nakano 1981). Furthermore, the mass spectrum of clumps in the cloud cores may be intimately related to the initial stellar mass function; this in turn has a profound effect on the chemical evolution of galaxies, since the nucleosynthetic processes which can occur in a star's interior during its lifetime are dependent on its mass. Also, conditions within cloud cores help to determine the structure and state of the protostellar disc, and hence affect the formation of planetary systems.

It is with such modelling, mainly using submillimetre molecular line data, that this thesis is concerned. The basic plan is as follows. In Chapter 2, I describe some of the basic concepts of molecular line astronomy, with reference to simple linear molecules, and give a critical review of the simple techniques which are commonly employed to analyse data presented in the literature. Chapter 3 explores the effects which different cloud model assumptions have on predicted line profiles, and discusses the feasibility of making model independent deductions about cloud densities, chemical constitutions and kinematical states. In Chapter 4, some of the issues relating to data taking and calibration are outlined. In the following 3 chapters, observations of molecular clouds are presented and analysed. The material of each of these originally constituted a paper, either published or in the press (Richardson et al. 1985a; Richardson et al. 1985b; Richardson et al. 1985c). I have retained the basic format of these, so that most of the chapters are fairly self-contained and can be read independently. This means that some of the matters discussed in a general way in Chapters 2-4 are returned
to later in more specific contexts. The conclusions are given separately at the end of each chapter. However, in Chapter 8, I very briefly recapitulate these, discussing some general points arising from them and outlining possible future developments.
REFERENCES


2.1 Introduction

Molecular line observations yield information on the intensity of a source as a function of both velocity (i.e. across the line profile) and position (i.e. across the source). If data are obtained in two or more different transitions of the same molecule (if possible, for two or more isotopes) one is in principle in a position to place many constraints on physical models.

In this chapter, we review the basic ideas encountered in analysing molecular line data, and give a critical account of the assumptions commonly made in simple modelling.

The associated practical observational problems will be discussed in Chapter 4. Here, we will provisionally assume that observations can be obtained with arbitrarily high signal to noise and spatial resolution, and that the effects of the atmosphere etc. can be corrected for by a suitable calibration procedure.

2.2 Basic definitions

The line intensity towards a particular point on a source, and at a particular velocity \( v \) on the line profile, if measured with a
perfectly efficient antenna above the atmosphere, is given by the radiation temperature, \( T_R \), defined by

\[
T_R(\nu) = \frac{c^2}{2k\nu} (I_\nu - I_{2.7}) ,
\]

where \( I_\nu \) and \( I_{2.7} \) are the respective specific radiation intensities from the source and from the cosmic background. It is also given in terms of the source properties by

\[
T_R(\nu) = \frac{h\nu}{k} \left\{ \frac{1}{\exp(h\nu/kT_{\text{ex}})-1} - \frac{1}{\exp(h\nu/2.7k)-1} \right\} (1 - \exp(-\tau_\nu))
\]

for a homogeneous source of excitation temperature \( T_{\text{ex}} \) and optical depth \( \tau_\nu \). This relates the observed quantity \( T_R \) to \( T_{\text{ex}} \) and \( \tau_\nu \), which are not directly observable but are in principle calculable from a particular cloud model. In the event that \( T_R(\nu) \) consists of contributions from different points along the line of sight with different excitation temperatures, equation 2.2 must be replaced by the integral expression

\[
T_R(\nu) = \frac{h\nu}{k} \int_0^{\tau_{\text{total}}} \left\{ \frac{1}{\exp(h\nu/kT_{\text{ex}}(\tau))-1} - \frac{1}{\exp(h\nu/2.7k)-1} \right\} \exp(-\tau_\nu) d\tau_\nu
\]

The excitation temperature is defined, in terms of the relative populations in the two levels \( i \) and \( j \) of the transition, by:
\[
\frac{n_j}{n_i} = \exp\left(-\frac{hv}{kT_{ex}}\right)
\]  

(2.4)

where \(n_j\) and \(n_i\) are the relative molecular populations per degenerate sublevel, being given by

\[
n_i = \frac{N_i}{g_i}
\]

(2.5)

with a similar expression for level \(j\), where \(N_i\) is the total level population and \(g_i\) is its degeneracy.

By definition, we have

\[
\sum_{\text{levels}} g_k n_k = 1
\]

(2.6)

Since real telescopes have finite beamwidths, it is often useful to convolve the predicted spatial distribution of \(T_R\) with a beam profile shape, giving the practically observed quantity \(T_{R*}\) (see Chapter 4; also Kutner and Ulich 1981).

2.3 Modelling

Construction of a cloud model consists essentially of 4 stages:

(i) Specification of free parameters e.g. densities, molecular abundances relative to \(H_2\), kinematical structure etc.;

(ii) Determination of the excitation temperatures of all transitions of interest, as a function of position in the cloud;

(iii) The evaluation of equation 2.3 to give the theoretically observable quantity \(T_R\) as a function both of position and frequency (velocity);

(iv) The convolution of the derived \(T_R\) with a beam profile to give predictions of the observable quantity \(T_{R*}\), again as a function of velocity and position.
Steps (i), (iii) and (iv) are essentially straightforward compared with (ii), which we now discuss in more detail, along which a consideration of the approximations and simplifying assumptions which are often made.

2.3.1. Energy levels and excitation temperatures

We consider a linear molecule which has a pure rotation spectrum without hyperfine structure. This case is appropriate to the molecular line observations described in this thesis. (An exception is HCN, which has hyperfine structure. This, though, is not usually resolved except in the lowest rotational transition).

The energy levels of such a molecule are given by

$$E_{Jv} = \hbar \omega (v + 1/2) - \hbar \omega (v + 1/2)^2 + J(J+1) \omega - DJ^2(J+1)^2\hbar - \alpha (v + 1/2) J(J+1)\hbar$$

(2.7)

where $v$ and $J$ are both integers $\geq 0$, (Townes and Schawlow 1955 - see this work also for definitions and meanings of the terms in 2.7).

We shall be concerned only with rotational transitions in the ground ($v = 0$) vibrational state, so the only relevant terms on the right hand side of 2.7 are the third and fourth. The constants $B$ and $D$ (both expressed in Hz) are respectively the rotational constant and the centrifugal distortion constant. $D$ is typically a few orders of magnitude smaller than $B$ so the centrifugal term can be neglected for the purpose of constructing models. The only radiative transitions allowed between rotational levels are those for which $\Delta J = \pm 1$, which gives a set of observed frequencies

$$v(J+1 \rightarrow J) = 2B(J + 1)$$

(2.8)

For example, for CO, the approximate frequencies of the 1st 3 transitions are 115 GHz ($J=1-0$), 230 GHz ($J=2-1$) and 345 GHz ($J=3-2$).
The population of each rotational level is in a state of dynamical equilibrium between the radiative and collisional processes tending to populate and depopulate it. The level populations are therefore given by a solution of the equations of statistical equilibrium. Having determined them, one can then specify the excitation temperatures $T_{\text{ex}}(J+1\rightarrow J)$ defined by equations 2.4 and 2.5, with

$$g_J = 2J + 1$$  \hspace{1cm} (2.9)

2.3.2. Radiative transitions

Consider first the radiative processes tending to populate or depopulate a rotational level $j$ of quantum number $J$. Because of the dipole selection rules, it is only necessary to deal with transitions to and from the levels immediately above and below level $j$. These will be denoted by the indices $k$ and $i$ and have rotational quantum numbers $J+1$ and $J-1$. The transition frequencies are $\nu_1 (j\rightarrow i)$ and $\nu_2 (k\rightarrow j)$ (see Figure 2.1).

The net rate of population of level $j$ by radiative processes at a particular point in the gas is then given by

$$\frac{\partial N_j}{\partial t} = \text{rad} = -B_{jk} \bar{J} \nu_2 N_j - B_{ji} \bar{J} \nu_1 N_j$$

$$+ B_{kj} \bar{J} \nu_2 N_k + B_{ij} \bar{J} \nu_1 N_i$$

$$- A_{ji} N_j + A_{kj} N_k$$  \hspace{1cm} (2.10)

In equation 2.10, $A_{ji}$, $B_{ji}$ and $B_{ij}$ are the familiar Einstein coefficients for spontaneous emission ($\Delta J = -1$), absorption ($\Delta J = +1$) and stimulated emission ($\Delta J = -1$), and are related through
\[ g_i B_{ij} = g_j B_{ji} = g_j \frac{c^2 A_{ji}}{2h\nu_{ji}} \]  \hspace{1cm} (2.11)

\( \bar{J}_\nu \) is the mean intensity of the radiation field, defined by

\[ \bar{J}_\nu = \frac{1}{4\pi} \int_{-\infty}^{\infty} J_\nu \, d\nu \]  \hspace{1cm} (2.12)

where \( I_\nu \) is the specific radiation intensity, and \( J_\nu \) the normalized line profile function (see equation 2.21) at that point.

From equations 2.9, 2.10 and 2.11 one can easily derive

\[ \frac{\partial n_{jrad}}{\partial t} = \frac{g_k}{g_j} \frac{A_{kj}}{\lambda_{kj}} (n_k + \frac{c^2}{2h\nu_2^3} n_k \bar{J}_{\nu_2} - \frac{c^2}{2h\nu_1^3} n_j \bar{J}_{\nu_1}) 
- A_{ji} (n_j + \frac{c^2}{2h\nu_1^3} n_j \bar{J}_{\nu_1} - \frac{c^2}{2h\nu_1^3} n_i \bar{J}_{\nu_1}) \]  \hspace{1cm} (2.13)

### 2.3.3 Collisional transitions

A molecule may also change its rotational level during a collision with another molecule. In molecular clouds, by far the most important collisional partners are \( \text{H}_2 \) and \( \text{He} \).

Collisionally induced transitions can occur between any pair of levels. For collisional transitions to and from level \( j \), we have

\[ \frac{\partial N_{J_{coll}}}{\partial t} = \sum_{L=J+1}^{\infty} \left\{ N_L C_{L+J} - N_J C_{J+L} \right\} 
+ \sum_{L=0}^{J-1} \left\{ N_L C_{L+J} - N_J C_{J+L} \right\} \]  \hspace{1cm} (2.14)
Figure 2.1

Labelling of energy levels for a diatomic molecule
The quantities $C_{L+J}$ etc. are the collisional rates between pairs of transitions, given by

$$C_{L+J} = R_{L+J} n_{H2} \quad (2.15)$$

The rate constants $R_{L+J}$ can be found theoretically by calculating collisional cross sections which are then averaged over the particle velocities, which follow a Boltzmann distribution (Spitzer 1978). The rate constants, therefore, vary with temperature.

Upward and downward rates are related through the principle of detailed balance,

$$\frac{C_{L\rightarrow J}}{C_{J\rightarrow L}} = \frac{g_J}{g_L} \exp \left\{ -\frac{\hbar B}{kT} (J+1) - L (L+1) \right\} \quad (2.16)$$

which has the convenient consequence that one needs only to input explicitly either the downward or the upward rates - not both - into the statistical equilibrium equations.

Combining equations 2.6, 2.14 and 2.16, we obtain

$$\frac{\partial n_J}{\partial t} = \sum_{L=J+1}^{\infty} \frac{C_{L\rightarrow J}}{g_J} g_L \left\{ n_L - n_J \exp \left( -\frac{\hbar B}{kT_k} (L+1) - J(J+1) \right) \right\}$$

$$+ \sum_{L=0}^{J-1} \frac{C_{J\rightarrow L}}{g_J} g_L \left\{ n_L \exp \left( -\frac{\hbar B}{kT_k} (J+1) - L(L+1) \right) - n_J \right\} \quad (2.17)$$

In this equation, the first bracketed terms after each summation sign are the downward collisional rates per magnetic sublevel. Goldreich and Kwan (1974) assumed that these were all equal, so they took them outside the summation signs and called
them all C. Since their work, however, theoretically derived rate constants for individual transitions have appeared in the literature for a number of molecules (e.g. Green and Thaddeus 1976; Green and Chapman 1978, Green and Thaddeus 1974; Monteiro 1984b; Monteiro; Flower and Launay 1985).

2.3.4. Determination of level populations

In equilibrium we have, for level $J$,

$$\frac{\partial n_J}{\partial t} = \frac{\partial n_J}{\partial t}^{\text{rad}} + \frac{\partial n_J}{\partial t}^{\text{coll}} = 0$$

where the radiative and collisional contributions are given by 2.13 and 2.17. Although they both involve summations to infinity, there will in practice be a level $J = J_{\text{max}}$ above which it may safely be assumed that the level populations are zero. In this thesis, I have set $J_{\text{max}} = 10$. If equation 2.18 is then used to express the equilibrium condition for the $J_{\text{max}} - 1$ lowest levels, and we also add the constraint

$$\sum_{J=0}^{J_{\text{max}}} (2J+1) n_J = 1$$

we now have a system of $J_{\text{max}}$ equations which can in principle be solved to give the values of $n_J$.

To achieve this, we need to know all the other quantities in equations 2.13 and 2.17, and this involves uncertainties.

Firstly, theoretical calculations of collisional cross sections are very difficult, and approximate methods have to be used (e.g. Monteiro 1984a). The published values often used in astrophysical modelling only claim accuracies of ~ 20-30%. Even if the errors had the same magnitude and sign for all transitions, any derived
H$_2$ densities would be subject to similar fractional uncertainty and, if the errors were more random, the situation might be even worse.

Goldsmith, Young and Langer (1983) examined predicted antenna temperatures for the lowest 2 transitions of CO using a simple LVG model. They investigated the sensitivity of predicted intensities for two alternative sets of collisional rates from the literature, and concluded that the discrepancy was small compared with other observational and modelling uncertainties. However, their statement that "for log n(H$_2$) < 5.5 the two transitions are optically thin, and thus differences due to different collision rates should be apparent" is misleading. Over much of the density range they considered ($10^2 - 10^7$ molecules per cm$^3$) the transitions are collisionally thermalised anyway, so the optical depth is irrelevant. When the collisional terms dominate the radiative terms in 2.18, emergent antenna temperatures are very insensitive to the assumed collisional rates. (The example they used was for a cloud with T$_K$ = 40 K, $X_{CO}/(dt/dr) = 10^{-8}$ km$^{-1}$s pc; in this case, T$_{ex}/T_k > 0.8$ for $n_{H_2} > 2 \times 10^3$ cm$^{-3}$ (CO J=1-0) and $n_{H_2} > 2 \times 10^4$ cm$^{-3}$ (CO J=2-1). It is likely that errors caused by inaccuracies in derived collisional rates will be much more serious when incompletely thermalised lines are used to derive local H$_2$ densities. The effect that this has on, for example, HCO$^+$ and CS results still needs to be thoroughly examined.

A second, and more fundamental problem lies in occurrence of the mean radiation intensity $\bar{J}_\nu$ in the statistical equilibrium equations. This expresses the fact that the radiation field will in general exert an influence on the level populations through the processes of absorption and stimulated emission. $\bar{J}_\nu$ is itself
dependent on the level populations, not only at the point under consideration, but at all points from which contributions to $J_\nu$ have originated. Thus, different parts of a cloud may be radiatively coupled together and the solution of the statistical equilibrium equations, being now a non-local problem, may require an iterative approach in which the global properties of the cloud participate. As well as the inevitably increased computing demands, this also imposes the inconvenience of an additional set of free parameters.

It is also conceivable that continuum emission from nearby infrared sources could contribute to the excitation of molecules. Carroll and Goldsmith (1981) examined the possibility of infrared pumping of the CS molecule via the vibrationally excited states. They concluded that the mechanism could be important for CS (much less so for HCN and CO) near the hot sources M17 a/b and W3-IRS 2/2a, where it might mimic the effect of high densities.

If, ultimately, the above difficulties can be surmounted and the excitation conditions found as a function of position in the cloud, then the predicted emergent radiation temperatures can also be evaluated for any frequency across the line profile, using equations 2.2 and 2.3. The optical depth increment $d\tau_\nu$ is given for each transition by

$$d\tau_\nu = \chi_\nu dz$$  \hspace{1cm} (2.20)

where $dz$ is an increment of distance along the line of sight and $\chi_\nu$ is the line opacity, expressible as

$$\chi_\nu = B_{ij} \frac{h\nu}{4\pi} g_i (n_i - n_j) \Phi_\nu X_{nH_2}$$  \hspace{1cm} (2.21)

Here, $\Phi_\nu$ is the normalised line profile function, corresponding to the line-of-sight Doppler velocity profile of the molecules at
that particular point in the cloud. Throughout this analysis, we make the usual assumption of complete redistribution of absorbed and emitted photons across the line profile, so that the local line profile function for emission is also given by $\phi_\nu$, and the excitation temperature at a particular point does not vary with particle velocity. The relaxation of this assumption for CO profiles was investigated by Deguchi and Kwan (1982), who found that it made little difference — a few percent at most — to computed antenna temperature predictions across the line profile.

The line emission coefficient $n_\nu$ is now expressed as

$$n_\nu = A_{ji} \frac{\hbar \nu}{4\pi} g_j n_j \phi_\nu X n_{H2}$$  \hspace{1cm} (2.22)

An alternative way of describing the excitation conditions at a point in the cloud is in terms of the source function, $S_\nu$, defined by

$$S_\nu = \frac{n_\nu}{X_\nu} = \frac{2h\nu^3}{c^2} \frac{1}{(n_i/n_j - 1)}$$  \hspace{1cm} (2.23)

It is clear that to find the excitation conditions at a particular point in a cloud can be formidably difficult, because they in general depend in a complex way on the $H_2$ and $He$ densities, the relative abundance $X$ of the observed molecule to $H_2$, and the kinematics (on a variety of length scales) in the cloud.

Various simplifying assumptions are nevertheless often possible, and I shall in the following sections discuss two which are used extensively both in the modelling presented in later chapters, and elsewhere in the literature.
2.4 The assumption of complete thermalisation

The collision rates, $C_{ji}$, in equation 2.17 can be expressed as $R_{ji} n_{H_2}$, where the $R_{ji}$ are the rates per colliding $H_2$ (or He) molecule and are assumed known from theoretical calculations. It then follows from inspection of 2.17 and 2.13 that, provided the local $H_2 + He$ density is high enough to satisfy

$$n_{H_2} R_{ji} > A_{ji}$$

then the collisional term in 2.18 will overwhelm the radiative term, and the excitation temperature will approach the kinetic temperature $T_k$. Inequality 2.24 therefore constitutes a sufficient condition for thermalisation of the line. It also enables us to define a characteristic density $n^*$, by

$$n^* = \frac{A_{ji}}{R_{ji}}$$

above which a particular transition will be thermalised (Evans 1980). Since $A_{ji}$ for a rotational transition of a symmetric molecule is given by

$$A_{J+1, J} = \frac{512}{3} n^4 \frac{\bar{\mu}^2}{hc^3} \frac{(J+1)^4}{(2J+3)}$$

where $\bar{\mu}$ is the electrical dipole moment of the molecule in esu, the simplistic application of 2.24 would imply that:

(a) for a particular molecule, higher $J$ transitions become thermalised at higher densities; and

(b) molecules with low dipole moments (e.g. CO, NH$_3$) become thermalised at lower densities than ones with higher dipole moments (e.g. CS, HCN, HCO$^+$).

Values of $n^*$ obtained from 2.25 are shown in Table 2.1 for the transitions relevant to this thesis.
If a particular transition is thermalised (or at least if we know its excitation temperature), the optical depth of a homogeneous region with line-of-sight extent L can be expressed, using 2.20 and 2.21, as

$$\tau_\nu = B_{ij} \frac{h\nu}{4\pi} g_i n_i (1 - \exp(-h\nu/kT_{ex})) \Phi \lambda n_{H_2}$$  \hspace{1cm} (2.27)

In the Rayleigh Jeans limit, $h\nu \ll kT_{ex}$, and, neglecting the 2.7 K background (as we shall also do throughout the rest of this section), we have, from 2.2:

$$T_R(\nu) = T_{ex} (1 - \exp(-\tau_\nu))$$  \hspace{1cm} (2.28)

If spectra are available in the same transition of 2 isotopes of the same molecule e.g. $^{12}$CO and $^{13}$CO, then 2.2 or 2.28 may be used to find their optical depth. If their excitation temperatures are equal, then

$$\frac{T_R(^{13}CO)}{T_R(^{12}CO)} = \frac{(1 - \exp(-\tau_{13}))}{(1 - \exp(-\tau_{13}))}$$  \hspace{1cm} (2.29)

where $I$ is the isotopic abundance ratio [$^{12}$CO]/[$^{13}$CO] and is variously assumed to have values between 40 (Dickman 1978) and 89 (the terrestrial value).

When two isotopes have optically thin transitions, the exponentials in 2.29 may be expanded to first order, giving the abundance ratio directly. Because they are optically thin, we are probably justified in assuming that their excitation temperatures are equal even if they are not thermalised, since the $J_\nu$ terms in 2.13 will usually be small, and it is they which can lead to different excitation temperatures between 2 isotopic lines of differing optical depths. This method has been used
<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Frequencies (GHz)</th>
<th>Dipole moment (debye) (1)</th>
<th>n_\text{rad} (cm^{-3})</th>
<th>n^* (cm^{-3})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>J=1-0</td>
<td>115.271</td>
<td>0.112</td>
<td>2x10^3</td>
<td>2x10^4</td>
</tr>
<tr>
<td></td>
<td>J=2-1</td>
<td>230.538</td>
<td>1.97</td>
<td>1x10^4</td>
<td>1x10^4</td>
</tr>
<tr>
<td></td>
<td>J=3-2</td>
<td>345.796</td>
<td>3.0</td>
<td>4x10^4</td>
<td>4x10^4</td>
</tr>
<tr>
<td></td>
<td>J=5-4</td>
<td>244.936</td>
<td>4.0</td>
<td>3x10^3</td>
<td>3x10^3</td>
</tr>
<tr>
<td></td>
<td>J=7-6</td>
<td>342.883</td>
<td></td>
<td>5x10^3</td>
<td>5x10^3</td>
</tr>
<tr>
<td></td>
<td>J=4-3</td>
<td>364.505</td>
<td></td>
<td>4x10^3</td>
<td>4x10^3</td>
</tr>
<tr>
<td></td>
<td>J=4-3</td>
<td>356.733</td>
<td></td>
<td>2x10^4</td>
<td>2x10^4</td>
</tr>
</tbody>
</table>

NOTE (1) 1 debye = 10^{-18} esu

### TABLE 2.1

- \( \frac{\langle \text{d}v/\text{d}r \rangle}{v} = 10^{-5} \)
- \( \frac{\langle \text{d}v/\text{d}r \rangle}{v} = 10^{-7} \)
by Wilson et al. (1976) and Frerking et al. (1980) to estimate

\[ I_{\text{CS}} = \frac{[^{13}\text{CS}]/[^{34}\text{S}]} \]

from the weighted integral ratio

\[
I_{\text{CS}} = \frac{\int T_A(^{13}\text{CS}) T_A(^{12}\text{CS}) \, dv}{\int T_A(^{34}\text{S}) T_A(^{12}\text{CS}) \, dv} \quad (2.30)
\]

A spectrum in a molecular transition which is both thermalised
and optically thin can be used to estimate the total molecular
column density along a line of sight. The population per magnetic
sublevel of a rotational level \( J \) is given by

\[
n_J = \frac{1}{Z} \exp \left[ -\frac{\hbar B J(J+1)}{kT} \right] \quad (2.31)
\]

where \( Z \) is the partition function. For \( \hbar B \ll kT \) and complete
thermalisation, \( Z \) can be approximated as

\[
Z = \frac{kT}{\hbar B} \quad (2.32)
\]

(e.g. See Townes and Schawlow 1955).

We can now combine 2.2, 2.11, 2.26, 2.27, 2.28, 2.31 and 2.32
to give, for the integrated intensity across the line \( J+1 \rightarrow J \),

\[
\int T_R(dv/km s^{-1}) = T \Delta V \\
= \frac{8\pi^2 \mu^2 (J+1) B N_{\text{col}}}{3 \times 10^5 k} \exp \left[ -\frac{\hbar B J(J+1)}{kT} \right] (1 - \exp \left[ -\frac{2\hbar B (J+1)}{kT} \right]) \quad (2.33)
\]

where \( N_{\text{col}} \) is the column density of the molecule along the line of
sight, which can hence be estimated from the integrated line
intensity. Additionally, with further input of an assumed value
for the line of sight extent of the cloud one can extract an approximate average number density of molecules. Knowledge (or a guess) of \( X \) then leads to an estimate of the average number density of \( \text{H}_2 \) molecules. The validity and reliability of this procedure, which has been extensively employed to interpret observations in e.g. the \(^{13}\text{CO} \) and \(^{18}\text{O} \) J=1-0 transitions (e.g. Bally and Lada 1983), will be assessed further in Chapter 5.

For 2 adjacent transitions of the same species (J+1->J and J->J-1, say), the ratio of their optical depths is given from 2.27 by

\[
\frac{T_{J+1, J}}{T_{J, J-1}} = \frac{(J+1)}{J} \exp \left\{ -\frac{2hBJ}{kT_{\text{ex}}(J, J-1)} \right\} \frac{(1-\exp(-2hBJ/kT_{\text{ex}}(J, J)))}{(1-\exp(-2hBJ/kT_{\text{ex}}(J, J-1)))}
\]

(2.34)

For optically thin lines of equal excitation temperatures, this is also the ratio of radiation temperatures. For transitions satisfying \( 2hBJ \ll kT_{\text{ex}} \) we have

\[
\frac{T_{R}(J+1, J)}{T_{R}(J, J-1)} = \left( \frac{J+1}{J} \right)^2
\]

(2.35)

In hot, optically thin molecular outflows, for example, the observed values of \( T_{R} \) for CO would be in the ratio 1(J=1-0): 4(J=2-1): 9(J=3-2) etc. for thermalised lines. Deviations from this behaviour in higher transitions have been used (van Vliet et al. 1981; Storey et al. 1981) to estimate excitation temperatures in the Orion molecular outflow. The procedure can give misleading results, though, and is discussed further in Chapter 5 for outflow sources.

Equation 2.34 was used also by Plambeck, Snell and Loren (1983)
to derive optical depths for the CO J=1-0 and CO J=2-1 transitions in various sources with high velocity wings, using assumed values for the excitation temperature. Again, for further discussion, see Chapter 5.

2.5 Local radiative excitation and the large velocity gradient (LVG) approximation

Although the equations derived in the last section are useful for CO and its isotopes, the assumption of thermalisation is frequently invalid even for this molecule, and is even more so for higher excitation lines of other species such as those listed in Table 2.1. Moreover, molecular line observations are often particularly informative over the regime of partial thermalisation because they are then a potential probe of local H$_2$ densities rather than the average values obtained using equations such as 2.33. However, relaxation of the thermalisation condition necessitates further consideration of the radiative terms contained in 2.13.

Under what conditions will a transition not be thermalised? It must be stressed here that inequality 2.24, though a sufficient condition for thermalisation, is not a necessary one since, if the terms containing $J_\nu$ in 2.13 are of appreciable magnitude, the collisional terms can still dominate 2.18, even if $A_{ji}$ is too high to satisfy 2.24.

We need expressions for the $J_\nu$ terms in 2.13. Many observed molecular line spectra are much larger (typically one or two orders of magnitude) than typical thermal line widths (~ 0.2 kms$^{-1}$), and it was postulated by Goldreich and Kwan (1974) that this is due to large scale gravitational collapse of the clouds. One can then make the Large Velocity Gradient (LVG) assumption that
\[ \frac{\Delta l}{l_0} = \frac{\Delta v_{\text{th}}}{v_0} \ll 1 \quad (2.36) \]

where \( v_0 \) and \( l_0 \) are typical systematic velocity and length scales in the cloud, \( \Delta v_{\text{th}} \) is the local Doppler line width and \( \Delta l \) is the distance from its point of emission over which a photon has an appreciable chance of being reabsorbed. The LVG condition \( 2.36 \) implies that such a photon, if not reabsorbed locally, will escape from the cloud because of the Doppler shifts created by the systematic velocity gradients.

Sobolev (1960) and Castor (1970) have shown that the values of \( J_v \) are then purely locally determined, so that any point in the cloud can be considered independently of any other. \( J_v \) at a point is then given by

\[ J_v = (1 - \beta) S_v + \beta I_{2.7} \quad (2.37) \]

where \( S_v \), the source function at that point, is determined by \( 2.23 \); also

\[ I_{2.7} = B_v(T = 2.7K) \quad (2.38) \]

and \( \beta \) is the probability that a photon of frequency \( v \), emitted at that point, will escape from the cloud. The second term in the right hand side of \( 2.37 \) represents the contribution to \( J_v \) from \( 2.7K \) background photons which have entered the cloud.

If the cloud collapse is homogeneous and isotropic, \( \beta \) is related to the optical depth by

\[ \beta = \frac{1 - \exp(-\tau)}{\tau} \quad (2.39) \]

(More general expressions for \( \beta \) will be given in Chapter 3.)

In the LVG case, the profile shape \( \Phi_v \) may be regarded (within an
infinitesimal volume of spatial extent \( \text{dr} \) as a top hat function of height \( 1/\text{dv} \) and width \( \text{dv} \), where

\[
\text{dv} = \frac{\nu}{c} \frac{\text{dv}}{\text{dr}} \text{ dr}
\]  

(2.40)

and \( \text{dv}/\text{dr} \) is the local velocity gradient in the cloud (here constant for all positions and orientations). So equation 2.27 now becomes

\[
\tau_\nu = B_{ij} \frac{hc}{4\pi} \frac{g_i n_i}{(\text{dv}/\text{dr})} (1 - \exp(-h\nu/kT_{\text{ex}})) \times n_{H2}
\]

\[
= \frac{c^3 A_{ji}}{8\pi^3} \frac{g_j n_i}{(\text{dv}/\text{dr})} (1 - \exp(-h\nu/kT_{\text{ex}})) \times n_{H2}
\]  

(2.41)

2.5.1 The 2 level molecule

Many features of the excitation conditions can be reproduced analytically by a simple model employing a 2 level molecule (Scoville and Solomon 1974), whose lower and upper levels we will index as \( i \) and \( j \) respectively. We drop the suffices from the downward collisional and spontaneous deexcitation rates \( \text{C} \) and \( \text{A} \), and neglect the 2.7 K background. Truncating equation 2.13, 2.17 and 2.18 to the 2 level case, and substituting into them 2.23 and 2.37, we find, after some manipulation,

\[
T_{\text{ex}} = \frac{T_k}{1 + \frac{kT_k}{h\nu} \ln (1 + \frac{BA}{C})}
\]  

(2.42)

From 2.39 it follows, for \( T \ll 1 \), that
\[
T_{\text{ex}}(\text{thin}) = \frac{T_k}{1 + \frac{kT_k}{h\nu} \ln \left( 1 + \frac{A}{C} \right)}
\]  
(2.43)

while for \(\tau >> 1\), we have

\[
T_{\text{ex}}(\text{thick}) = \frac{T_k}{1 + \frac{kT_k}{h\nu} \ln \left( 1 + \frac{A}{\tau C} \right)}
\]  
(2.44)

These two limiting expressions, which were derived by Scoville and Solomon (1974), differ only in the occurrence of \(\tau\) in 2.44. The latter equation shows that in conditions of high optical depth the spontaneous deexcitation coefficient, \(A\), has effectively been replaced by \(A/\tau\); consequently, a line may be thermalised without condition 2.24 being satisfied. Thus, because of this radiative trapping effect, the values of \(T_R\) for all molecular lines, regardless of their dipole moments and of the local molecular hydrogen densities, approach the kinetic temperature \(T_k\) in the limit of high \(\tau\). In fact, even before this point is reached, the value of \(T_{\text{ex}}\) attained becomes independent of \(A\), because of the proportionality of \(\tau\) to \(A\) (see equation 2.41).

The frequently made assertion that "molecules of high dipole moment require high densities to excite them and so are excellent tracers of regions of high density" therefore requires very heavy qualification: it is only valid when the transition is optically thin. If, for example, CS or HCN were as abundant in the galaxy as CO is, they would probably be as widely observed, despite their high dipole moments.

To emphasise the importance of radiative trapping, we give in Table 2.1 some illustrative examples of its influence on the
approximate local $\text{H}_2$ densities needed to thermalise a line. For
relative molecular abundances of $X = 10^{-7}$ and $10^{-5}$ are tabulated
values of $n^{*}_{\text{rad}}$ for each transition, where $n^{*}_{\text{rad}}$ is the $\text{H}_2 + \text{He}$
density required to raise the excitation temperature of the
transition to 75% of the kinetic temperature. (I have used the
simple multilevel LVG model described in subsection 2.5.2. for
a cloud kinetic temperature of 40K and a uniform velocity gradient
of 1 kms$^{-1}$ pc$^{-1}$). It is evident that, even for $X/(dv/dr) = 10^{-7}$
kms pc, the transitions have ceased to provide any meaningful
discriminant between different regimes of $\text{H}_2$ density above
$\sim 10^4$ cm$^{-3}$. Although such relative abundances are somewhat higher
than values which have been presented in the literature (except for
CO), they are by no means implausible. Many previous estimates have
been derived from LVG modelling, often together with the implicit
assumption that the sources are extended relative to the telescope
beam. Recent papers have tended to present upward revisions of
abundances. Frerking et al. (1980) derived values of $X_{\text{CS}}/(dv/dr)$
which were factors of from 5 to 50 times greater than those previously
found by Linke and Goldsmith (1980) and fell in the range $5 \times 10^{-10}$
to $1 \times 10^{-8}$ km$^{-1}$ s pc. Snell et al. (1984) in their LVG analysis
of apparently clumpy clouds remarked on the uncertainty in our
knowledge of $X_{\text{CS}}$ and raised the possibility that, as an explanation
of the large variance in their measurements of CS column density
at different positions across the same cloud, the fractional
abundance of CS could be over an order of magnitude greater at the
centre of cloud cores than at their edges. Recently quoted values
for $X_{\text{HCO}^+}$ towards the outflow sources NGC 2071 and Cepheus A are
$\sim 10^{-8}$ and $3 - 6 \times 10^{-9}$ respectively (Wootten et al. 1984, Loren et
al. 1984) — again, much higher than many previously presented results
(e.g. $X_{\text{HCO}^+} \sim 10^{-11}$ in hot central clouds; see Wootten, Snell and Evans 1980). Another recent estimate of $X_{\text{HCO}^+}$ by Vogel et al. (1984) for Orion A gave $\sim 10^{-9}$ for the core material and a lower limit of $10^{-8}$ for the outflow.

Bearing in mind these wide variations between values of $X$ estimated for high dipole moment species, the great model-sensitivity of the derivations, and also the strong suspicion both from observations and theoretical chemical modelling that $X$ may vary drastically throughout a cloud, we are led to the conclusion that molecules such as CS, HCO$^+$ and HCN, though their detection may be suggestive of high densities, are not uniquely diagnostic of them.

However, the detection of a relatively transparent isotopic line in addition to the corresponding main line does constitute much more convincing evidence for high local $H_2$ densities e.g. see the discussion of the data in the $J=4-3$ transition of HCO$^+$ and $H^{13}CO^+$ in S255 and DR21 in Chapters 6 and 7. Such isotopic observations (or good upper limits) are therefore essential to any reliable estimate of cloud densities from molecular line data, unless there is good reason to believe that the main isotopic lines are not too opaque (e.g. see the analysis of the CO wing data in Chapter 5).

2.5.2. A simple multilevel LVG model

Although LVG kinematics are at best an oversimplification of conditions within molecular clouds, such a model is often used in interpreting observations. A more detailed critique of its merits and demerits will be given in Chapter 3; suffice it to say here that it has a number of convenient attributes:

Firstly, it is superior to the simple thermalised models described earlier in the sense that it is capable of dealing with conditions of
partial thermalisation. In addition, by employing the local Sobolev expression for the radiation intensity $\tilde{J}_\nu$, one is able to make some correction for the effect of radiative trapping on local excitation temperatures, especially if a likely value of the local velocity gradient, $dv/dr$, which appears in the expression for $\tau$, can be estimated. Even in a situation of total ignorance of the cloud kinematics, use of an LVG model is still likely to be superior to a cruder treatment which either assumes total thermalisation and/or neglects radiative terms.

Furthermore - and this is especially true for a highly symmetrical cloud - an LVG model makes very specific predictions about the variation of intensity with velocity at a fixed line of sight (i.e. the spectrum) and its relationship to the variation of intensity with position at a fixed velocity (e.g. drift scan profile), essentially because radiation at a particular velocity comes from one position along the line of sight.

It is convenient firstly to consider a point where the local velocity gradient is isotropic. (This would be the case for all points within a cloud which was contracting or expanding with a velocity proportional to radial distance). A program has been developed in which the equations of statistical equilibrium 2.18 were solved, with the radiative terms given by 2.13 and the collisional terms by 2.17. The ladder of energy levels was truncated at $J=10$. Equations 2.18 were used for $J=0,1,2,...,9$, together with constraint 2.19 (for $J_{\text{MAX}} = 10$). The expressions 2.4, 2.8, 2.9, 2.23, 2.37, 2.39 and 2.41 were used to express the values of $J_\nu$ in terms of the level populations $n_J$ ($J=0,1,2,...,10$). This gave a system of 11 non-linear equations which could be solved for the 11 unknown values of $n_J$. The routine used for this was
CO5NBF of the Numerical Algorithms Library (NAG). Finally, the emergent radiation temperature was calculated from 2.2 and 2.4. The whole program (with associated plotting routines) was run on the Queen Mary College ICL 2988 computer.

Tabulated values of collisional rates were taken from the literature, and for any chosen gas kinetic temperature $T_k$, relative molecular abundance $X$, local velocity gradient $(dV/dr)$ and local gas density $n_{H_2}$, a printout could be obtained which consisted of the calculated values of $n_J$, $T_{ex}$, $\tau$ and $T_R$ for each transition. An alternative way of displaying the results was on a 2 dimensional contour plot, on logarithmic axes of $n_{H_2}$ and $X/(dV/dr)$. Contours of $T_R$, $T_{ex}$ or $\tau$ could be plotted for any transition, as well as ratios of any of these quantities between 2 transitions and/or 2 different isotopes of the same molecule.

2.5.3. Results

Examples of plots from the model for an assumed kinetic temperature of 40K are shown in Figures 2.2 - 2.5, which have been chosen to illustrate the diversity of excitation conditions, and more specifically to delimit the regimes over which a number of common assumptions in molecular line astronomy are really applicable. Figure 2.2 refers to the CO $J=1-0$ transition and shows contours of $T_R$, of the excitation temperature $T_{ex}$, and of the optical depth $\tau$. Also shown are 2 contours of optical depth for the $^{13}$CO isotope ($\tau_{13} = 0.1$ and $\tau_{13} = 0.5$) determined on the assumption of a $[^{12}$CO]/[$^{13}$CO] abundance ratio of 40 (Dickman 1978). Figure 2.3 shows similar information for the CO $J=3-2$ transition (omitting details for $^{13}$CO, whose $J=3-2$ transition falls in a region of relatively high atmospheric opacity). In Figure 2.4, ratios of $T_R$ between the $J=3-2$ and $J=1-0$ lines are plotted, while in Figure 2.5, the contours are of $T_R$ for the $J=1-0$ and $J=4-3$ transitions.
Figure 2.2

LVG results for the CO J=1-0 transition

Contour levels:

- $T_R$ (solid line) = 2-36K, interval = 2K
- $T_{ex}$ (dashed line) = 4, 10, 20, 30, 40, 50, 60K
  (showing the regime of superthermal excitation)
- $\tau$ (dotted line) = 1, 10, 100
- $\tau$ ($^{13}$CO, crossed line) = 0.1, 0.5
  (for an assumed isotopic abundance ratio of 40)

Units:

- $n(H_2 + He)/cm^{-3}$
- $X/(dv/dr)/km^{-1}s pc$
Figure 2.3
LVG results for the CO 3-2 transition

Contour levels:
\( T_R \) (solid line) = 2, 6, 10, 14, 18, 22, 26, 30, 32K
\( T_{ex} \) (dashed line) = 6, 10, 20, 30, 38K
(The deviation of \( T_{ex} \) contours from the vertical shows the effects of radiative trapping).
\( \tau \) (dotted line) = 1, 10, 100
Units as for Figure 2.2
of HCO\(^+\). (Note that for HCO\(^+\) the abundance range chosen is much wider than is usually measured from observations. This is simply to compare the behaviour of a high dipole moment molecule with that of CO over a similar abundance range).

The following features are noteworthy:

(i) **Radiation temperatures**

Over a substantial area of the \(X/(dv/dr), n_{\text{H}_2}\) plane, the value of \(T_R\) even for the \(J=1-0\) line is significantly lower than the 36.5K which would be obtained for an optically thick, thermalised line. As an example, for \(X/(dv/dr) = 3 \times 10^{-5} \text{ km}^{-1}\text{s pc}\), an \(\text{H}_2\) density of \(> 2 \times 10^3 \text{ cm}^{-3}\) is required for \(T_R\) to exceed 30K. Over a wider abundance range this is also the approximate density needed for \(T_{\text{ex}}\) to exceed the same value. This is of interest because the \(J=1-0\) transition is often assumed to be both thermalised and optically thick, and therefore to provide a measure of the gas kinetic temperature. Figure 2.2 shows that although this is probably valid for relatively dense regions (\(n_{\text{H}_2} > 10^4 \text{ cm}^{-3}\)), it may in more diffuse molecular gas give a serious underestimate of the kinetic temperature.

(ii) **Excitation temperature**

The contours of excitation temperature in Figures 2.2 and 2.3 show the effect of radiative trapping, while Figure 2.5 shows it in a more spectacular way for a molecule of high dipole moment. Herein lies a problem for the applicability of equation 2.29, since it will not in general be the case that the excitation temperatures of 2 isotopes in the same transition are equal. For examples of where this might be occurring, see the data in the lines HCO\(^+\) \(J=4-3\) and H\(^{13}\)CO\(^+\) \(J=4-3\) for S255 and DR21 in Chapters 6 and 7.

A particular feature of the CO \(J=1-0\) transition is that it may become superthermally excited, as noticed by Leung and Liszt (1976).
Figure 2.4

LVG results for the ratio

\[
\frac{T_R(C_0 J = 3-2)}{T_R(C_0 J = 1-0)}
\]

Contour levels:

0.1 to 3.3, interval = 0.1

(This shows the relative enhancement of the higher transition for dense, optically thin gas; see equations 2.34 and 2.35.)

Units as for Figure 2.2
UVG results for HCO⁺ transitions

Contour levels:

\[ T_R(J=1-0) = 4 \times 10^4 \text{K} \]
\[ T_R(J=3-2)/T_R(J=1-0) \] (dashed line)
\[ T_e(J=4-3) \] (dotted line) 10^4, 1.0, 3.0K

Units as for Figure 2.2

Figure 2.5

![Graph showing HCO⁺ transitions with contour levels and temperature values.](image-url)
This is because collisional excitations from J=0 to J=2 occur at a comparable rate to those from J=0 to J=1, while spontaneous radiative decays are faster for J=2-1 than for J=1-0. As a result, the J=1 level may become overpopulated. The effect tends to be quenched at higher optical depths.

(iii) **Optical depths**

Figures 2.2 and 2.3 show a few representative contours of optical depth for the respective transitions. It is evident that the J=3-2 line is often more opaque than the J=1-0 transition. Also shown in Figure 2.2 are contours of τ = 0.1 and τ = 0.5 for the $^{13}$CO J=1-0 line (again, with an assumed isotopic abundance ratio of 40). For an equation such as 2.33 to be true, the line must be both thermalised and optically thin (say, $T_{\text{ex}}/T_k > 0.75$ and $\tau \leq 0.5$). Figure 2.2 shows that this assumption would only be true for $^{13}$CO J = 1-0 over a limited domain, so the use of 2.33 is not always justified. Superthermal excitation of $^{13}$CO, though, does not invalidate 2.33 as a means of estimating column density (nor 2.29 as a way of finding $\tau$ for $^{12}$CO).

When $T_{\text{ex}}$ is large, $T_{13}$ becomes small and inversely proportional to $T_{\text{ex}}$ (see equation 2.27). The observed $T_k$ is then $\approx T_{\text{ex}} T_{13}$, so (for a fixed number density of radiating molecules) is independent of $T_{\text{ex}}$, while the optically thin approximation becomes quite accurate.

(iv) **Line ratios**

Figure 2.4 shows the ratio of $T_R$ (J=3-2) to $T_R$ (J=1-0) for $^{12}$CO. The increase in $T_R$ is seen as one goes to higher transitions in the thermalised, optically thin limit. Also, for low optical depths, we see that the line ratios become independent of $X/(dv/dr)$. One can then estimate the gas density without needing to know the relative molecular abundance $X_{\text{CO}}$. 
2.6 Summary

In this Chapter, we have reviewed some of the basic theoretical concepts of molecular line astronomy, and some of the simple modelling techniques which are widely used. We have seen that some of the assumptions often made (e.g. thermalisation, optical thinness etc.), though sometimes forced on the observer by the incompleteness of real data and the need to deal with manageable numbers of free parameters, are nonetheless only valid within quite restricted ranges of the relevant parameters. Specifically, the CO J=1-0 line is often not thermalised, $^{13}$CO J=1-0 line is not always optically thin, and excitation temperatures in a main line and its isotope are not necessarily equal, due to the complicating effect of radiative trapping. Also, even under conditions of incomplete thermalisation, observations in single lines of molecules of different dipole moments do not enable us to distinguish reliably between dense and less dense regions, unless the transitions can be shown to be optically thin. This is because for optically thick lines, the excitation temperatures are independent of dipole moment. It is therefore essential in mapping density variations to observe also in an optically thin isotopic line.

Since we have so far examined one, particularly simple, cloud model, we have not yet established the extent to which cloud properties derived from observation are model dependent. Neither have we concerned ourselves with the limitations imposed by finite signal-to-noise and spatial resolution.

These issues are addressed in more detail in Chapters 3 and 4.
CHAPTER 2

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CHAPTER 3

ALTERNATIVE CLOUD MODELS

3.1 Introduction

A knowledge of the kinematical and density structure of an evolving molecular cloud, also its chemical composition, is integral to an understanding of star formation. However a theoretical treatment of the evolution processes is formidably complex. Because of the non-linearities which occur in gas moving under gravitational forces, numerical techniques are necessary to investigate the processes involved. They have to cope with the wide range of different time scales characteristic of aspects of the cloud evolution/stellar formation process (Tscharnutter 1980).

A complete theoretical treatment would entail a 3 dimensional dynamical simulation taking into account magnetic, gravitational and radiation fields, chemical changes, collapse and rotation, and has not yet been achieved. In particular, the physics of turbulence in the clouds is poorly understood (especially at Mach numbers too high to be investigated by laboratory experiments) and there are doubts about the extent to which magnetic fields can inhibit collapse (Mouschovias 1978; Nakano 1979). Neither is it clear whether the phenomenon of fragmentation for which there is evidence is essentially gravitational in origin (Rozyczka 1983) or due, for example, to chemical instabilities (Gilden 1984). Nor do different models agree on the length and time scales over which
fragmentation might be expected (Tohline 1980; Rozyczka 1983; Silk 1982; Tohline 1985).

Given all these uncertainties, it is desirable to know whether, and with what reliability, the kinematics and structure of a cloud can be inferred from observations, independently of model assumptions.

An issue of special uncertainty is that of the kinematical structure of the clouds. Typical observed line widths, particularly in hot-centred clouds, are highly supersonic (Goldreich and Kwan 1974) and this has been variously attributed to large or small scale motions, or to combinations of the two (e.g. Kwan 1978). One would like to isolate the effect of kinematics from other variable factors such as local densities and relative molecular abundances. We shall therefore need to investigate the effect that various kinds of cloud kinematics have on emergent line profiles and maps. The ultimate goals are to identify:

(i) Features of predicted spectra and maps which are diagnostic of particular kinematical structures; and

(ii) Observed data which are largely independent of kinematics, but which, in a model independent way, yield information on, for example, gas densities and relative molecular abundances and their variation with position.

Unfortunately, it is not obvious what degree of generality to allow in cloud models. Many so far investigated have been restricted to one dimensional spherical or slab symmetries. This contrasts with observed clouds, many of which are conspicuously asymmetrical in appearance and show spatial inhomogeneities on all scales down to the available telescope resolution.

Nevertheless, idealised models can give valuable indications of the range of conditions encountered and general trends in the
data expected, and we now review some of those which have been used.

3.2 Review of cloud models

It is clear that the large linewidths observed towards many molecular clouds cannot be explained solely on the basis of thermal Doppler broadening, and there has been a diversity of kinematical models proposed to account for them. To some extent these have tended to become polarised between two extreme cases, according as the observed linewidths are assumed due respectively to:

(i) large scale, systematic motions e.g. gravitational collapse (Goldreich and Kwan 1974; de Jong, Chu and Dalgarno 1975); or
(ii) small scale "microturbulence", a conveniently vague term signifying that velocity correlation lengths in a cloud are much smaller than a photon mean free path (e.g. Leung and Liszt 1976).

In this limit, the local microturbulent velocities can be treated similarly to thermal velocities, giving a local "microturbulent" line width, $\Delta \nu_D$:

$$\Delta \nu_D = \frac{v_0}{c} \left( \frac{2kT}{m} + v_{turb}^2 \right)^{1/2}$$

where $v_0$ is the line centre frequency (Liszt and Leung 1977).

It has been suggested (White 1977) that although both these two extreme postulates are likely to be gross oversimplifications of real cloud kinematics, they nonetheless represent two useful, well-defined, contrasting pictures. This, it is argued, is because the situation in any real cloud is likely to fall between these two poles, and a theoretical examination of purely systematic motion and pure microturbulence in turn can enable an assessment to be made of their relative importance.
In arguing in favour of LVG kinematics, Goldreich and Kwan (1974) pointed out that the thermal pressures deduced from observed cloud kinetic temperatures are insufficient to support the clouds kinematically, so they would almost certainly be gravitationally unstable. Furthermore, the maintenance of a state of microturbulence requires a strong source of mechanical energy, since its decay time is of the order of the time for a shock to propagate across a turbulent eddy (~ $10^5 - 10^6$ years). (However, Turner (1984) has argued that such a supply of energy is available from the "global turbulence" originating from galactic rotation).

Also supporting the LVG hypothesis was the observation that lines of different isotopes (and also different transitions of the same isotope) often have similar shapes, though different intensities, even when the line ratios strongly indicate very different optical depths (Linke and Goldsmith 1980). As we shall see later, microturbulent models have a strong tendency to predict self-reversed profiles for optically thick lines, and qualitatively different profile shapes for lines of different optical depth. This is particularly true when the excitation temperature decreases towards the cloud edge (Leung 1978). Such features are not observed in most clouds.

There are nevertheless powerful objections to an LVG model. Firstly, the profiles of a significant minority of clouds do exhibit self reversals (Loren 1981, Loren et al. 1981). Secondly, and more fundamentally, the assumption that all clouds are in a state of gravitational free-fall tends to predict a galactic rate of star formation greater by one or two orders of magnitude than that which is observed (Zuckerman and Palmer 1974).

The mean lifetime $t_{\text{CL}}$ of a cloud may be expressed as:
where \( n \) is the efficiency of star formation, \( \sigma \) is the surface density of molecular material and \( M \) is the star formation rate, all in the solar neighbourhood, while the free fall collapse time \( t_{ff} \) is given by

\[
t_{ff} = 4.4 \times 10^5 (n_{H_2}/10^4)^{-1/2} \text{ year}
\]

(Silk and Norman 1980).

The fraction \( F \) of clouds likely to be in free fall collapse is then estimated as the ratio \( t_{ff}/t_{cl} \). Insertion of the values \( M = 4 \times 10^{-9} M_\odot \text{ yr}^{-1} \text{ pc}^{-2} \) (Miller and Scalo 1979), \( \sigma = 5.2 M_\odot \text{ pc}^{-2} \) (Sanders, Solomon and Scoville 1984) and \( n \sim 0.1 \) (Cohen and Kuhi 1979) one derives

\[
F \sim 3 \times 10^{-3} (n/10^4)^{-1/2}
\]

However, this estimate refers to all the molecular gas, whereas in this thesis we are concerned with the relatively dense regions visible in submillimetre transitions. To estimate whether they are likely to be collapsing we need to multiply \( \sigma \) by a number \( \alpha \) (<1) which represents the fraction by mass of molecular gas in the dense regions—say, greater than \( 10^4 \text{ cm}^{-3} \) as compared with the values of \( \sim 10^2 \text{ cm}^{-3} \) characteristic of the larger cloud complexes. Unfortunately, this fraction is very uncertain; the large scale distribution of molecular gas has been mapped mainly using the CO J=1-0 and \( ^{13}\text{CO} \) J=1-0 lines (e.g. Sanders, Solomon and Scoville 1984) and they are not very useful for determining densities \( > 10^4 \text{ cm}^{-3} \). However, if we take \( \sim 10^2 \text{ pc} \) and \( \sim 10^5 M_\odot \) as a typical size and mass of a giant molecular complex (e.g. Blitz 1980) and 1-10 pc and \( 10^3 M_\odot \) as the values for the relatively dense cores (e.g. the centre of S255, DR21, DR21 (OH)) of which there might be only 2 or 3 in a GMC, then it seems not implausible that \( \alpha \) could be \( \sim 10^{-2} \). In
this case the likelihood of free fall collapse would be correspondingly increased.

We suggest then that the case against large scale collapse in the dense regions is not here so clear cut as in the more diffuse gas, and that in interpreting data from dense hot-centred clouds such as Orion A, S255, DR21 and DR21(OH), such a mechanism as an at least partial explanation of large line widths cannot be rejected a priori.

Nevertheless, the above considerations do weigh against the automatic use of LVG models to analyse data and they, together with the accumulating number of observed self-reversed profiles have led other authors to examine microturbulence as a possible source of line broadening.

A difficulty with such models is that the radiation intensities $J_\nu$ at a point, which partially determine the level populations $n_i$ (see equation 2.13) now include contributions from the whole cloud and are therefore dependent on the level populations (or source functions) at remote points. An iterative solution may therefore be needed.

The level populations can be expressed as a set of rate equations

$$A_{ij} n_j = b_i$$  \hspace{1cm} (3.5)

$A_{ij}$ is the sum of 2 matrices representing radiative and collisional processes, of which the former is tridiagonal. The equations are linear if the $J_\nu$ terms are explicitly given, or can be estimated, and can be solved to give values for the $n_j$.

Feautrier (1964) showed that the transfer equation along any ray direction could be closed and expressed as a two point boundary value problem. The resulting differential equation could then be
reexpressed as a finite difference scheme and solved for one ray direction at a time. As a result, revised values for $J_\nu$ could be found and resubstituted into the rate equations, 3.5.

Other methods of solving the problem have involved the use of variable Eddington factors (e.g. Leung and Liszt 1976) and various degrees of linearisation in which the equations of statistical equilibrium were incorporated into the transfer equation and the whole system linearised (Auer 1973).

The situation in which both large and small scale motions are present in a cloud has been treated by the core saturation comoving frame technique (Rybicki 1971; Bastian et al. 1980; Stenholm 1980 and references therein). This involves defining a portion of the local line profile over which the medium is optically thick, and over this range putting $I_\nu = S$. An expression for the source of function $S$ (independent of $\nu$ if complete redistribution is assumed) can then be written for each point (Bastian et al. 1980), involving integrals of $J_\nu$ only over the non-saturated portions of the profile. An iterative procedure can then give a solution for both the source functions $S(r)$ and the radiation intensities $I(\nu, \mu, r)$ throughout the cloud.

Leung and Liszt (1976) constructed microturbulent models for CO and found that the $J=2-1$ profile showed self reversal in many cases while the $J=1-0$ generally did not. The self reversal was due to a decreasing excitation temperature towards the cloud edge. They found also that the $J=1-0$ line could be superthermally excited, in fact over a similar range of $n_{H_2}$ and $X_{CO}$ as in the simple LGV model discussed in Chapter 2. A similar analysis has also been carried out for CS (Liszt and Leung 1977).

Another approach which has been used to solve the radiative
transfer problem in molecular clouds has been by the use of Monte Carlo techniques (Fleck 1963; House and Avery 1969; Bernes 1979). These have the advantages firstly of very modest memory storage space requirements, and secondly that increases in the complexity of cloud considered do not usually require a correspondingly greater complexity in the program. It is thus quite feasible to treat asymmetric or inhomogeneous clouds and also to relax the condition of complete redistribution. However, because of the essentially photon-counting nature of the technique, the random noise decreases proportionally only to the inverse square root of the number of photons processed (although various biasing and weighting schemes can ameliorate this to some extent). Decreasing the number of photons increases the statistical noise in the data output. Also, because the number of zones into which the cloud has to be divided must be at least of the order of the maximum optical depth, the technique tends to be rather extravagant of computer time for optically thick transitions. As developing observational techniques reveal more and more detailed structure and asymmetry in clouds, however, the ability of Monte Carlo methods to deal with such complexities becomes increasingly valuable.

Snell and Loren (1977) argued that the self reversed profiles observed towards some clouds (e.g. Mon R2, W3, NGC 1333 and Oph) could be explained on the basis of an LVG model if it was assumed that the collapse velocity decreased with radius, according to a law such as $v \propto r^{-1/2}$. In such a case, there will often be 2 points along a given line of sight which have the same velocity component towards the observer, and which therefore contribute to the same frequency point on the line profile. There is then the possibility that radiation emitted near the cloud centre can
be absorbed further towards the edge, possibly in an envelope of lower excitation temperature. The frequently observed displacement of self reversals towards the red end of the profile (e.g. Loren et al. 1981) is then interpreted as an indication that the cloud is collapsing rather than expanding.

However, a result of their model was that the predicted optically thin $^{13}$CO $J=1-0$ line had a central dip, due not in this case to self absorption, but to a variation of optical depth across the profile caused by the varying line-of-sight velocity gradient (see equation 2.41). This prompted them to add some microturbulence to their model, in order to smear out the cusps in the $^{13}$CO profile.

Leung and Brown (1977) objected that this transgressed the fundamental premise of LVG theory, namely that the ratio $\alpha$ of systematic to turbulent velocities in the cloud be $>> 1$. In fact, in Snell and Loren's model, $\alpha$ was $< 1$ over more than 96% of the cloud radius.

Another criticism was that with a decreasing velocity law the excitation temperature at a point in the cloud is to some extent determined by the conditions elsewhere, because of the form of the velocity field. In fact, though, the LVG approach has been generalised to such cases by Rybicki and Hummer (1978) who dealt with a 2 level atom in a moving atmosphere. We now develop this approximation for the multilevel molecular line problem of relevance to molecular clouds.

### 3.3 A generalised LVG model

For a velocity law $v \propto r^\alpha$ where $\alpha < 0$, equation 2.37 no longer holds since, for a point $r$ in the cloud, there in general exists a
Figure 3.1

CP Surfaces for $v \propto r^{-0.5}$ collapse law, for different fractional radii $r/R$
(The core edge is at $r/R = 0.01$.)
surface $S'$ on which all points $r'$ have zero radial velocity with respect to $r$. A photon escaping from $r$ would therefore have a second chance to be absorbed when it reached $S'$. For $r$, then there exists a common point (CP) surface (Rybicki and Hummer 1978). Example of such surfaces for $\alpha = -0.5$ are shown in Figure 3.1.

Rybicki and Hummer deal with the case of a spherical envelope round an opaque core. For our purposes, this is replaced by the contribution from the 2.7 K background, which comes from the whole $4\pi$ solid angle. The equation for $J(r)$, with this trivial modification, is now

$$J(r) = (1 - \beta_r) S(r) + \beta_{2.7}(r) I_{2.7}$$

$$+ \frac{1}{4\pi} \int d\Omega (1 - e^{-\tau'}) \frac{1 - e^{-\tau}}{\tau} S(r')$$

(3.6)

where the integral on the right hand side extends over all the solid angle for which the surface $S'$ exists, and where

$$\beta_{2.7} = \frac{1}{4\pi} \int d\Omega e^{-\tau'} \frac{1 - e^{-\tau}}{\tau}$$

(3.7)

and

$$\beta_r = \frac{1}{4\pi} \int d\Omega \frac{1 - e^{-\tau}}{\tau}$$

(3.8)

The $e^{-\tau'}$ term in 3.7 represents absorption of the 2.7 K background by the $S'$ surface as it enters the cloud.

For a pair of levels indexed by $j$ and $k$ (with $k$ the upper), we have
\[ S(r) = \frac{2\hbar \nu}{c^2} \left[ \frac{n_j}{n_k} - 1 \right]^{-1} \quad (3.9) \]

and
\[ I_{2.7} = \frac{2\hbar \nu}{c^2} \left[ \exp \left( \frac{\hbar \nu}{2.7k} \right) - 1 \right]^{-1} \quad (3.10) \]

Substituting in 3.6, we find
\[ \bar{J}(r) = \frac{2\hbar \nu}{c^2} \left[ \frac{n_j}{n_k} - 1 \right]^{-1} (1 - \beta_r) \]

\[ + \frac{2\hbar \nu}{c^2} \left[ \exp \left( \frac{\hbar \nu}{2.7k} \right) - 1 \right]^{-1} \beta_{2.7} \]

\[ + \frac{2\hbar \nu}{c^2} \phi \quad (3.11) \]

where
\[ \phi = \frac{1}{4\pi} \int d\Omega (1 - \tau') \frac{1 - e^{-\tau}}{\tau} \left[ \frac{n_j'}{n_{k'}} - 1 \right]^{-1} \quad (3.12) \]

Again, the dashes on quantities such as \( \tau' \), \( n_j' \) mean that they are evaluated over surface \( S' \). The third term on the right hand side of 3.11 represents the radiative coupling between \( r \) and the surface \( S' \).

We can now substitute 3.11 into 2.13. On rearranging, and expressing the \( A_{J+1,J} \) etc., in terms of \( A_{10} \) through

\[ A_{J+1,J} = \frac{3(J+1)^4}{2J+3} A_{10} \quad , \quad (3.13) \]
we eventually obtain, for a state of dynamical equilibrium between the level populations:

\[
0 = \frac{(J+1)^4}{(2J+1)} \left\{ x_{J+1} - \Phi_{J+1,J} \left( n_{J+1} - n_J \right) \right\} \\
- \frac{J^4}{(2J+1)} \left\{ x_J - \Phi_{J,J-1} \left( n_{J-1} - n_J \right) \right\} + \frac{1}{3A_{10}} \frac{\delta n_J}{\delta t} \text{coll}
\]

where

\[
x_J = \beta_{J,J-1} n_J - \frac{\beta_{J+1,J}^2 \left( n_{J-1} - n_J \right)}{\exp \left( \frac{2hBJ}{2.7k} \right) - 1}
\]

(3.14)

with a similar expression for \( x_{J+1} \), and where \( (\delta n_J/\delta t) \text{coll} \) is given by 2.17.

The system of equations 3.14 is now identical in form to those given by Goldreich and Kwan (1974) except in two respects:

(i) There are now new terms \( \Phi \) which represent the degree of radiative coupling between any point \( r \) and all points \( r' \) on the CP velocity surface;

(ii) There is a distinction between \( \beta_{J+1,J} \) and \( \beta_{J+1,J}^2 \), involving a factor \( e^{-T'} \) inside the integral for the latter quantity. (The effect of this upon emergent antenna temperatures, though, is probably very small.)

Since the \( \Phi \) terms in 3.14 contain the level populations \( n' \) and optical depths over the CP velocity surface \( s' \), the solution is no longer a purely local one, but involves calculating the degree of radiative coupling between separated points in the cloud.

The equations were solved iteratively. The values of gas
kinetic temperature, density, relative molecular abundance and collapse velocity were specified throughout the cloud, and solutions, initially ignoring the $\phi$ terms, were found for the populations $n_j$ at each of 100 radial points in the cloud (which was assumed to be spherical). (The solution for each radial point was used as the initial estimate for the next.) For each point the CP velocity surface was determined. Equations 3.14 were then solved again for improved values of $n_j$ by using the initial estimates as values for the $n_j'$. The convergence was found to be very rapid and only one reiteration was usually needed for the excitation temperatures to converge to values which were constant to $<1\%$.

The convergence of excitation temperature and optical depth for a typical cloud model with $\alpha = -0.5$ is shown in Figure 3.2, which represents a rerun of the model of Snell and Loren (1977). It is evident that for the J=1-0 CO line the deduced excitation temperature changes hardly at all on iteration. However, the change is more marked with higher transitions. Changes of up to 20\% are seen for $T_{\text{ex}}(J=3-2)$ and up to 70\% for $T_{\text{ex}}(J=6-5)$.

However, since the change in optical depth upon iteration generally occurs in the reverse sense to that in the excitation temperature, the two effects tend to cancel out in the final computed line profile. The J=1-0 profiles are visually indistinguishable after 0 and 1 iterations, while the J=3-2 profiles differed by $<1\text{K}$ over the line. This suggests that in most circumstances one is probably justified in only performing one iteration. For the lowest 3 CO transitions even this may not be necessary, but the effect is more likely to be significant for non-thermalised lines of moderate optical depth. It is however limited by the fraction of of the solid angle over which a point $r$ in the cloud can "see" a CP surface e.g.
Figure 3.2 Excitation temperatures and optical depths in a generalised LVG model - the effect of iteration. The broken dashed and solid lines show the solutions after 0, 1 and 2 iterations. See text for further details.
for a point on the cloud edge, and \( \alpha = -0.5 \), this fraction is only \( \approx 0.1 \).

Note that equations 2.39 and 2.41 for \( \beta \) and \( \tau \) need to be generalised for any case where \( \alpha \neq 1 \), since the variation of velocity gradient over solid angle implies a variation in \( \tau \) also. The optical depth along a particular direction is now given by

\[
\tau_{J+1,J} = \frac{8\pi^3}{3h|Q|} \chi_{\text{mol}} n_{\text{H}_2} (n_J - n_{J+1})
\]

(3.16)

where \( Q \) is the local velocity gradient component in the direction under consideration and, for a radial velocity law and a direction \( \hat{n} \) is given by

\[
Q(r, \hat{n}) = \frac{d\nu}{d\varphi} = \mu^2 \frac{\partial v}{\partial \varphi} + (1 - \mu^2) \frac{v}{r}
\]

(3.17)

where \( \mu \) is the cosine of the angle between \( \hat{n} \) and the radius through the point.

For a power law collapse

\[
v = v_0 \left( \frac{r}{r_0} \right)^\alpha
\]

(3.18)

we have

\[
Q(r, \mu) = \frac{\nu}{r} \left\{ (\alpha - 1) \mu^2 + 1 \right\}
\]

(3.19)

The expression for \( \beta \) is given by equation 3.8 and is evaluated in the program as a Gaussian quadrature sum. (Note also that Rybicki and Hummer (1978) do not include the stimulated emission term in their expression for the absorption coefficient, but we do include it here).

Having calculated the run of excitation temperatures (or source functions) throughout the cloud, one can then with comparative ease find the emergent \( T_R \) for any line of sight. For the assumed velocity
Figure 3.3
Examples of constant velocity (CV) curves for various velocity laws.
(c) \( \alpha = -0.5 \)  

Figure 3.3  
(continued)

Showing the possibility of having 2 points having the same velocity component along the same line of sight. 

(d) \( \alpha = 1 \)

with a varying angular velocity \( \omega \propto r^{-2} \). The rotational velocity at the cloud edge is \( 0.4 \times \) the edge collapse velocity. Inside the core region, \( \omega \) is constant and the collapse velocity is \( \alpha \) \( r \)
law, it is first necessary to know the point(s) \( z \) along the line of sight which have a velocity component \( v_z \) corresponding to each point on the profile. For \( \alpha > 0 \) (see 3.18), there will be at most one such point for each \( v_z \). Examples of contour diagrams of equal line of sight velocity are shown in Figure 3.3, including one example each in which \( \alpha < 0, 0 < \alpha < 1 \) and \( \alpha > 1 \). (The case \( \alpha = 1 \), not shown, would give a set of equally spaced straight contours). By combining collapse with rotation, both varying with radial distance, it is actually possible to have more than two points along the same line of sight with the same velocity component. An example is shown in Figure 3.3(d), and the program has been generalised to deal with such cases.

For a collapse velocity

\[
v_r = v_{r0} \left( \frac{r}{r_0} \right)^\alpha
\]

and an angular velocity \( \omega \) satisfying

\[
\omega = \omega_0 \left( \frac{r}{r_0} \right)^{-s}
\]

where

\[
\omega_0 = \frac{v_{t0}}{r_0}
\]

and where \( r_0, v_{r0} \) and \( v_{t0} \) are the cloud radius, and the radial and tangential components of velocity measured at the cloud edge in the equatorial plane, the quantity \( Q \) (defined by 3.19) is then given for the equatorial plane by

\[
Q = \frac{v_0}{r_0} \left( \frac{r}{r_0} \right)^{\alpha-1} \left\{ (\alpha-1) \mu^2 + 1 \right\} + f \frac{v_0}{r_0} \left( \frac{r}{r_0} \right)^{-s} (2-s) \mu (1-\mu^2)^{1/2}
\]

where \( f \) is the ratio of tangential to collapse velocities measured
Figure 3.4

Symbols used in generalised LVG model
at the cloud edge. Since the second, rotational term on the right hand side of 3.22 is antisymmetric in $\mu$, one would not expect local excitation temperatures, which are dependent on the integral of $\beta(Q)$ over solid angle, to be much affected by rotation, although the emergent line profiles clearly would be.

Whenever the line of sight passes through 2 points, $r'$ and $r$, having the same $v_z$ and with $r'$ further from the observer, the observed $T_R$ is given by

$$T_R(v) = \frac{c^2}{2k v^2} \left[ (e^{-\tau} - 1) I_{2.7} + e^{-\tau}(1-e^{-\tau'}) S' \right] \left( \frac{1}{1-e^{-\tau}} \right) S$$

(3.23)

where $\tau'$ and $\tau$; $S'$ and $S$, are the respective optical depths and source functions at the 2 points, evaluated from 3.16, 3.19 and 2.23. (The values of $\mu$ are of course different for the 2 points, unless $\mu = 1$). The geometry of the situation is illustrated in Figure 3.4

In the program employed here, the emergent $T_R$ is calculated for 101 equally spaced values of impact parameter $p$ from 0 to 1, for each point on the line profile. It is then possible to output the results in 3 alternative graphical forms, for each transition:

(i) Spectra, at any chosen impact parameter $p$;

(ii) Scans across the source diameter, for any chosen velocity $v_z$;

(iii) A velocity-displacement plot of contours of $T_R$.

In addition, the program gives the option of convolving the values of $T_R$ with a Gaussian beam of any size, and plotting the results in any of the above 3 ways.
3.4 LVG models with pure gravitational collapse

To demonstrate the variety of line profiles which may be obtained using LVG kinematics we now present the results from a series of model clouds under pure gravitational collapse. In each model, the cloud radius is 10 pc and the average molecular hydrogen density is $n_{H_2} = 8.4 \times 10^2$ cm$^{-3}$. These values give a total cloud mass of $2.3 \times 10^5 M_\odot$ and, for cases where the collapse velocity increases monotonically with radial distance, an edge collapse velocity of 10 kms$^{-1}$. The abundance $X_{CO}$ of CO relative to $H_2$ is taken to be $5 \times 10^{-5}$ and is constant throughout the clouds.

For a cloud whose collapse velocity $v$ and density $n$ satisfy respectively,

$$v \propto r^\alpha,$$

and

$$n \propto r^{-\beta},$$

we have, for pure gravitational collapse,

$$\beta = 2 - 2\alpha \quad (3.24)$$

5 models were run, for different values of $\alpha$, and the details are given in Table 3.1. To avoid singularities, the velocity gradient and density were assumed to be constant within a central core. In general, the density was also assumed to be continuous across the core boundary and the density exponent $\beta$ was chosen to satisfy (3.24). Exceptions to these general rules were:

(i) In model E, a constant density was chosen ($\beta = 0$), the material on the boundary being subject to unretarded gravitational collapse. The value of $\beta$ given by 3.24 was rejected because it would imply a density which increased with radial distance, a situation which seems physically unlikely;
(ii) Model A has a collapse velocity which decreases with radial distance and is therefore a maximum at the core boundary. The size and density of the core were chosen so that material just outside the core, under the assumed unretarded gravitational collapse, would have a radial velocity of 10 kms$^{-1}$.

In each case, the emergent radiation temperatures were convolved with a Gaussian beam of width (FWHM) 0.1 times the cloud radius. A convenient way of representing the results of the models is in the form of velocity - displacement diagrams, and examples of these, mainly for the CO J=3-2 transition, are shown in Figures 3.5 - 3.9. The following features are noticeable:

(i) Since in an LVG model, emission at particular velocities originates from individual points within the cloud, different velocity laws give rise to different shapes of velocity - displacement plots. For example, models where $0 < \alpha < 1$ tend to give relatively flat-topped spectra but sharply peaked intensity distributions (e.g. models B and C). For $\alpha > 1$ (e.g. model F), the situation is reversed.

This in principle gives a method of distinguishing observationally between different velocity laws, if LVG kinematics are assumed. In practice, though, finite beam sizes, noise and the irregular shapes of many clouds are often a problem.

(ii) Model A, in which the velocity exponent is negative, shows both self reversal and high velocity wings. Both these features are spatially compact relative to the cloud size. The self-reversal is due to absorption of radiation originating from within and around the core by lower excitation material situated further out. The wings are in this model produced by the collapse of material around the core boundary. However, a similar feature could equally well be produced if the region consisted of outflowing gas (see Chapter 5).
### Table 3.1 LVG gravitational collapse models

(a) Variations in parameters used

<table>
<thead>
<tr>
<th>QUANTITY</th>
<th>VARIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Outside core</td>
</tr>
<tr>
<td>Collapse velocity</td>
<td>( v = v_{\text{core}} \left( \frac{r}{r_{\text{core}}} \right)^{\alpha} )</td>
</tr>
<tr>
<td>Density</td>
<td>( n = n_{\text{core}} \left( \frac{r}{r_{\text{core}}} \right)^{-\beta} )</td>
</tr>
<tr>
<td>Gas temperature</td>
<td>( T = T_{\text{core}} \left( \frac{r}{r_{\text{core}}} \right)^{-\gamma} )</td>
</tr>
</tbody>
</table>

(b) Details of Models

<table>
<thead>
<tr>
<th>MODEL</th>
<th>( \alpha )</th>
<th>( \beta )</th>
<th>( \gamma )</th>
<th>( r_{\text{core}} ) pc</th>
<th>( n_{\text{core}} ) cm(^{-3} )</th>
<th>( T_{\text{core}} ) K</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>-0.5</td>
<td>3.0</td>
<td>0.2</td>
<td>0.5</td>
<td>3.35x10(^5) (^{(1)})</td>
<td>40</td>
</tr>
<tr>
<td>B</td>
<td>0.1</td>
<td>1.8</td>
<td>0.2</td>
<td>0.1</td>
<td>1.34x10(^6)</td>
<td>40</td>
</tr>
<tr>
<td>C</td>
<td>0.5</td>
<td>1.0</td>
<td>0.2</td>
<td>0.1</td>
<td>5.6x10(^4)</td>
<td>40</td>
</tr>
<tr>
<td>D</td>
<td>1.0</td>
<td>0.0</td>
<td>0.2</td>
<td>0.1</td>
<td>8x4x10(^2)</td>
<td>40</td>
</tr>
<tr>
<td>E</td>
<td>2.0</td>
<td>0.0(^{(2)})</td>
<td>0.2</td>
<td>0.1</td>
<td>8x4x10(^2)</td>
<td>40</td>
</tr>
</tbody>
</table>

**NOTES**

1. Density just outside core assumed to be \( 1.1 \times 10^5 \) cm\(^{-3} \)
2. Does not satisfy equation 3.7. See text for discussion.
Figure 3.5

Predicted position-velocity map for gravitational collapse model D, in the CO $J=3-2$ (above) and $J=1-0$ (below) transitions. Contours of $T_R^N$ for a beam (FWHM) = 0.05 x the cloud diameter, plotted on axes of impact parameter $p$ (horizontal) and LSR velocity in $\text{km s}^{-1}$ (vertical). See Table 3.1 for further details.
Figure 3.6: Same as Fig. 3.5, for Model C, CO J=3-2. See Table 3.1

Figure 3.7: Same as Fig. 3.5, for Model E, CO J=3-2. See Table 3.1
Figure 3.8: Same as Fig. 3.5, for Model A, CO J=3-2. See Table 3.1

Figure 3.9: Same as Fig. 3.5, for Model B, CO J=3-2. See Table 3.1
The same models were also run for the molecule HCO⁺, which was assumed to have an abundance relative to H₂ of $2 \times 10^{-10}$. Predicted central spectra are shown in Figure 3.10 for the HCO⁺ J=1-0 transition. For this chosen set of alternative models, the line is very sensitive to the value of the maximum density of the cloud, and so provides a sensitive probe of the density structure. However, it must be stressed that this would not have been the case had we chosen a much larger value for $X_{\text{HCO}^+}$ (see the discussion of radiative trapping in Section 2.5.1).

The above examples illustrate how, by combining results from different molecular lines, and making assumptions about the basic nature of the kinematics, one can extract information about the velocity and density structure of a cloud.

Nonetheless, although it is easy to construct a variety of theoretical models which predict markedly contrasting spectra and maps, the reverse process, of modelling actual data in a unique way, is much more insecure. Even if one is prepared to assume, for example, the validity of LVG kinematics, the enormous number of free parameters involved requires the acquisition of data which are both as complete in velocity and spatial coverage, and of as high a quality, as possible. For each molecule observed, it is highly desirable to obtain data in at least two transitions. For a simple linear molecule, these will be at very different frequencies and will almost always be taken either with different telescopes or with different beam sizes, or both. One is then, of necessity, embroiled in the hazardous tasks of data comparison to be discussed in Chapter 4.

These problems are encountered even for the relatively straightforward case of an LVG model with molecules of constant abundance relative to H₂ throughout the cloud. The arguments against the
Figure 3.10

Predicted central spectra in the HCO$^+$ J=1-0 transition, for the LVG gravitational collapse models described in Table 3.1. Beam (FWHM) = 0.05 of the cloud diameter. Model D and E gave no detectable emission.
universal applicability of LVG kinematics have already been discussed. Also, many chemical models predict a variation in relative molecular abundances even within the same cloud, as well as between clouds.

We must now address the thorny question of the effect of different kinematical assumptions on predicted profiles.

3.5 Comparison of LVG and microturbulent models

When molecular line data are presented in the literature and used to deduce hydrogen densities and molecular abundances, the work of White (1977) is often cited in support of the assertion that the derived densities are not very dependent on the kinematical model used. To the extent that this is true, one is then justified in employing, for example, a simple LVG model on the grounds of computational convenience, confident that this choice should not have too determining an influence on derived densities (e.g. Snell et al. 1984). White's approach was in 2 stages: firstly, an analytical discussion of the 2 level molecule in which it was shown that, in both the optically thin and optically thick limits, the dependence upon optical depth of the photon escape probability $\beta$ was very similar for both the microturbulent and LVG cases; secondly, grids of values of $T_R$ in the lowest 2 CO transitions for the multilevel molecule in an isothermal homogenous cloud. The general conclusion was that both peak and integrated line intensities agreed between the 2 kinematical models within the degree of uncertainty attributable to ignorance of the cloud geometry.

However, since we are now able to observe in a much wider range of transitions than were available to White, and since also it is clear that real clouds - particularly in their cores - are very far from homogeneous and isothermal, we must reexamine his assumptions. The
similarity between the results of the two kinematical models in the optically thin limits seems secure. In these circumstances, radiative trapping has a negligible influence on the source function, which is then determined solely by the degree of collisional excitation.

But the optically thick case is more problematic. For LVG kinematics, the peak intensity in the line is \( S_{\text{max}} \), where \( S_{\text{max}} \) is the maximum source function in the cloud (probably at the cloud centre). At every point on the profile, one sees right through the cloud. In arguing that a similar relationship would hold even in the microturbulent case, White appealed to the Eddington-Barbier relationship, which states that for a 1 dimensional atmosphere, the emergent intensity, along a ray direction inclined at an angle \( \cos^{-1} \mu \) with the normal, is characteristic of the value of the source function at an optical depth \( \tau = \mu \) (i.e. \( \tau = 1 \) for normal incidence). As one moves outwards from the line centre, the intensity becomes characteristic of points further into the cloud interior, and reaches a maximum at a point on the profile for which an optical depth of unity occurs at the cloud centre. This accounts for self reversed profiles since the source function generally increases towards the interior.

But the Eddington-Barbier relation in this simple forms assumes a linear variation of the source function with optical depth, and this will not always be a valid approximation for a molecular cloud.

Consider a plane parallel slab geometry. The radiation intensity observed along a line of sight \( \mu \) is given by

\[
I(\nu, \mu) = \int_{0}^{\infty} S(\tau) \exp\left(-\frac{\tau(\nu)}{\mu}\right) \frac{d\tau}{\mu} 
\]

We now express \( S(\nu) \) as a Taylor expansion up to second order, about the mid-plane of the slab, whose optical depth (measured
from the surface) is $\tau_m$, say. Thus

$$S = S_m + \frac{3S}{\partial \tau} \left[ (\tau - \tau_m) + \frac{1}{2} \frac{3^2 S}{\partial^2 \tau} \right] (\tau - \tau_m)^2. \quad (3.26)$$

Substituting 3.26 into 3.25, we obtain

$$I(\nu, \mu) = S_m + \mu \frac{dS}{d\tau} \left[ (1 - \frac{\tau_m}{\mu}) + \frac{\mu^2}{2} \frac{3^2 S}{\partial^2 \tau} \right] m \left( \frac{\tau_m^2}{\mu^2} - \frac{2\tau_m}{\mu} + 2 \right) \quad (3.27)$$

(If we had expressed $S$ as $S_0 + \frac{3S}{\partial \tau} \tau_0$ where the zero subscript denotes the cloud surface, we should have obtained $I = S$ ($\tau = \mu$), the simple Eddington-Barbier result).

In the cloud we are considering here, $\frac{3S}{\partial \tau}$ will be zero, due to symmetry, and the important term is the second order one. It is now not necessarily the case that $I_\nu = S_m$, although it is true that $I_\nu$ most closely approximates to $S_m$ at a frequency such that $\tau_m = 1$ (for $\mu = 1$). We then have

$$\frac{I_\nu}{S_m} = 1 + \frac{1}{2S_m} \frac{3^2 S}{\partial^2 \tau} \quad (3.28)$$

Consider a cloud in which $S$ peaks at the centre and falls off appreciably towards the edge, because of density, abundance or temperature gradients or some combination of the three. The value of $d^2S/d\tau^2$ may then be $-S_m/\tau_m^2$. Equation 3.28 then shows that the peak value of $I_\nu$ may fall very considerably below $S_m$. (For the CO transitions considered by White, $S$ would be constant over much of the central region for a homogeneous cloud so the simple Eddington Barbier result would be satisfactory here.)

For a spherical cloud with a pronounced central density and/or temperature peak, dilution effects would probably make the discre-
3.6 Description of models

The above considerations lead us to attempt a comparison of LVG and microturbulent models over a wider range of cloud structures and conditions. The number of free parameters, though, is dauntingly large and one can hope only to make a representative selection. The LVG program used is the one described in Section 3.3. For the microturbulent approximation I have used the Monte Carlo radiative transfer program of Dr. L.W. Avery (Avery 1983).

We begin by adopting a somewhat philatelic approach. This is deliberate, since we wish to allow for the possibility that currently used values for densities and (especially) relative molecular abundances may be seriously in error. We will therefore investigate the effect of varying these two free parameters over a wide range, thereby avoiding prejudgements about their likely values. Our object is to examine any very obvious tendencies in predicted spectra.

For each of the several categories of model under consideration, we compute spectra towards the cloud centre, in the lowest CO transitions, for each point on a 5 x 5 logarithmic grid of $n_{H_2}$ and $X_{CO}$. The models have been chosen to achieve a reasonable diversity of free parameters and to provide comparable models with different kinematics. Full details of the models run are given in Tables 3.2-3.4, but a brief description is as follows:

The models run were all for spherical clouds of radius 2 pc and the central spectra were convolved with a Gaussian beam of width (FWHM) equal to 0.2 x the cloud diameter. The densities were parametrised in terms of average values and extended from $n_{H_2} = 10^2$...
cm$^{-3}$ to $10^6$ cm$^{-3}$. The fractional abundance of CO relative to H$_2$ ranged from $X_{CO} = 5 \times 10^{-8}$ to $5 \times 10^{-4}$.

For the microturbulent models, a constant microturbulent velocity width of 10 km s$^{-1}$ (FWHM) was initially chosen; in all the LVG models the maximum collapse velocity was taken to be 10 km s$^{-1}$.

In most of the models run, the density was made to decrease with radial distance ($n_{H_2} \propto r^{-2}$ was chosen) since it was anticipated that the most interesting differences between molecular lines of differing transition probabilities and/or optical depths might occur when density gradients were present. Also, such gradients might plausibly be expected to occur in real gas clouds, either over a cloud as a whole or within individual clumps. However, one grid of completely homogeneous clouds was also run for each form of kinematics (grids MTI and LVGI) i.e. the situation investigated by White (1978).

Apart from the constant density grid MTI, the microturbulent grids correspond to different radial temperature variations: in grid MTII, the temperature was constant, in grid MTIII it decreased with radius (so as to give the same mass-weighted average temperature as MTII), and, in grid MTIV, an exponential function was included so that near the cloud edge the temperature rose rapidly to 50K (from a central value of 25K).

For LVG models, the effect of radial temperature variations was not thought to be so interesting - radiation at particular points on the spectral line come from particular, identifiable points in the cloud, so radial temperature gradients have predictable effects on profiles. Instead, the radial dependence of the collapse velocity was varied.

The nomenclature used to identify each model is specified in Table 3.2. As an example, LVGIII B4 refers to the LVG model in
Table 3.2
Details of grids of models

\[ \begin{array}{cccccc}
\times_{\text{CO}} & E1 & E2 & E3 & E4 & E5 \\
5 \times 10^{-4} & & & & & \\
5 \times 10^{-5} & D1 & D2 & D3 & D4 & D5 \\
5 \times 10^{-6} & C1 & C2 & C3 & C4 & C5 \\
5 \times 10^{-7} & B1 & B2 & B3 & B4 & B5 \\
5 \times 10^{-8} & A1 & A2 & A3 & A4 & A5 \\
\end{array} \]

\[ n_{\text{H}_2} = \text{average cloud density (cm}^{-3}\text{)} \]

\[ \times_{\text{CO}} = \text{molecular abundance relative to H}_2 \]

For the HCO\(^+\) grids the values of \( X_{\text{HCO}^+} \) extend from \( 5 \times 10^{-8} \) to \( 5 \times 10^{-12} \).

Cloud radius = 2pc

Beam FWHM = 0.2 \( \times \) cloud diameter

Microturbulent models: Local microturbulent line width = 10 \( \text{km} \text{s}^{-1} \) (FWHM)

LVG models: Maximum collapse velocity = 10 \( \text{km} \text{s}^{-1} \)
grid III for which \( X_{\text{CO}} = 5 \times 10^{-7} \) and the average \( \text{H}_2 + \text{He} \) density is \( 10^5 \text{ cm}^{-3} \).

Some grids were run also for \(^{13}\text{CO} \), using an assumed ratio of \( X_{\text{CO}}/X^{^{13}\text{CO}} = 40 \). In addition, grids LVGI, LVGII, MTI and MTII were obtained also for \( \text{HCO}^+ \); here the assumed values of \( X_{\text{HCO}^+} \) ranged from \( 5 \times 10^{-12} \) to \( 5 \times 10^{-8} \) and central spectra in the transitions \( J=1-0 \) and \( J=4-3 \) were plotted.

The results from the models are shown in Figures 3.11 to 3.19. The LVG models need no further description than that already given in Sections 3.3 and 3.4. Each one took about 300s of OCP time on the QMC ICL 2988 computer. In the microturbulent models (Avery 1983), iterations of the program were continued until satisfactory convergence was obtained, each iteration taking about 200s on the ICL 2988. The criterion for convergence was that the change \( \Delta T_{\text{ex}} \) in average excitation temperature, for each transition averaged over the cloud, was less than some specified value (usually 0.1 to 0.2 K) between one iteration and the next.

Sometimes this criterion was relaxed for the \( J=1-0 \) line if it fell into the regime of superthermal excitation; in such cases \( T_{\text{ex}} \) might change markedly between iterations while the observable quantity \( T_{\text{ex}}T \) remained quite constant (see discussion in Section 2.5.3). For some high optical depth cases, the number of required zones was so great that the computing time would have been prohibitive, hence the blank spaces towards the high density - high abundance corner of some of the grids. Sometimes also the convergence was very slow, especially in non-thermalised but optically thick models e.g. MTII E3 \( \text{HCO}^+ \) and MTIII D3 \( \text{HCO}^+ \), to the extent that small values of \( \Delta T_{\text{ex}} \) were not deemed to constitute sufficient evidence that the program has converged. For these cases, the model
Table 3.3
LVG Grids

<table>
<thead>
<tr>
<th>Grid</th>
<th>$\beta$</th>
<th>Collapse velocity variation</th>
</tr>
</thead>
<tbody>
<tr>
<td>LVGI</td>
<td>0</td>
<td>$v \propto r$</td>
</tr>
<tr>
<td>LVGII</td>
<td>2</td>
<td>$v \propto r$</td>
</tr>
<tr>
<td>LVGIII</td>
<td>2</td>
<td>$v \propto r^{0.1}$</td>
</tr>
<tr>
<td>LVGIV</td>
<td>2</td>
<td>$v \propto r^{-0.5}$</td>
</tr>
</tbody>
</table>

The constant density and velocity gradient core extends to 0.02 pc from the centre for all grids except IV, for which the value is 0.1 pc. In all grids, the gas temperature is a constant 40K.

The maximum collapse velocity in each case is 10 kms$^{-1}$. This occurs at the cloud edge for all cases except LVGIV, for which it occurs at the edge of the core.
### Table 3.4

**Microturbulent Grids**

<table>
<thead>
<tr>
<th>Grid</th>
<th>$\beta$</th>
<th>Kinetic temp variation</th>
</tr>
</thead>
<tbody>
<tr>
<td>MTI</td>
<td>0</td>
<td>Constant 40K</td>
</tr>
<tr>
<td>MTII</td>
<td>2</td>
<td>Constant 40K</td>
</tr>
<tr>
<td>MTIII</td>
<td>2</td>
<td>$T = 15 \left( \frac{r}{r_0} \right)^{-0.625}$</td>
</tr>
<tr>
<td>MTIV</td>
<td>2</td>
<td>$T = 15 + 10 \exp \left( \frac{r}{(r_0 \times 0.8)} \right)$</td>
</tr>
</tbody>
</table>

$r_0 = 2$ pc
was rerun with different initial estimates of excitation temperatures, and iterated as many as 15-20 times in order to ensure that consistent results were obtained between different starting points.

For one microturbulent model, MTII D3, CO spectra are shown in Figure 3.19 for different positions on the cloud. In the same figure are displayed also the resultant spectra for microturbulent clouds where the local microturbulent velocity width respectively decreases and increases with radial distance.

3.7 Results from the modelling

3.7.1. Homogeneous clouds

Figures 3.11(a) and (b) show the predicted CO and $^{13}$CO spectra for constant temperature and density clouds (grids LVGI and MTI). In agreement with the results of White (1978) we see that the peak temperatures are for the most part equal between the two kinematic models to within ~ 20%. The LVG profiles are flat-topped, a consequence of the chosen $v \propto r$ collapse velocity variation. For low molecular hydrogen densities and high $X_{CO}$ there is a tendency for the microturbulent spectra to be self reversed, particularly in the J=3-2 transition (e.g. see MTI E2 (CO)). This may be interpreted as due to the decrease in excitation temperature towards the cloud edge, which occurs because of the higher photon escape probabilities there. In most of the spectra, though, the self absorption is either non-existent or is so weak that in real data it might well be obscured by the noise.

For the HCO$^+$ spectra (Figure 3.12) the peak antenna temperatures are still quite similar between the 2 kinematical models, although for grid point 3B (which occurs at a point of incomplete thermalisation but high optical depth) the peak intensity especially in continued on p99
Figures 3.11 - 3.18

In each of these Figures, predicted spectra towards the centre of the cloud are shown for a grid of values of mean \( H_2 \) density and molecular abundance relative to \( H_2 + \text{He} \), as specified in Table 3.2.

For each spectrum, the height of the box represents \( T_R^* = 40\)K and the width represents the velocity range \( \pm 15 \) kms\(^{-1}\).

Full details of each model are given in Tables 3.2, 3.3 and 3.4.

\[
\begin{align*}
\text{CO transitions:} & & J = 1 - 0 \text{ (dotted)} \\
& & J = 2 - 1 \text{ (dashed)} \\
& & J = 3 - 2 \text{ (solid)} \\

\text{HCO}^+ \text{ transitions:} & & J = 1 - 0 \text{ (dotted)} \\
& & J = 4 - 3 \text{ (solid)}
\end{align*}
\]

For transitions of \( ^{13}\text{CO} \), the grid points along the vertical direction still refer to \( X_{^{12}\text{CO}} \), and an isotopic abundance ratio of 40 is assumed.
Homogeneous isothermal clouds, in CO transitions. Grid LVGI (overlay) compared with grid MTI. The approximate similarity in peak intensities between the two kinematic models is in agreement with the work of White (1978).
Homogeneous isothermal clouds, in CO transitions. Grid LVGI (overlay) compared with grid MTI. The approximate similarity in peak intensities between the two kinematic models is in agreement with the work of White (1978).
Homogeneous isothermal microturbulent clouds. Predicted spectra in transitions of $^{12}$CO.
the J=1-0 line is predicted to be much lower in the microturbulent than in the LVG model.

We see in Figure 3.12 that even for homogeneous clouds the HCO⁺ J=4-3 spectrum shows a conspicuous self reversal for most cases in which it is detected with appreciable intensity. Such a feature is not usually seen in observed spectra in this line (e.g. see the HCO⁺ spectra in Chapters 6 and 7; also White et al. 1985; Padman, Scott and Webster 1982), although one does appear in the HCO⁺ J=3-2 profile towards G35.2N (Matthews et al. 1984). This would seem to constitute evidence against the applicability of this model to real clouds. However, since it now seems that many clouds have a small scale clumpy structure, any self reversal produced by an individual clump would be smeared out by the summation of radiation from many such clumps with different velocities within the telescope beam. Then, the observed intensities in different transitions would be highly dependent on the density and kinematical structure of an individual clump, which however would not be directly observable because of the dilution in both physical and velocity space.

3.7.2 Constant temperature models with centrally peaked density

We now compare the results from grids LVGII and MTII (Figures 3.13(a) and (b), both of which represent clouds having a constant kinetic temperature of 40K, and a density law \( n_\text{H}_2 \propto r^{-2} \). In the former grid, a constant velocity gradient \((v \propto r)\) was assumed; in the latter, a constant microturbulent velocity width.

For high \( X_\text{CO} \) and \( n_\text{H}_2 \), both kinematical models predict flat-topped spectra. For intermediate optical depths and degrees of thermalisation, the LVG profiles have a triangular appearance while those for microturbulent clouds exhibit self reversals.
Figure 3.12

Homogeneous isothermal clouds, in HCO⁺ transitions. Grid LVGI (overlay) compared with grid MTI.
Figure 3.12

Homogeneous isothermal clouds, in HCO⁺ transitions. Grid LVGI (overlay) compared with grid MTI.
Figure 3.13(a)

Isothermal clouds with radially decreasing density ($\propto r^{-2}$), in CO transitions. Grid LVGII (overlay) compared with grid MTII.
Figure 3.13(a)

Isothermal clouds with radially decreasing density ($\alpha r^{-2}$), in CO transitions. Grid LVGII (overlay) compared with grid MTII.
Figure 3.13(b)

Isothermal clouds with radially decreasing density ($\alpha r^{-2}$), in $^{13}$CO transitions. Grid LVGII (overlay) compared with grid MTII.
Figure 3.13(b)

Isothermal clouds with radially decreasing density (\(\alpha r^{-2}\)) in \(^{13}\text{CO}\) transitions. Grid LVGII (overlay) compared with grid MTII.
which are often more pronounced than in the homogeneous clouds. Unlike the CO spectra for the homogeneous clouds, the peak antenna temperatures do not appear to agree very well between the 2 kinematical models, except at low optical depths.

The differences are even more apparent for the HCO+ spectra (Figure 3.14), particularly in the low density/high optical depth regime, where the peak intensities are significantly greater in the LVG clouds. A possible explanation is that in the latter case one is actually able to see right through to the dense cloud centre, whereas in a microturbulent cloud significant optical depths in the outer layers prevent this. An alternative perspective is given by equation 3.28 since, for a source function which is strongly peaked at the cloud centre, \( \frac{\partial^2 S}{\partial \tau^2} \) will have a large negative value there, and the observed intensity will fall well below the central value of \( S \). This effect will be more pronounced for high J transitions.

The discrepancies between predicted intensities (both peak and integrated values) between the 2 kinematical situations have serious implications for the validity of modelling since, given a particular set of observed data, it is evident that the answers one will get for derived densities and relative molecular abundances within clouds will be highly dependent on the assumed model which is used to analyse the data. For example, the peak intensities predicted by model LVGII E2 (HCO+) (which corresponds to average values of \( n_{H_2} = 10^3 \text{ cm}^{-3} \) and \( X_{HCO^+} = 5 \times 10^{-8} \)) are quite similar to those predicted by MTII B4 (HCO+) (where the parameters are \( n_{H_2} = 10^5 \text{ cm}^{-3} \) and \( X_{HCO^+} = 5 \times 10^{-11} \)).

Of course, for these particular clouds a choice could be made between the different kinematic extremes on the basis of their
Isothermal clouds with radially decreasing density ($\alpha r^{-2}$) in HCO$^+$ transitions. Grid LVGII (overlay) compared with grid MTII.
Figure 3.14

Isothermal clouds with radially decreasing density ($\alpha r^{-2}$) in HCO$^+$ transitions. Grid LGIII (overlay) compared with grid MTII.
qualitative shapes, e.g. whether the HCO$^+$ J=4-3 profile was self reversed in a given piece of data. However, if the actual observed cloud was clumpy, this feature would be washed out by dilution in both physical and velocity space. The internal structure of individual clumps would then have a crucially determining influence on the observed intensities.

Fortunately, as for CO, the agreement is much better at lower optical depths, both in peak and integrated values.

3.7.3 Effects of different radial temperature variations

Figures 3.15 and 3.16 are for microturbulent clouds with the same parameters as Grid MTII but for kinetic temperatures which respectively decrease and increase with radial distance, as detailed in Table 3.4. In the decreasing temperature case, we see that the self absorptions in CO spectra are extremely prominent and broad (contrary to most actual observations). It has been noted (e.g. Young et al. 1982) that a temperature increase towards the outer part of a cloud can tend to remove self absorptions. Although we do not see this in our grid MTIV, this is almost certainly because the effect of increasing temperature is masked by that of the rapidly decreasing density law we have chosen, so that the excitation temperatures in the transitions of interest do not increase towards the edge. Another effect which may tend to remove self absorptions, but which we have not considered, is the destruction of CO in the outer cloud layers by absorption of UV radiation.
Figure 3.15

Microturbulent clouds with radially decreasing density and temperature. $^{13}\text{CO}$ spectra (overlay superimposed on $^{12}\text{CO}$ spectra for grid MTIII. See Table 3.4 for details.
Figure 3.15

Microturbulent clouds with radially decreasing density and temperature. $^{13}$CO spectra (overlay superimposed on $^{12}$CO spectra for grid MTIII.
See Table 3.4 for details.
Figure 3.16

Microturbulent clouds with radially decreasing density and radially increasing temperature. $^{13}$CO spectra (overlay) superimposed on $^{12}$CO spectra for grid MTIV. See Table 3.4 for details.
Figure 3.16

Microturbulent clouds with radially decreasing density and radially increasing temperature. $^{13}$CO spectra (overlay) superimposed on $^{12}$CO spectra for grid MTIV. See Table 3.4 for details.
3.7.4 **Variation of collapse velocity law in LVG models**

The grid with a density law $n_{\text{H}_2} \propto r^{-2}$ was also run for velocity laws $v \propto r^{0.1}$ and $v \propto r^{-0.5}$ and the results are displayed in Figures 3.17 to 3.18. The variation in spectra and maps obtained from different velocity laws has been discussed in Section 3.4. Here we simply note two features:

(i) The "cusped" appearance of CO J=1-0 spectra noted by Snell and Loren (1977) e.g. in LVGIII C3 and LVGIV A3;
(ii) The asymmetries produced by absorption in the outer cloud layers e.g. in LVGIV CI and LVGIV DI. (These have to a large extent been washed out for most of the spectra in grid LVGIV by dilution in the relatively large assumed beam).

3.7.5 **Radial variations of microturbulent velocity width**

In Figure 3.19 are shown the observed spectra predicted from model MTII D3 for impact parameters $p = 0, 0.2, 0.4$, and 0.6. Also shown are corresponding plots for 2 similar clouds which have been given radially varying microturbulent velocity widths. In the model for which this width increases towards the outside of the cloud, the profiles, do not differ much from the constant case, except that the self absorption is not quite so deep. However, in the cloud where the velocity dispersion increases towards the inside, the self absorption has disappeared; also, the linewidth has become narrower towards the cloud edge. This last case might intuitively be expected to correspond the most closely of the three to reality if the microturbulence were maintained by energetic outflows in the cloud interior. It is also the most similar of the three to the profiles which would be given by an LVG model in that the linewidths decrease away from the source centre.
Figure 3.17
LVG clouds with radially decreasing density and slowly increasing velocity (var 0.1). $^{13}$CO spectra (overlay) superimposed on $^{12}$CO spectra for grid LVGIII. See Table 3.3 for details.
LVG clouds with radially decreasing density and slowly increasing velocity \( (v \propto r^{0.1}) \). \(^{13}\)CO spectra (overlay) superimposed on \(^{12}\)CO spectra for grid LVGIII. See Table 3.3 for details.
LVG clouds with radially decreasing density and decreasing collapse velocity ($v \propto r^{-0.5}$). The asymmetry of spectra is apparent in several cases, although the beam has diluted this out to a considerable extent. Grid LVGIV (see Table 3.3).
Figure 3.19

Effect of radially varying microturbulent linewidth for CO spectra at impact parameters 0.0, 0.2, 0.4 and 0.6.

Left: constant microturbulent linewidth ($\Delta v$FWHM = 10 kms$^{-1}$)

Centre: $\Delta v \propto r$ (15 kms$^{-1}$ at cloud edge)

Right: $\Delta v \propto r^{-2}$ (0.4 kms$^{-1}$ at cloud edge)

Otherwise models same as MTII D2 (see Tables 3.2 and 3.4)
We note that where self reversals are present they tend to be spatially extended (see Figure 3.19), whereas in real clouds they are often compact relative to the total cloud size (Phillips et al. 1981; also, see DR21 in Chapter 7).

3.8 Summary of deductions from the models

As is evident from the foregoing discussion, attempts at a systematic investigation of predicted line profiles and maps from alternative cloud models are always in danger of ending up by floundering in a free-parameter space of unlimited dimensionality. Even so, a few results are suggested by the above computations.

Firstly, real clouds would not appear to be uniformly micro-turbulent. This is because such models often predict prominent self reversals in spectra, which would be seen over a large fraction of the cloud. This is not, as a general rule, observed. The contrast between theory and observations is especially stark for the HCO$^+$ J=4-3 transition, where deep and wide self absorptions are widely predicted but not seen.

We must, though, qualify the above by pointing out that:

(i) Self reversals can be to some extent removed by arranging for the excitation temperatures to increase towards the cloud edge e.g. due to cosmic ray heating (Young et al. 1982). Keene et al. (1980) also suggested that heating could be effected by the interstellar UV radiation field. Although this mechanism was subsequently discounted as a major heating source for B335 (Keene et al. 1983), it would still remain true that such contribution as there was would be concentrated towards the surface layers. However, this mechanism is probably less likely to be effective for hot-centred clouds;
(ii) In the above models we have taken the abundances of CO and HCO$^+$ relative to H$_2$ to be constant. The truth of this seems very doubtful. The time scale for most molecules (including CO and HCO$^+$) to condense out on to dust grains is $\sim 1-4 \times 10^6$ years (Iglesias 1977) — much shorter than the estimated cloud lifetimes (a few $\times 10^7$ years). It is probably necessary therefore to identify a particular mechanism for the evaporation of molecules from grain surfaces. Ones which have been put forward include energy supplied from relatively hot infrared sources (Iglesias 1977), low velocity shocks (Williams and Hartquist 1984) and turbulent mixing Boland and de Jong 1982). All of these (especially the first two) would probably give rise to a highly inhomogeneous abundance distribution. In their detailed cloud model, Gerola and Glassgold (1978) also predicted homogeneous and time dependent abundances. Such inhomogeneities could possibly remove predicted self absorptions.

However, simple LVG models would also in many cases appear to be inadequate, quite apart from the considerations of star formation rate discussed in Section 3.2. In order to fit the much smaller source sizes seen in high excitation molecular lines such as those of CS, HCN and HCO$^+$ it seems necessary to postulate radial gradients in the local H$_2$ densities. But in an LVG model this would also imply smaller linewidths in higher transitions (e.g. CO J=3-2 as compared with CO J=1-0). These appear not be observed (Linke and Goldsmith 1980; White et al. 1985; Martin, Sanders and Hills 1984; Plambeck, Williams and Goldsmith 1977; see also the CO spectra of S255 in Chapter 6 of DR21 in Chapter 7 and of various other sources in Chapter 5). Most LVG models with gradients in local density, as well as most microturbulent models, tend also to predict line profiles which are of qualitatively different shape for optically thick than for
optically thin lines. Although such differences are sometimes seen (e.g. in the HCO$^+$ and H$^{13}$CO$^+$ J=1-0 data of Wootten et al. 1984), in the other cases they are not (e.g. see the HCO$^+$ and H$^{13}$CO$^+$ J=4-3 spectra presented in Chapters 6 and 7).

3.9. Clumpy models

Results such as these have led many authors (e.g. Zuckerman and Palmer 1974; Little et al. 1980; Martin, Sanders and Hills 1984; Snell et al. 1984; Matthews et al. 1984; see also Chapters 6 and 7) to consider various types of clumpy model. These can readily explain the similarity of line profiles between molecular lines of very different optical depths. Variations in intensity across a line are now interpreted in terms of beam dilution effects due to the different number of clumps at different velocities.

Also, small scale structure has now been observed directly in some clouds, for example, in transitions of NH$_3$ (e.g. Matsakis et al. 1981; Zheng et al. 1985; see also Chapters 6 and 7) in both lines and the continuum, and at various wavelengths.

If real clouds have small scale structure, how are we to model actual observations, if the beam size is too large to resolve the individual fragments? White (1978) argued that such models, involving as they do a mixture of large and small scale motions, should give predicted antenna temperatures intermediate between the micro-turbulent and LVG cases.

The easiest clumpy model to visualise is one in which each fragment is homogenous in excitation temperature, and is small compared with the size of the region. If, in addition, the dispersion in clump velocities is sufficiently large compared with the linewidth of an individual clump, then one may have the situation in which a given
line of sight only intersects at most one clump at every velocity. (There may still be many clumps along the line of sight, but the velocity dispersion will be sufficient that radiation from one clump is not absorbed by another on its way to the observer). The intensity at each point on the observed profile will then consist of a superposition of radiation from fragments situated at different positions within the beam, but not along the same line of sight. This could constitute an essentially similar kinematic situation to the LVG case i.e. single velocities along a line of sight would correspond to a specific point within the cloud, and excitation conditions would be approximately locally determined. One could then probably without too much error use an LVG program to analyse observations, although due to the dilution occurring in both physical and velocity space it would be necessary to acquire data in a suitable selection of lines, chosen to give contours of beam-independent intensity ratios. These would have to intersect on LVG contour diagrams at sufficiently large angles that values of $n_{\text{H}_2}$ and $X(dv/dr)$ (but not $X$ by itself) could be uniquely determined. The problems of separating the velocity and spatial dilutions are discussed further in Chapter 7, where a more quantitative treatment of clumping is also given for the case of DR21.

The above, though, is a particularly simple form of clumpy model. It seems more reasonable to suppose that each individual clump may have some non-uniform structure, such as a centrally peaked density, and an excitation temperature which for a given transition may vary with radial position within the clump. Although observations in all molecular lines would then still sample positions at all points within the cloud i.e. would still "see" through the whole region, it could well be that the more opaque lines would preferentially sample the outer regions of individual clumps, while the less
opaque ones would penetrate more into the dense centres. If, on the other hand, the individual fragments were gravitationally collapsing, one would be back to the LVG situation again. In either case, the beam and velocity dilutions would mean that one would have to rely on observed line ratios rather than absolute values. Also, predicted model profile shapes for an individual clump would not be directly useable for comparison against observations — only integrated values which would themselves be beam diluted.

We have seen earlier how regimes of cloud excitation structure more generalised than those treated by White (1978) can give predicted intensities (both peak and integrated) that are dependent on the kinematics. We are therefore forced to the conclusion that the detailed, small scale, unresolved cloud structure can for optically thick lines have a sufficiently strong influence on emergent line profiles that densities and molecular abundances derived from observations are sensitive to the assumed cloud model.

3.10 Summary and Conclusions

This Chapter has offered very few direct diagnostic tests to distinguish between cloud models and derive cloud conditions from observations; the general import has been to cast doubt on currently used methods. It would seem that genuine progress can only be made by the accumulation of as complete data as possible on selected clouds (including submillimetre continuum and infrared data).

However, the results of the modelling described do suggest two complementary lines of attack:

(i) Line intensities are much less model dependent for optically thin transitions e.g. those of relatively rare isotopes. Observations in, say, $\text{H}^{13}\text{C}^+ J=1-0$, $J=3-2$, $J=4-3$, or $\text{C}^{34}\text{S} J=1-0$ up to $J=7-6$, could
be the most useful in deriving densities. The conveniently simple LVG model should be quite satisfactory here, although it would have to be borne in mind that, for an inhomogeneous cloud density structure, any derived results would be some sort of weighted mean (see Chapter 7). In this optically thin limit, one might confidently expect that the higher dipole moment molecules would preferentially sample the denser regions. One might then be able to gain information about the degree of inhomogeneity by comparing the densities derived from line ratios such as $^1{C^{180}}_0 J=2-1/^1{C^{180}}_0 J=1-0$, $^3{C^{34S}}_0 J=3-2/^3{C^{34S}}_0 J=2-1$, $^1{H^{13CO^+}} J=4-3/^1{H^{13CO^+}} J=1-0$ etc. as well as any derived dilution factors. This procedure would not give abundance information (e.g. see Figure 2.4). For that, it could be advantageous to combine absolute integrated intensities with continuum information and/or more optically thick isotopes as we will do in Chapter 7 to derive a value for $X_{H^{13CO^+}}$ in DR21.

For such optically thin data, where the intensities are likely to be low, a high signal to noise ratio may be more important than high spatial or velocity resolution.

(ii) Direct observation of small scale structure requires, of course, sufficiently small beam sizes. The great disparity of profile shapes between kinematic models occurs for optically thick lines in regimes where radiative trapping is important (i.e. densities which are insufficiently high to thermalise the lines purely by collisions). It is possible that significant further elucidation of the detailed cloud and clump kinematic structures will require significantly smaller beamsizes at submillimetre wavelengths (e.g. as will be available on the Millimetre Wave Telescope). By observing in optically thick lines with relatively high spontaneous deexcitation coefficients (e.g. $^{12}HCO^+ J=4-3$) one might hope to detect variations in
line profile shapes and widths over small length scales (Matthews et al. 1984). Indeed, strong indications of the power of submillimetre techniques in this respect are given by our HCO\(^+\), HCN and submillimetre continuum data on S255 and DR21 presented in later Chapters. For these sources we will give further consideration to the evidence for clumping.

The results discussed in this Chapter very much represent work in progress rather than definitive solutions to the problems posed. We have chosen to concentrate most on the variety of results predicted by variation of the average density and relative molecular abundance parameters. In future work, the nettle of inhomogeneous cloud structure will have to grasped more firmly. Particularly important is the matter of variable molecular abundances throughout the cloud. Because chemical modelling often predicts variations between hot and cold, dense and rarefied regions, it is important for direct observations to be made which measure these. Recent analyses (e.g. Snell et al. 1984) have used LVG programs to treat data from apparently clumpy clouds, and have examined the goodness of fit of the data in several transitions, on LVG contour plots. We need to check whether clumpy models in which the LVG criterion 2.36 did not apply would still predict values of \( T_R \) which gave constant intersections on LVG plots and, if so, whether the densities and molecular abundances predicted would be reliable. In other words, do statistical tests of self consistency really provide a valid criterion for the applicability of a particular kinematic model, or for the reliability of cloud properties derived from them?

In the approximate formulae discussed in Chapter 2, also the speed and convenience of LVG programs, and the power and capacity for generality of Monte Carlo methods, we now have at our disposal a
panoply of techniques which we can bring to bear on the observational determination of cloud structure. However, the main problems at the moment seem to be incompleteness in available data, and the question of how to cut down the enormous number of free parameters.
CHAPTER 3
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4.1 Introduction

Molecular cloud gas temperatures deduced from CO or NH$_3$ observations - also dust temperatures derived from continuum data - are typically ~ 30-40K for hot centred clouds, and < 20K for dark clouds showing no evidence of massive star formation. These are therefore the approximate values of the radiation temperature $T_R$ which might be observed for a thermalised and optically thick molecular line. However, the discussions of the previous chapters have shown that molecular line data may be most informative when the transitions are optically thin and/or only partially thermalised. These factors will reduce observed antenna temperatures to a fraction of the kinetic temperature. Moreover, beam and velocity dilution effects will tend to lower these still further, with the result that the most potentially valuable observations may have antenna temperatures of a few K or less and so be vulnerable distortion by receiver... noise. Thus, the least easily observed lines may be the most diagnostically useful. Indeed, as in the strange incident of the dog in the night time, a negative detection with a good upper limit on the noise may be just as valuable as a positive one.

We have further seen the desirability of acquiring data at different frequencies on the same source, and it is clearly essential to make sure that these are truly comparable.
In this Chapter, therefore, we give a brief summary of the methods of calibration and reduction applied to the data presented in this thesis and elsewhere in the literature; also, of the question of comparability between data from different telescopes. The discussions are also intended as a link between the somewhat idealised arguments of the preceding chapters and the necessarily more pragmatic approach of the later ones, which are concerned with the analysis of real data.

4.2 Instrumentation and data acquisition

The QMC heterodyne system with which the data were acquired employs an InSb hot electron bolometer as mixer. The required local oscillator power of ~ 1 mW was provided by a millimetre wave klystron driving a Shottky diode harmonic generator. A description of the receiver's construction and operation is beyond the scope of this thesis; details of the QMC system are given in White, Phillips and Watt (1981) and Watt (1980). The use of an InSb hot electron bolometer as a mixer in heterodyne receivers has also been discussed by Phillips and Jefferts (1973) and Phillips (1981). This type of mixer is more efficient at submillimetre wavelengths than the room temperature Schottky diode mixers widely used at lower frequencies. The reason is that the achievable signal-to-noise ratio for a heterodyne mixer is \( \alpha \sqrt{AV/T} \), and the mixer noise temperature for the room temperature Schottky diode increases with frequency much more rapidly than that of the InSb bolometer. At frequencies > 300 GHz, this effect overwhelms the superiority of the former device in instantaneous bandwidth (~ 100 MHz as compared with ~ 1 MHz for InSb).

Unfortunately, the bandwidth of the InSb bolometer is much less than typically observed molecular linewidths (~ 100 MHz). It is therefore necessary in observing a line to sweep the local oscillator
across the required frequency range.

For all the data presented here, the telescope used was the 3.8 m United Kingdom Infra Red Telescope (UKIRT), situated at an altitude of 14000 ft on the summit of Mauna Kea, Hawaii. More specific details of the particular observing runs are given in later chapters. The procedure followed when observing a line towards a particular source was as follows. The spectral range and resolution required were estimated, usually from observations at lower frequencies taken from the literature and/or guesses about the nature of the source. The central LSR velocity of the source also had to be estimated sufficiently accurately for all appreciable emission to fall within the frequency range covered. A suitable IF filter was chosen to give the required spectral resolution; this was typically of similar width to the chosen frequency step. The integration time per step as the local oscillator swept across the line was 100 ms but in practice a number of successive back and forth sweeps was performed to give a total observation time of ~ 5 minutes. One then had the choice of restarting the integration, or moving the telescope to a new position. An equal amount of integration was carried out off, the source, at an adjacent point on the sky (typically ~ 1° away) where there was believed to be no emission. The sequence of integrations on and off source was ON OFF OFF ON ON OFF etc. The substracted ON-OFF pairs were co-added in a buffer, and integration continued until a satisfactory signal to noise ratio was obtained. It was usually necessary also to subtract a linear baseline from the coadded scans. The data acquisition and storage were controlled by a DEC LSI-11 (MINC) minicomputer, on which it was also possible to perform on-line data reduction while observing. The data were stored on floppy discs so that a more thorough reduction could be carried out later.
An alternative mode of observation was to perform drift scans across the source. Here, the frequency step chosen was zero, and the telescope drives were stopped simultaneously with the beginning of integration, so that the source drifted through the beam at the sidereal rate. Different channels in the first scan then corresponded to different points on the sky. This provided a fairly quick method of mapping a source at a given velocity.

For sources which it was intended to observe in detail (e.g. DR21 and S255 in this thesis), spectral mapping was carried out. A set of positions on the source was chosen (A, B, C, D etc., say) and successive integrations and calibrations were performed in an order such as, calibration OFF ON(A) ON(A) calibration OFF and ON(B) ON(B) calibration OFF ON(C) ON(C) calibration OFF etc. Such a sequence has a number of advantages. Firstly, it is only necessary to spend about a third of the total time on the OFF position, because the same OFF integration can be used for the two different ON positions preceding and following it. Secondly, the fact that successive ON/OFF pairs for the same position are taken in opposite order means that the effect of any steady component of drift in sky conditions cancels out in the final coaddition. Also, this sequence is quite efficient in minimising the time taken to move the telescope and calibrate the data. Finally, such spectral mapping fully exploits the capability of a molecular line receiver to achieve both velocity and spatial coverage of a source.

4.3 Calibration

The raw data stored to disc consists not just of the signal from the source, but also of contributions from noise generated in the instrument, from radiation at ambient temperature emitted by the
ground, dome, various parts of the telescope etc., and the atmosphere. Any signal from the source will also have been attenuated in the atmosphere by an amount which can change significantly over very short time scales (Cunningham 1982; Ade et al. 1984). In order to convert the data to physically meaningful source intensities, it is necessary to correct for these other effects.

We have used the chopper wheel method to calibrate the data (Davis & Vanden Bout 1973, Kutner and Ulich 1981). Since this procedure is by now standard, full details are not given here. The method is discussed more exhaustively in the last-mentioned references; see also Ulich and Haas (1976), Ulich (1980), and Kutner, Mundy and Howard (1984).

Essentially, at suitable intervals, integration is carried out with an ambient temperature vane filling the telescope beam, giving a digital reading of, say \(D_{\text{cal}}\). This is repeated with the vane removed, and the telescope pointing at blank sky (i.e. at the "OFF" position of the source). One can then evaluate a "chopper calibration factor" \(C_{\text{cal}}\), given by

\[
C_{\text{cal}} = \frac{D_{\text{cal}} - D_{\text{sky}}}{T'}
\]  

(4.1)

where \(T'\) is related to the ambient temperature \(T_{\text{amb}}\) through

\[
T' = \frac{h\nu}{k} \left\{ \frac{1}{\exp (h\nu/kT_{\text{amb}}) - 1} - \frac{1}{\exp (h\nu/2.7k) - 1} \right\}
\]  

(4.2)

If the raw data for an ON-OFF pair of observations on a source are divided by \(C_{\text{cal}}\), the result is an antenna temperature \(T_{A*}\) which is corrected for all ambient temperature contributions to the signal.
(e.g. ohmic losses in the reflecting surfaces, blockage by the secondary and other parts of the telescope, rearward spillover etc.) and also for attenuation of the source intensity by the atmosphere.

For the data presented in this thesis, calibration was carried out typically after every two ON-OFF pairs (i.e. every 15-20 minutes). This enabled each pair to be corrected by a factor obtained for similar source elevation and atmospheric conditions. The succession of chopper calibration factors obtained throughout the observing period was also useful as a means of monitoring the stability of the atmosphere. On a good and stable submillimetre night, the successive values of $C_{\text{cal}}$ showed typical fluctuations of a few percent, superimposed upon a steady drift (~10-40% per hour) attributable to varying air mass as the source moved across the sky. Sometimes, however, much more sudden changes could occur in the submillimetre sky transparency over a period of 15 minutes. Such unpredictable fluctuations, which are not necessarily accompanied by any palpable deterioration in the state of the atmosphere in the vicinity of the observatory, nor visible changes in the cloud cover, are probably due to the passage of clumps of water vapour through the telescope beam (Cunningham 1982; Ade et al. 1984).

It should be noted also that the chopper wheel calibration technique assumes that the temperature of the absorbing layer in the atmosphere is the same, as that of the chopper vane, whereas in practice this might not be the case. For continuum observations at 3.5 mm, Ulich (1980) has found that failure to correct for this can lead to an error of up to ±10% in the final calculated intensity. Equation 4.1 shows that the errors would be most serious under conditions of high sky opacity. As this becomes large, the value of $C_{\text{cal}}$ should tend to zero. However, if the temperature of the atmosphere was
significantly lower than that of the chopper vane, a finite value
would be obtained for $C_{\text{cal}}$, leading to an erroneously low final value
for $T_R$. For the observations described in this thesis, though, the
principal source of opacity is water vapour which is probably situated
at a similar altitude to the telescope and likely therefore to have
a temperature in deficit of the ambient value by $\leq 10$K (Kutner 1978;
Ulich 1980). Over many observing periods on UKIRT we have found in
practice, for reasonably good sky transparency and frequent calibrat-
ions, that values of $T_A^*$ measured towards frequently observed sources
such as Orion A and DR21 are repeatable to within $\pm 10\%$, which is
generally less than uncertainties due to other factors such as unknown
beam coupling efficiency factors.

There are two further potential sources of error which are not
removed by the aforementioned calibration technique, but for which we
need to account in order to arrive at physically meaningful intensit-
ies:

(i) Forward spillover. This refers to the fraction of the
antenna beam contained in the forward hemisphere which has not hit the
secondary, and which may therefore consist of contributions from over
the whole sky. (Spillover in the rearward hemisphere is assumed to
terminate at some object at ambient temperature and is therefore
corrected for in the chopper calibration). It is represented by
the efficiency factor $\eta_{fss}$ (see Kutner and Ulich 1981), whose value can
be found by calculation (from a knowledge of the receiver and tele-
scope optics; L{\o}surf 1981), or by direct measurement on an extended
object of known brightness temperature (usually the moon).

For the QMC receiver on UKIRT, both methods were used and found
to give a consistent value of $\eta_{fss} = 0.9$. Division of $T_A^*$ by $\eta_{fss}$
gives the quantity $T_R^*$ which has been recommended (Kutner and Ulich
1981) as the most useful for reporting observational results in a relatively model independent way.

(ii) Coupling of the antenna pattern onto the source. Submillimetre telescope beams may have typical widths of ~ 1 arcmin (55" FWHM for UKIRT at 345 GHz) but may also have sidelobes and/or error patterns extending over a wider area. Since source intensity distributions may also vary appreciably over such scales (especially for cloud core regions), it is clear that the coupling of the antenna pattern onto the source brightness distribution must be taken into account in deriving the real source intensities.

It is to some extent arbitrary what part of the antenna power pattern to designate as beam and what as forward spillover. One self consistent definition (Kutner and Ulich 1981), motivated by the method of estimating $n_{fss}$, is to choose a solid angle $\Omega_d$ (almost always that subtended by the Moon), then to regard everything within that as beam and everything outside as forward spillover.

One may then define a source coupling efficiency $n_c$ by

$$n_c = \frac{\iint_{\Omega_s} P_n(\psi - \Omega) B_n(\psi) d\psi}{\iint_{\Omega_d} P_n(\Omega) d\Omega}$$

(4.3)

where $B_n$ is the normalised source brightness distribution and $P_n$ is the antenna power pattern, while $n_{fss}$ is expressible as

$$n_{fss} = \frac{\iint_{\Omega_d} P_n(\Omega) d\Omega}{\iint_{2\pi} P_R(\Omega) d\Omega}$$

(4.4)

The integral in the denominator is performed over the forward hemi-
sphere (Kutner and Ulich 1981).

The factor $n_c$, when divided into $T_R^*$, yields a value for the brightness temperature $T_R$ at the centre of the beam; this corresponds to a physical point intensity.

In summary, we have

$$T_R^* = \frac{T_A^*}{n_{fss}}$$  (4.5)

where $T_A^*$ is the antenna temperature obtained after using the chopper calibration, and

$$T_R = \frac{T_R^*}{n_c}$$  (4.6)

where $n_c$ depends both on the source size and intensity distribution, and on the position of the beam on the source. Many observational results are now presented in terms of $T_R^*$ with $n_{fss}$ defined as above, so that in correcting for coupling onto the source one simply has to correct for $n_c$, normalised to unity for a 30' diameter disc.

However, there are wide variations in forward spillover factors $n_{fss}$ for different telescopes, and also between the error beam characteristics due e.g. to imperfections in the antenna's reflecting surfaces. Although the size of a particular telescope's diffraction limited beam may be well known, the presence of an error beam extending (typically) over a region a few arc minutes in extent can obviously make it very difficult to calibrate data reliably. This is a particularly serious problem in view of the lack of genuinely extended molecular line sources which can be used as standards. Although measurements on such intense sources as Orion A and DR21 are often used as a guide, they are not totally satisfactory because their intensities vary over length scales of $\sim 1$ arc minute or less. To illustrate the problem, we show in Table 4.1 some measurements of
$T_A^*$ towards Orion A in the lowest 3 CO transitions, all of which are thought to be optically thick and thermalised and which might therefore be expected to be very similar to one another. However, the values of $T_A^*$ show wide variations. For most of the work cited in Table 4.1 the authors have gone on to make some corrections for beam dilution and obtained a value for $T_R$ or $T_R^*$, which to some extent (though not always) reduces the disparity in the results. However, any attempt at such corrections beyond the standard $n_{fss}$ measurements onto the Moon's disc are highly model dependent, and particular to the individual telescope. The values of $T_A^*$ shown in Table 4.1 probably give a more realistic impression of the problems of data comparability. A cursory glance at this Table together with Figures such as 2.2, 2.3 and 2.4 serve to emphasise the hazards of employing e.g. LVG modelling, using data in different molecular transitions observed with different telescopes, in order to estimate local $H_2$ densities and relative molecular abundances.

4.4 Comparability of data

Despite the concomitant calibration difficulties mentioned in the previous section, it is often desired to combine observations of a particular source in different transitions of the same molecular species. Since these will almost invariably be at very different wavelengths, the lines need to be observed with different telescopes, if similar bandwidths are to be obtained. These will in general have different antenna patterns. Valid comparison of data can in principle be achieved if the telescope antenna patterns are known; any predicted model intensity distribution can then be convolved with the beam shapes to give predicted values of $T_R^*$.

It is sometimes more convenient, though, to convert observed
Table 4.1

Measured values of $T_A^*$ towards Orion A in CO transitions

<table>
<thead>
<tr>
<th>CO transition</th>
<th>Telescope</th>
<th>$T_A^*$ (K) (unless otherwise stated)</th>
<th>Beam FWHM arc sec</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J = 1 - 0$</td>
<td>Nobeyama 45m</td>
<td>26</td>
<td>15</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>NRAO 11m</td>
<td>57</td>
<td>64</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>OVRO</td>
<td>70$^a$</td>
<td>60</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>Hat Creek 6m</td>
<td>46 (77)$^b$</td>
<td>110</td>
<td>4</td>
</tr>
<tr>
<td>$J = 2 - 1$</td>
<td>UKIRT 3.8 m</td>
<td>58</td>
<td>85</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>NRAO 12m</td>
<td>70</td>
<td>30</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>MWO 5m</td>
<td>71</td>
<td>75</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Hat Creek 6m</td>
<td>35 (88)$^b$</td>
<td>55</td>
<td>4</td>
</tr>
<tr>
<td>$J = 3 - 2$</td>
<td>UKIRT</td>
<td>70</td>
<td>55</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>MMT</td>
<td>67</td>
<td>26</td>
<td>5</td>
</tr>
<tr>
<td>$J = 4 - 3$</td>
<td>UKIRT</td>
<td>48</td>
<td>35</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>UKIRT</td>
<td>82</td>
<td>35</td>
<td>6</td>
</tr>
</tbody>
</table>

$^a T_R^*$

$^b$ Numbers in brackets are authors' estimates of $T_R$, corrected for coupling onto a 4 arc min diameter uniform source (which Orion A is not).

values of $T_R^*$ to $T_R$, using equation 4.6. An example is when carrying out a basic analysis on data taken at one position. This, however, assumes knowledge of $n_c$, which cannot be derived rigorously since the true source brightness distribution $B_n$ is unknown. Nevertheless, for simple modelling, and observations towards the central peak of a source, values of $n_c$ can be estimated on the assumption that the source has some simple brightness distribution (e.g. a uniform disc). Values for $T_R$ may thence be derived and then used in an analysis which, through crude, is nonetheless superior to one which assumes the source to be extended with respect to the telescope beam, and which therefore implicitly equates $T_R$ with $T_R^*$.

There are two alternative paths towards obtaining comparable data at different frequencies. One is to observe different lines on different telescopes, chosen to give beamwidths which are as similar as possible. It will still in general be necessary to correct the observations for different source coupling efficiencies, since the antenna patterns will never be identical. This approach is used for the CO data on high velocity wing sources in Chapter 5, where the three telescopes were NRAO 11m (CO J=1-0), MWO (CO J=2-1) and UKIRT (CO J=3-2). They have beamwidths (FWHM), for those transitions, of 64, 75 and 55 arc seconds respectively, and their beam coupling efficiencies as a function of source diameter (onto a uniform disc) are shown in Figure 4.1.

An alternative approach is to observe in two or more transitions on the same telescope with the same receiver. One advantage here is that the procedures for observing, calibrating, and calculating beam efficiencies are likely to be more internally consistent. Also, the various sources of emission and absorption for which one attempts to correct in calibration - for example, atmospheric absorption and
Figure 4.1
Beam coupling efficiencies $\eta_c$:

- NRAO 11m at 115GHz (Kutner, Mundy and Howard 1984)
- MWO 5m at 230GHz (Loren, private communication)
- UKIRT 3.8m at 345GHz (Lesurf 1981)
Figure 4.2

UKIRT

Ratio $\eta_c(345 \text{ GHz})/\eta_c(230 \text{ GHz})$ as a function of source diameter for a uniform disc, and as a function of source FWHM for a Gaussian source.
emission, and both forward and rearward spillover – are likely to be relatively similar. Any hidden systematic errors which may be present in the calibration (for example due to error in the assumption that the telescope, dome and atmosphere are all at the same temperature: see, for example, Kutner 1978; Ulich 1980) are more likely to have the same sign for the two frequencies, and will hopefully tend to cancel out when ratios of line intensities are calculated.

It is of course necessary to allow for the fact that the beamwidths are different at the two frequencies. Figure 4.2 shows the calculated ratio $n_C (345 \text{ GHz}) / n_C (230 \text{ GHz})$ for UKIRT, plotted against source diameter, for both a uniform disc and a Gaussian source. We see from this that the ratios are never different from one another by more than ~ 12%, and often by much less. Thus, derived corrected ratios of $T_R$ are not likely to be too sensitive to errors in the assumed source brightness distribution. A further point is that for source diameters between, say, 1.5 and 6 arc minutes, the disparity between $n_C (230 \text{ GHz})$ and $n_C (345 \text{ GHz})$ for UKIRT is actually less than the variations between the values for the telescope represented in Figure 4.1, which were chosen on the basis of roughly equal beamwidths.

It is probable that the agreement would not be so good in the case of an antenna used near the upper limit of its useful frequency range, since the quality of the reflecting surface might be appreciably different between the 2 transitions. For example, use of the formulae given by Kutner, Howard and Mundy (1984) for the NRAO 11m antenna before its recent resurfacing, predicts an error beam at 115 GHz which has FWHM = 35' and contains 25% of the power, whereas at 230 GHz the respective figures are 17' and 75%. Nonetheless, for frequencies where reflecting surface irregularity is not a
problem, it may be better to obtain data at different frequencies with the same telescope and receiver, rather than with different ones chosen to give more equal nominal beamwidths. Examples of pairs of lines where this would be the case are CO J=3–2 and J=2–1, HCO+ J=4–3 and J=3–2, and CS J=7–6 and J=5–4 (and their isotopes), all of which can be observed at UKIRT with an InSb receiver.

4.5 Data reduction

The data obtained were reduced using the GEC 4070 Multi User Minicomputer (MUM) at Queen Mary College. The reduction program was a revised version of one already available on the DEC LSI-11 and mentioned in Section 4.2, but was extended to have a wider range of reduction routines and graphics facilities. It was found convenient to make extensive use of the CERN HBOOK and HPLOT histogramming and plotting packages (Brun, Ivanchenko and Palazzi 1979; Brun and Watkins 1981). Routines available included ones for combining scans in various ways including scaling and coadding them (weighted if necessary according to noisiness), for fitting Gaussians, subtracting linear baselines, and for producing spectra and contour diagrams etc. It was also possible to have simultaneous access to data obtained on different observing runs, so that observations could be compared or combined in a flexible way.

The estimation of error bars for the data is somewhat problematic, as also is the process of coadding scans so as to minimise errors. As described earlier, the data for each frequency bin in a spectrum consists of many 100 ms integrations, and error bars should in principle be calculable from the standard deviations of these. Each bin of each 5 minute scan would then have a completely independent error bar assigned to it, and instrumental spikes
occurring in individual 100 ms integrations could be rejected on purely objective criteria. Unfortunately, due to restricted storage space this has not yet been put into practice - merely the accumulated sums for each channel over the 5 minute scans were stored to disc. For most observations, the noise level had therefore to be roughly estimated from the channel to channel fluctuations in the baseline.

For observations with longer integration times (for example 6 ON-OFF pairs) some statistical weighting and despiking in individual channels was possible by means of an iterative routine in the data reduction program. Each ON-OFF pair was divided by its appropriate chopper calibration factor and a linear baseline fitted. For each channel, i, a mean intensity $T_i$ of the $N_s$ scan-pairs was calculated. Also for each channel a sample standard deviation $\sigma_i$ was evaluated from

$$\sigma_i = \left( \frac{\sum_{j=1}^{N_s} (T_{ji} - \bar{T}_i)^2}{N_s - 1} \right)^{0.5}$$

(4.7)

where $T_{ji}$ is the intensity in the ith channel of the jth scan. Individual values of $T_{ji}$ were rejected if they deviated by more than $3\sigma_i$ from the mean for that particular channel. An estimate $\sigma'_j$ of the noise level for each scan $j$ was then made by computing

$$\sigma'_j = \left( \frac{\sum_{i=1}^{N_C} (T_{ji} - \bar{T}_i)^2}{N_C - 1} \right)^{0.5}$$

(4.8)

where $N_C$ is the number of channels, and a weighted average $T_i'$ then found using
New values of $\sigma_i$ were then found with this as a new average, and the iterative process repeated until satisfactory convergence was obtained. The exit point from the iteration was determined by visual inspection. Usually, two or three iterations were sufficient.

For most cases in which this iterative procedure was used, the resulting spectrum was very similar to the one obtained by taking a straight average of the calibrated pairs. The process was nevertheless found to be useful for observations with very long integration times (e.g. 1 hr of real time) e.g. the $^{13}$CO$^+$ $J$=4-3 spectrum towards S255 (Chapter 6) and the CS $J$=7-6 spectrum towards DR21(OH) (Chapter 7), since in these cases the source elevation changed significantly over the period of observation.

4.6. Conclusions

We have given a brief overview of the various issues relating to the acquisition, reduction and calibration of submillimetre molecular line data.

The process of reducing the data inevitably entails a certain amount of subjective sifting by the observer, because of the difficulty of observing at these wavelengths and the consequently small data sets. If one could achieve the computing speed and memory necessary to examine data in smaller time intervals (e.g. 100 ms chunks) then a more objective reduction could be performed using more satisfactory statistical techniques, in a way which could account both for random noise and for secular drift in both the
receiver and the atmosphere.

In the meantime, it would seem essential that data should be taken with as few preconceptions as possible, bearing in mind the great variety of profiles and intensities predicted by the various rival models. Since, for example, clouds may contain clumpy structure, and the local densities within a clump may or may not be the same at points near the cloud centre and the cloud edge, there is no justification for presupposing that there will be any difference in linewidths between optically thin and optically thick lines, nor between higher than lower excitation lines. In taking data to compare against cloud models it is therefore necessary to use similar velocity coverage for all transitions, regardless of intensity.

We have also considered the need to correct observed intensities for the coupling of the beam onto the source, especially when comparing results taken at very different frequencies. If the frequency range is very wide (e.g. 115-345 GHz) it is probably necessary to use more than one telescope, in order not to have excessively different beamwidths for the lines observed. In this case it is still essential to allow for the different antenna patterns of the telescopes used. In other circumstances, the advantages of using the same telescope and receiver for different frequency lines may outweigh those gained by using different telescopes even with more closely similar nominal beamwidths.

In the remaining Chapters, we present submillimetre molecular line data acquired over several observing sessions on UKIRT. We shall return to some of the issues addressed in this and the previous chapters, but this time within the context of specific sources and sets of data.
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CHAPTER 5

CO J=3-2 OBSERVATIONS OF MOLECULAR LINE SOURCES HAVING HIGH VELOCITY WINGS

5.1. Summary

13 molecular line sources which exhibit high velocity wings in the CO J=1-0 rotational transition have been observed in the CO J=3-2 line. In all cases we have detected high velocity wings in this transition. LVG modelling of the relative line intensities of the lowest three transitions indicates, for some of the sources, that densities are present which are considerably higher than previously quoted estimates of average hydrogen density determined only from CO J=1-0 data. The CO J=1-0 line is often thermalised, and has an optical depth < 1, but the CO J=3-2 transition may be subthermally excited, and can be more optically thick (τ > 1).

We also derive low values of apparent CO fractional abundance per unit velocity gradient, which may be due to a depletion of CO in the outflow regions, or alternatively to clumping of the outflowing molecular gas.

The more compact (< 0.5 pc) outflows exhibit a higher degree of thermalisation, indicating higher densities, and also a higher ratio of kinetic to gravitational potential energy. The results are consistent with a model in which an expanding but decelerating shell of molecular material is swept up by a pre-main sequence stellar wind or a magnetically driven shock.
5.2. Introduction

High velocity wings have now been observed in a number of molecular clouds, particularly in the J=1-0 and J=2-1 transitions of CO. (For surveys and references, see Loren 1981; Plambeck, Snell, and Loren 1983; Bally and Lada 1983; and Loren et al. 1981).

The wing emission of many of these sources exhibits a bipolar structure which is usually less spatially extended than the emission in the line core. The concurrence of high velocities and small spatial extents has in many cases led to their being modelled as high velocity outflows, possibly driven by intense stellar winds occurring during a pre-main sequence phase of stellar evolution, or, alternatively, by a magnetically driven shock wave or a centrifugally driven wind (Draine 1983; Pudritz and Norman 1983). This is in contrast to the narrower line core, which is thought to emanate from the surrounding molecular cloud.

Despite growing recognition of their astrophysical significance, there remain great gaps in our knowledge of conditions in these regions; in particular, of their temperatures, gas densities, kinematical states, and optical depths in various molecular rotational transitions. Partly, this is because of the special observational difficulties of investigating compact regions of low intensity.

Much of the previous investigation of the outflow regions has been carried out using the J=1-0 transitions of \(^{12}\)CO and \(^{13}\)CO. From spectral observations of the regions in these lines it is possible, given certain assumptions, to estimate optical depths, excitation temperatures, outflow masses and average molecular hydrogen densities, using the method described by Bally and Lada (1983). This is subject, however, to some serious uncertainties:

(i) The optical depth is estimated from the ratio of observed
$^{13}$CO and $^{12}$CO intensities. This can be unreliable because the $^{13}$CO wings are so weak (usually much less than 1K or not detected at all). It is also necessary to assume a value for the isotopic abundance ratio, which itself may be uncertain by a factor $> 2$.

(ii) After the $^{13}$CO column density has been derived, a value for the ratio $^{13}$CO/$H_2$+He is required, in order to estimate the region's mass. Wootten et al (1978) have found that this ratio can, in hot, dense regions, be reduced by an order of magnitude or more, relative to that estimated for dark clouds (Dickman 1978). Since the $^{12}$CO transitions are usually optically thick for most of the cloud material, the $^{12}$CO/$H_2$+He ratio is even more uncertain; its value is needed, together with the sometimes unjustified assumption of optical thinness, in cases where $^{13}$CO data are not available.

(iii) To convert from masses to average hydrogen densities, assumptions are needed about the source size and geometry.

An alternative procedure, adopted by Plambeck, Snell, and Loren (1983) is to combine observations in different transitions (in their case, CO J=1-0 and CO J=2-1), which enables optical depths to be estimated without recourse to $^{13}$CO data. By assuming effectively that the lowest two transitions are thermalised at the temperature of the surrounding cloud, these authors have derived line optical depths which are sometimes greater than unity. Their conclusion is that the outflows may consist of a number of small clumps which are individually much smaller than the beam size, even though the outflow region may be large enough to fill the beam.

The assumption of equal excitation temperatures, however, requires the local hydrogen densities to be high enough to thermalise the transitions. For a typical kinetic temperature of 40K, and assuming no radiative trapping, local molecular hydrogen densities $> 10^4$ cm$^{-3}$
are needed for the excitation temperature of the J=2-1 transition to exceed 30K, which is higher than all but one of the average densities derived by Bally and Lada (1983). Such higher local densities might be present, if the material was clumped; also, radiative trapping effects might help to thermalise the transitions. Nevertheless, in view of its dependence on the degree of inhomogeneity of the material, there would appear to be inadequate grounds for adopting complete thermalisation as an initial premise.

The CO J=3-2 transition of CO at 345.9 GHz provides another potential probe of conditions in these regions (White, Phillips, and Watt 1981; Phillips et al. 1981; Phillips et al.1982; White 1982; Phillips, White and Watt 1982; Erickson et al. 1982; this transition is fairly easily excited, but at higher densities (> $10^4$ H$_2$ molecules per cm$^3$) than are the CO J=1-0 and CO J=2-1 lines. Over a wide range of conditions it has a higher opacity than the lower CO transitions, and this fact can hinder unique interpretation of data from the lower velocity dispersion line core. But in outflow regions, the behaviour of the CO J=3-2 transition can differ significantly from those of the lower lines, and, in combination with them, can therefore yield independent information on the disturbed gas. In particular, the fact that it may not be fully thermalised can allow a more direct determination to be made of the molecular hydrogen density, obviating the need to assume a value for the abundance of CO relative to H$_2$, or to make assumptions about the optical depth or degree of thermalisation of the transitions.

5.3 Observations

The observations were carried out using the 3.8 m United Kingdom Infra Red Telescope (UKIRT) on Mauna Kea, Hawaii, during the periods
26th August to 1st September and 29th November to 6th December, 1982 (together with a few additional observations during May 1983).

The receiver used in each case was an indium antimonide hot electron mixer. In the latter period, we used the Queen Mary College submillimetre heterodyne system, which typically achieved total system noise temperatures of 275-600K at the CO J=3-2 frequency, and which was also found to have highly stable baseline repeatability. Observing conditions were mostly very good, with atmospheric transmission at the zenith often being between 85% and 90%, and included an exceptional period in December 1982, immediately after the passage of Hurricane Iwa, with transmission greater than 95%. Observations in the earlier period were obtained using the UKIRT InSb heterodyne common user system (White, Phillips and Watt 1981).

Calibration was carried out at approximately 15-30 minute intervals, using a chopper wheel calibration technique (Kutner and Ulich 1981). This technique has, over the last four years, given calibrated intensities on the Orion CO peak which agree to within 5%. From scans across Saturn, the beam width (FWHM) was measured to be 55". The forward spillover efficiency (\(\eta_{fss}\)) was estimated to be 0.9, from Moon scans. Both these values are consistent with theoretical calculations of the antenna pattern and previous measurements of heterodyne receiver systems on UKIRT (Lesurf 1981). A weak sidelobe at the -20db level is present with a FWHM of 3 arc minutes. Pointing with UKIRT, as determined with an on-axis TV guider, was generally found to be excellent, with an rms uncertainty of less than 5 arc seconds.

5.4 Problems of data comparability

As discussed in Chapter 4, the valid comparison of molecular line data taken at different frequencies, often by different observers,
using different receivers and telescopes with different antenna patterns is a practice fraught with difficulties. These become particularly acute for observations of weak high velocity wing emission. The sizes of the emitting regions are often similar to or smaller than the telescope beamwidths, and the absolute intensities are frequently low. Not only might the beam coupling efficiency of a particular telescope be sensitive to variations in assumed source size, but also, for a given size, different telescopes will in general have different efficiencies. It is therefore important to compare data only between telescopes whose beam properties are well known, and preferably similar.

We have, for the most part, chosen to compare our CO J=3-2 data with CO J=1-0 and CO J=2-1 results from the literature, taken respectively with the NRAO llm and the University of Texas Millimetre Wave Observatory (MWO) 4.9 m antennae. The CO J=3-2 data, with CO J=1-0 and CO J=2-1 spectra superimposed, are presented in Figures 5.1-5.11. The telescopes have beamwidths (FWHM) of 64" (NRAO at 115 GHz), 75" (MWO at 230 GHz) and 55" (UKIRT at 345 GHz). For each telescope, we have tabulated coupling efficiencies $n_c$ for a range of source sizes (assumed to be uniform discs), as described in Chapter 4. However, where authors actually quote efficiencies for NRAO or MWO which differ from those given in Chapter 4 we use their quoted values.

As a measure of the intensity in the line wings we define the quantity $T_{\text{wing}}$, given by

$$T_{\text{wing}} = \frac{\int_{V_1}^{V_2} T_A^* dv}{(V_2-V_1) \eta_{fss} n_c(\theta)} = \frac{\int_{V_1}^{V_2} T_A^* dv}{(V_2-V_1) n_c(\theta)}$$

(5.1)
where the integral is carried out over the velocity range $V_1$ to $V_2$ of wing emission (but excluding the line core) and $\eta_c(\theta)$ is the coupling efficiency for source angular size $\theta$. ($\eta_c(\theta)$ will also, in general, vary across the line profile. We have employed average efficiencies for the assumed velocity ranges). For a velocity interval which contains wing emission having a triangular profile, $T_{\text{wing}}$ represents the best available estimate of the peak wing radiation temperature $T_R$, corrected for beam dilution (given an assumed source size). If there is further dilution within the assumed extent of the source, for example due to small scale inhomogeneities (clumping), or if, as is likely, the wing component reaches a peak at a velocity where it is dominated by emission from the core component, then $T_{\text{wing}}$ provides a lower limit on the true value of $T_R$. (For HH7-11 and L1551, the wing component is sufficiently distinct that a peak value can be taken directly). For some sources, one wing is much weaker than the other. For these, only the stronger one has been used in the analysis.

There is some arbitrariness in the specification of the wing interval limits, especially the inner ones. These were generally taken from existing CO J=1-0 velocity/position maps, or from comparisons of $^{13}$CO or higher excitation molecular spectra with those of $^{12}$CO, and are given in Table 5.1.

Limitations of observing time prevented our determining sizes for some of the sources, so for these we have used sizes taken from mapping observations reported at lower CO frequencies. For source sizes $> 1.5'$, the ratios of efficiencies between all three telescopes are constant to within about 10%. Consequently, although source size errors may lead to substantial ($\approx 30\%$) errors in absolute values of $T_{\text{wing}}$, the ratios of line temperatures are much better determined,
Table 5.1

Source positions, assumed distances and velocity ranges

<table>
<thead>
<tr>
<th>Source</th>
<th>RA (1950)</th>
<th>Dec (1950)</th>
<th>Distance (pc)</th>
<th>Wing intervals: (kms⁻¹)</th>
<th>J=1-0 and J=2-1 refs.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Blue</td>
<td>Red</td>
</tr>
<tr>
<td>GL490</td>
<td>03 23 41</td>
<td>58 36 52</td>
<td>900</td>
<td>-36, -16</td>
<td>-8, 10</td>
</tr>
<tr>
<td>HH7-11</td>
<td>03 25 58.2</td>
<td>31 05 46</td>
<td>500</td>
<td>...</td>
<td>11,25</td>
</tr>
<tr>
<td>L1551</td>
<td>04 28 31.6</td>
<td>17 59 52</td>
<td>120</td>
<td>-5+5</td>
<td>...</td>
</tr>
<tr>
<td>T Tau</td>
<td>04 19 03</td>
<td>19 24 26</td>
<td>140</td>
<td>-1,7</td>
<td>9,15</td>
</tr>
<tr>
<td>Ori A</td>
<td>05 32 47</td>
<td>-05 24 17</td>
<td>500</td>
<td>-30,0</td>
<td>20,50</td>
</tr>
<tr>
<td>NGC2024</td>
<td>05 39 14</td>
<td>-01 56 57</td>
<td>500</td>
<td>...</td>
<td>14,18</td>
</tr>
<tr>
<td>NGC2071</td>
<td>05 44 30.5</td>
<td>00 20 17</td>
<td>450</td>
<td>0.6</td>
<td>12,20</td>
</tr>
<tr>
<td>S255</td>
<td>06 09 59</td>
<td>18 00 15</td>
<td>2500</td>
<td>...</td>
<td>11,14</td>
</tr>
<tr>
<td>GL61</td>
<td>06 31 59</td>
<td>04 15 03</td>
<td>1600</td>
<td>0.9</td>
<td>16,25</td>
</tr>
<tr>
<td>M17(SW)</td>
<td>18 17 26</td>
<td>-16 14 54</td>
<td>2000</td>
<td>10,15</td>
<td>...</td>
</tr>
<tr>
<td>Serpens</td>
<td>18 27 17</td>
<td>01 12 40</td>
<td>440</td>
<td>0.6</td>
<td>11,17</td>
</tr>
<tr>
<td>DR21</td>
<td>20 37 10</td>
<td>42 09 00</td>
<td>3000</td>
<td>-12, -28</td>
<td>4,20</td>
</tr>
<tr>
<td>Elias 1-12</td>
<td>21 45 26.8</td>
<td>47 18 08</td>
<td>900</td>
<td>-7.5, 0.3</td>
<td>6.8, 17.2</td>
</tr>
</tbody>
</table>

and it is these which largely determine our estimates of hydrogen densities in the present analysis. Accordingly, our estimates of hydrogen density should be more reliable than those of the relative CO abundance.

Values of assumed angular source size and of $T_{\text{wing}}$ are given in Table 5.2.

5.5 Modelling

A large velocity gradient (LVG) model has been used to calculate $T_R$ in the lowest 3 CO transitions. In such a model, $T_R$ can be calculated as function of gas kinetic temperature $T_K$, the combined $H_2$ and He density $n(H_2 + He)$, and the fractional abundance per unit velocity gradient of CO relative to hydrogen plus helium, $X_{CO}/(dv/dr)$, expressed in pc km$^{-1}$s. These last two quantities will be referred to as $n_{H2}$ and $x$ respectively.

For each of a series of kinetic temperatures between 10K and 100K, a diagram was produced, in which contours of both $T_R$ and the line intensity ratios were plotted on axes of log $x$ and log $n_{H2}$, as described in Chapter 2.

The LVG model considered here refers to a homogeneous and uniformly expanding volume of gas. Such a model may not represent the actual conditions within an outflow region, for several reasons, especially:

(i) the $v \propto r$ relationship may not be obeyed in the outflow; for example, Genzel et al. (1981) give $v \propto r^\alpha$ where $\alpha = 0.3 \pm 0.1$ from $H_2O$ maser observations in Orion, and Loren (1981) suggests $v \propto r^{-0.5}$ for the sources he observed in the CO J=1-0 transition;

(ii) the average gas density may vary with radial distance; this would mean that the CO J=3-2 radiation would be likely to be emitted
<table>
<thead>
<tr>
<th>Assumed Source size (arc min)</th>
<th>T\textsubscript{wing}(K)</th>
<th>Ref. for assumed size</th>
</tr>
</thead>
<tbody>
<tr>
<td>GL490</td>
<td>2.5</td>
<td>1</td>
</tr>
<tr>
<td>HH7-11\textsuperscript{c}</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>L1551\textsuperscript{b}</td>
<td>8\textsuperscript{d}</td>
<td>3</td>
</tr>
<tr>
<td>T Tau\textsuperscript{b}</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Ori A</td>
<td>0.7</td>
<td>5</td>
</tr>
<tr>
<td>NGC2024</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>NGC2071</td>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>S255</td>
<td>0.7</td>
<td>7</td>
</tr>
<tr>
<td>GL961</td>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>M17(SW)\textsuperscript{b}</td>
<td>6</td>
<td>9, 10</td>
</tr>
<tr>
<td>Serpens</td>
<td>6</td>
<td>11</td>
</tr>
<tr>
<td>DR21</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Elias 1-12\textsuperscript{c}</td>
<td>1</td>
<td>12</td>
</tr>
</tbody>
</table>

\textsuperscript{a} Values of T\textsubscript{wing} for the sources read directly (see section 5.4).
\textsuperscript{b} Blue wing only.
\textsuperscript{c} Red wing only.
\textsuperscript{d} Harmonic mean size.

from a smaller volume than that from the lower transitions;

(iii) the radiation may come from optically thick clumps, in which the conditions required for valid application of an LVG model might not exist.

However, because of the above-mentioned uncertainties in the actual data, it seems undesirable and unjustifiable to introduce the extra free parameters which would be needed for a more complex model. Any gas densities we derive will be interpreted as being characteristic of the volume corresponding to the assumed source size. As discussed below, for most sources we deduce values of $x$ which are at least an order of magnitude lower than typical values ($\sim 8 \times 10^{-5}$) found for the more quiescent cloud material, and consequent optical depths which are seldom much greater than unity. We do not therefore expect the results to be very sensitive to the assumed outflow kinematics. The LVG model employed here may be regarded as a first order method of correcting for radiative trapping in the solution of the statistical equilibrium equations.

If no beam dilution is assumed, and $T_{\text{wing}}$ is taken as an estimate of $T_R$ in each transition, then the 3 values of $T_{\text{wing}}$ will each define a line in the log $n_\text{H}_2$/$\log x$ plane, given an assumed kinetic temperature for the source. Ideally, these should intersect at the same point and define unique values of $n_\text{H}_2$ and $x$; in practice, the scatter in their intersection points will give an estimate of the errors, which are typically up to half an order of magnitude in $n_\text{H}_2$ and an order of magnitude in $x$. Since the beam efficiencies for NRAO and UKIRT have been extensively checked observationally (Kutner, Mundy and Howard 1984; Lesurf 1981), while those for MWO are theoretically derived (and also in general smaller than for the other two antennae), we have used the data from the first two telescopes in deriving values for $n_\text{H}_2$.
and x. However, we have found that the $T_{\text{wing}}$ data in the J=2-1 transition are consistent with those for the J=1-0 and J=3-2 lines, within the likely ranges of error.

As an example of the modelling, the relevant contour intersections for a representative sample of the sources are shown in Figures 5.12 to 5.16 together with an indication of the effect of ± 30% errors in the observed values of $T_{\text{wing}}$ (which would tend to have the same sign if due to an incorrect assumed source size).

If the possibility of beam dilution is admitted, then we have $T_{\text{wing}} = W T_R$ where the beam dilution factor, W is <1, and is unknown. In this case, the method described above may give an underestimate both of $n_{H_2}$ and of x in individual clumps. For a non-thermalised CO J=3-2 transition, though, the effect on $n_{H_2}$ is usually small.

The ratio

$$R_{31} = \frac{T_{\text{wing}} (J = 3 - 2)}{T_{\text{wing}} (J = 1 - 0)} \quad (5.2)$$

may be taken as a estimate of the quantity

$$r_{31} = \frac{T_R (J = 3 - 2)}{T_R (J = 1 - 0)} \quad (5.3)$$

This is, to first order, independent of beam dilution and gives a useful lower limit to $n_{H_2}$ since, for a non-thermalised CO J=3-2 transition in the limit of low optical depth, the contour of $r_{31}$ tends to a line of constant density, independent of x, which will be referred to as $n_{H_2}$ (thin) (e.g. see Figure 5.12).
Appropriate kinetic temperatures were assumed from the CO J=1-0 intensities in the line core, although for 3 sources, L1551, HH7-11 and NGC 2024, a higher temperature was needed in order to account for the relative enhancements observed in the CO J=3-2 and CO J=2-1 wing intensities, compared with those in the CO J=1-0 line.

Results from the modelling are given in Table 5.3, which includes one source, L1551, for which the data have been presented previously (White, Phillips and Watt 1981) and also S255, which is the subject of Chapter 6. For some sources, it is found that all 3 lines are thermalised; for these we can only place a lower limit on the density. In such cases the value of log nH2 given in the table may be replaced by log nH2 + Δ, where Δ is an arbitrary positive number, provided log x is replaced by log x - Δ, thereby preserving the same number density of CO molecules (e.g. see Figures 5.13 and 5.14).

5.6 Comments on Individual Sources

GL490

The spectrum for this source is shown in Figure 5.1. J=3-2 wing emission is detected over most of the velocity range in which wings have already been observed in the lower transitions (Lada and Harvey 1981; Plambeck, Snell and Loren 1983; Kawabe et al. 1984). An LVG solution gives a gas density of 2 x 10^4 cm^{-3}. Thronson and Lada (1984) quote a peak wing temperature of T_A^* = 0.059 K for the CS J=2-1 transition, and no emission over most of the CO wing velocity range. Taking a typical X_{CS} of 5 x 10^{-10} (Linke and Goldsmith 1980) and V/R = 100 kms^{-1} pc^{-1}, the CS observation gives nH2 < 3 x 10^4 cm^{-3}, consistent with our CO result.
Appropriate kinetic temperatures were assumed from the CO J=1-0 intensities in the line core, although for 3 sources, L1551, HH7-11 and NGC 2024, a higher temperature was needed in order to account for the relative enhancements observed in the CO J=3-2 and CO J=2-1 wing intensities, compared with those in the CO J=1-0 line.

Results from the modelling are given in Table 5.3, which includes one source, L1551, for which the data have been presented previously (White, Phillips and Watt 1981) and also S255, which is the subject of Chapter 6. For some sources, it is found that all 3 lines are thermalised; for these we can only place a lower limit on the density. In such cases the value of log $n_{H_2}$ given in the table may be replaced by log $n_{H_2} + \Delta$, where $\Delta$ is an arbitrary positive number, provided log $x$ is replaced by log $x - \Delta$, thereby preserving the same number density of CO molecules (e.g. see Figures 5.13 and 5.14).

5.6 Comments on Individual Sources

G1490

The spectrum for this source is shown in Figure 5.1. J=3-2 wing emission is detected over most of the velocity range in which wings have already been observed in the lower transitions (Lada and Harvey 1981; Plambeck, Snell and Loren 1983; Kawabe et al. 1984). An LVG solution gives a gas density of $2 \times 10^4$ cm$^{-3}$. Thronson and Lada (1984) quote a peak wing temperature of $T_A^* = 0.059$ K for the CS J=2-1 transition, and no emission over most of the CO wing velocity range. Taking a typical $X_{CS}$ of $5 \times 10^{-10}$ (Linke and Goldsmith 1980) and $V/R = 100$ kms$^{-1}$ pc$^{-1}$, the CS observation gives $n_{H_2} < 3 \times 10^4$ cm$^{-3}$, consistent with our CO result.
Table 5.3

Results from modelling

<table>
<thead>
<tr>
<th>Source</th>
<th>Assumed Temp of outflow(K)</th>
<th>log ( n_{\text{H}_2} ) (cm(^{-3}))</th>
<th>log ( n_{\text{H}_2}(\text{thin}) ) (cm(^{-3}))</th>
<th>log ( x )</th>
<th>log ( x_{\text{est}} )</th>
<th>Optical Depth 1-0</th>
<th>Optical Depth 3-2</th>
<th>Tex 1-0</th>
<th>Tex 3-2</th>
<th>( R )</th>
</tr>
</thead>
<tbody>
<tr>
<td>GL490</td>
<td>20</td>
<td>4.3</td>
<td>4.1</td>
<td>-7.2</td>
<td>-6.0</td>
<td>0.2</td>
<td>0.8</td>
<td>22</td>
<td>14</td>
<td>900</td>
</tr>
<tr>
<td>HH7-11</td>
<td>80</td>
<td>4.6+Δ</td>
<td>4.2</td>
<td>-7.1-Δ</td>
<td>-6.1</td>
<td>0.03</td>
<td>0.4</td>
<td>142</td>
<td>63</td>
<td>300</td>
</tr>
<tr>
<td>L1551</td>
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<td>4.6+Δ</td>
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<td>-7.4-Δ</td>
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<td>300</td>
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<tr>
<td>Ori A</td>
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<td>6000</td>
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<tr>
<td>NGC 2024</td>
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<td>5.0+Δ</td>
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<td>-7.5-Δ</td>
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</tr>
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<td>M17(SW)</td>
<td>60</td>
<td>3.5</td>
<td>3.4</td>
<td>-6.0</td>
<td>-4.7</td>
<td>0.08</td>
<td>1.9</td>
<td>119</td>
<td>17</td>
<td>3</td>
</tr>
<tr>
<td>Serpens</td>
<td>20</td>
<td>4.3</td>
<td>4.1</td>
<td>-7.1</td>
<td>-5.3</td>
<td>0.3</td>
<td>1.0</td>
<td>22</td>
<td>14</td>
<td>10</td>
</tr>
<tr>
<td>DR21</td>
<td>30</td>
<td>3.9</td>
<td>3.8</td>
<td>-6.7</td>
<td>-5.4</td>
<td>0.1</td>
<td>1.0</td>
<td>41</td>
<td>14</td>
<td>20</td>
</tr>
<tr>
<td>Elias 1-12</td>
<td>15</td>
<td>5.0+Δ</td>
<td>5.0</td>
<td>-8.0-Δ</td>
<td>-6.0</td>
<td>0.3</td>
<td>0.6</td>
<td>15</td>
<td>14</td>
<td>90</td>
</tr>
</tbody>
</table>
This bipolar high velocity outflow source has been mapped in the CO J=1-0 and CO J=2-1 transitions by Snell and Edwards (1981). We have observed the CO J=3-2 line towards their central position (which is displaced 0.5 arc minutes to the west of the position of White, Phillips and Watt (1981), where the spectrum has a similar appearance).

A striking feature of the CO J=3-2 spectrum for this source, shown in Figure 5.2, is that the central velocity component, at 7.0 kms\(^{-1}\), has a markedly reduced intensity compared with the CO J=1-0 and CO J=2-1 line cores, while the red-shifted high velocity emission is strongly enhanced. Drift scans across the source in a single velocity channel of width 0.65 kms\(^{-1}\) centred at a velocity of 15.0 km/s indicate a source diameter of ~ 3 arc minutes, similar to that seen in the CO J=1-0 line. Our value of 1.9 for the CO J=3-2 to CO J=2-1 intensity ratio is indicative of hot (\(\geq 80\) K), optically thin gas. A temperature of 80K has been assumed in the analysis.

CO observations on this source have been presented for the J=1-0 and J=2-1 transitions by Snell, Loren and Plambeck (1980) and for CO J=3-2 by White, Phillips and Watt (1981); Phillips et al. (1982) and Phillips, White and Watt (1982). The position we consider here is 2'S and 2'W of IRS5 (Beichman and Harris 1981) where the CO blue shifted wing is particularly distinct.

It is not possible to obtain a consistent solution using a kinetic temperature of 15K, taken from the line core. The assumed temperature of 30K is near the upper limit given by Snell, Loren and Plambeck (1980) and somewhat lower than the 40K deduced for the dust temperature by Phillips et al. (1982) on the basis of a \(\lambda^{-1}\) dust emissivity
Figure 5.2 CO J=3-2 spectra of HH7-11, superimposed on the J=2-1 and J=1-0 spectra of Snell and Edwards (1981).
variation. Higher temperatures cannot be excluded.

**T Tau**

T Tau has been extensively observed in one or both of the lowest 2 CO transitions by several authors (Bally and Lada 1983; Plambeck, Snell and Loren 1983; Edwards and Snell 1982; Calvet, Cantó and Rodriguez 1983). The CO J=3-2 spectrum is shown in Figure 5.3. Assumptions of a temperature of 15K and a source size of 3' give, for the ratio $R_{31}$ (defined in Section 5.5), an absolute lower limit to $n_{H_2}$ of $10^4$ cm$^{-3}$. This is higher by a factor of 70 than the estimate of Bally and Lada (1983) and illustrates the way in which the use of CO J=1-0 data alone can seriously underestimate local densities.

**OriA (KL)**

Molecular line observations of this high velocity source have been presented by many authors (e.g. Zuckerman, Kuiper, and Kuiper 1976; Kuiper Zuckerman and Rodriguez-Kuiper 1981; Erickson et al. 1982; Phillips, White and Watt 1982). We have assumed a kinetic temperature of 80K, from the line core. This is close to the value of 68K derived from observations of sulphur dioxide (Picket and Davis 1979), and to the 90K assumed by Plambeck, Snell and Loren (1983).

The J=3-2 spectrum, shown in Figure 5.4, tends to corroborate the conclusion of the last-named authors that the CO 2-1 line is moderately optically thick since, assuming a source diameter of 0.7' (Phillips, White and Watt 1982; Erickson et al. 1982), we estimate a value of $T_{\text{wing}}$ in the J=3-2 transition which is similar to that in the J=2-1 line. The derived hydrogen density is here a lower limit;
Figure 5.3  T Tau, otherwise same as Fig. 5.1
Figure 5.4 Ori A(KL), otherwise same as Fig. 5.1
observations of submillimetre lines of higher dipole moment species (e.g. HCN and HCO+) indicate densities in excess of $10^5 \text{ cm}^{-3}$ in the outflow (White et al. 1984).

The data for the lowest 3 transitions are poorly fit by the model of van Vliet et al. (1981), which predicts an optical depth $< 0.15$ in the CO $J=3-2$ transition, and a kinetic temperature $> 600\text{K}$. However, our simple model cannot account for the observations of the $J=27-26$ and $J=30-29$ CO transitions (Storey et al. 1981). Whether it is consistent with published data in the CO $J=6-5$ transition is less obvious. For the peak radiation temperature of the source in this transition, Koepf et al. (1982) give $180 \pm 36\text{K}$, their observations having been calibrated against Jupiter. Both these observations used a 35 arc second beam and would seem to imply that our assumed temperature is too low.

But valid comparison of these with our own data is very difficult. Apart from the large difference in beam size, there exists the problem of separating the spike and wing emission components since, at the molecular hydrogen densities thought to exist within the surrounding cloud material (Goldsmith et al. 1980), all the CO transitions up to $J=6-5$ are thermalised and optically thick. For any antenna having significant spillover and/or sidelobe structure, there would be inevitable contamination of the wing emission by that from the surrounding cloud, and associated uncertainty in the effective beam coupling efficiency.

In view of these uncertainties, the existing data up to $J=6-5$ would not appear inconsistent with a single temperature optically thick model, but other data (e.g. Storey et al. 1981; White et al. 1984) suggest that the outflow has smaller scale density and temperature structure.
Figure 5.5 CO J=3-2 spectrum of NGC2024, superimposed in the J=2-1 and J=1-0 spectra of Loren, Plambeck, Davis, and Snell (1981).
NGC 2024

This source was observed by Loren et al. (1981), who categorised it as one showing self absorption but no high velocity wings. Bally and Lada (1983) have subsequently detected weak wings extending over 35 kms$^{-1}$ at the 100 mk level.

We have detected CO J=3-2 emission in the velocity range 14 to 18 kms$^{-1}$ which is significantly enhanced over that observed in this range by the above authors (see Figure 5.5). A drift scan at a velocity of 16 kms$^{-1}$ has revealed a compact source ( ~ 1' EW diameter) at the CO J=3-2 frequency. This suggests the possibility of a hot, optically thin outflow. A higher temperature than the 40K given by the CO J=1-0 line core is needed to model the data; here we assume 80K, the same as for Orion A.

NGC 2071

This source has been studied and modelled by White and Phillips (1981); and White, Phillips and Watt (1981). More recently, CO J=1-0 observations by Lichten (1982) and Bally (1982), have shown it to contain a bipolar outflow, directed along the axis of a dense molecular disc. We have observed the object using a wide spectral coverage to measure the intensities of the CO J=3-2 wings, which after correcting for beam efficiencies, we find to be lower than those in either the J=1-0 or the J=2-1 line wings (see Figure 5.6). This implies that the CO J=3-2 transition is not thermalised and we derive a molecular hydrogen density of 6x10$^3$ cm$^{-3}$.

GL961

The CO J=3-2 spectrum of GL961 is presented in Figure 5.7. The fact that wings are detected in this transition at an intensity com-
Figure 5.6  NGC2071, otherwise same as Fig. 5.5

![Diagram showing CO J=1-0, J=2-1, and J=3-2 transitions with temperature (K) and V$_{LSR}$ (km/s) axes.]
parable to those in the CO J=1-0 and CO J=2-1 line wings implies an outflow density, $n_{H2}$, which is $> 10^4$ cm$^{-3}$, as compared with the estimate of Bally and Lada (1983), of $0.8 \times 10^2$ cm$^{-3}$ for the average density.

M17(SW)

This prominent star formation region has been mapped in the CO J=1-0 transition by Lada (1976) and more recently by Thronson and Lada (1983).

It has been observed in the CO J=1-0 and CO J=3-2 transitions by Martin, Sanders and Hills (1984), who interpret the data using a model which comprises randomly moving fragments. We present the CO J=3-2 spectrum in Figure 5.7.

Loren (1981) includes M17(SW) in his list of high velocity sources and presents a highly symmetrical spectrum. If we define the wing to be the velocity range where CO, but no appreciable CS (Linke and Goldsmith 1982) emission occurs ($10-15$ kms$^{-1}$), we may compare the integrated emission in each line, and find that the J=3-2 intensity is rather similar to that of the J=1-0 transition. (We do not see the marked enhancement observed by Phillips et al. (1979) in J=2-1).

The present CO observations alone do not enable us to identify the high velocity wing unambiguously as an outflow, but such a process is indicated from observations of Br$\gamma$ line emission from M17 IRS1 (Simon et al. 1981).

Serpens

The spectrum for this source is presented in Figure 5.9. The CO J=3-2 line core, like those of the CO J=1-0 and CO J=2-1 transitions,
Figure 5.8  CO J=3-2 spectrum of M17(SW), superimposed on the J=1-0 spectrum of Loren (1981).
Figure 5.9 Serpens, otherwise same as Fig. 5.5
exhibits self absorption, a feature which is characteristic both of turbulent models in which the CO excitation temperature decreases towards the cloud edge, and of collapsing models in which the collapse velocity decreases outwards.

**DR21**

High quality CO J=1-0 spectra showing high velocity wings have been obtained towards DR21 by Plambeck, Snell and Loren (1983), who also give a J=2-1 spectrum, and by Bally and Lada (1983). The source is of particular interest because of the presence of extended H$_2$ emission (Fischer et al. 1980, Garden et al., work in preparation), which is symptomatic of shock excitation within the cloud, and whose luminosity is similar to that of the Orion H$_2$ source.

We have mapped this region in the CO (J=3-2) transition and detect CO wings which are extended (~4′) along the EW direction, but are more compact (~1.5′) along the NS direction. The CO J=3-2 spectrum is shown in Figure 5.10. We find no evidence of a bipolar structure, nor do we detect any wing emission towards DR21 (OH), which probably has a higher central density. A detailed discussion of this region is given in Chapter 7.

**Elias 1-12**

This molecular source, which is associated with an FU Orionis star, has been observed in the CO J=1-0, CO J=2-1, $^{13}$CO J=1-0, $^{13}$CO J=2-1, HCO$^+$ J=1-0, and HCO$^+$ (J=3-2) transitions by Levreault (1983), who gives spectra which have already been corrected for beam coupling efficiency on to a source of diameter 2′. Correcting our CO J=3-2 spectrum (see Figure 5.11) for this size, we find a lower J=3-2
Figure 5.10  DR21, otherwise same as Fig. 5.1
Figure 5.11 CO J=3-2 spectrum of Elias 1-12, superimposed on the J=2-1 and J=1-0 spectra of Levreault (1983). The spectra have been corrected for coupling on to a 2 arc minute diameter source.
Contours of $T_R$ corresponding to the observed values of $T_{\text{wing}}$ for the $J=1-0$, $J=2-1$ and $J=3-2$ transitions of CO in DR21, for the LVG model described in Section 5.5. The arrows show the effect of ±30% errors in the observations of each line. Also shown are the lines of $x = x_{\text{est}}$ and $n_{\text{H}_2} = n_{\text{H}_2}$ (thin) and the line of constant $r_{31}$ appropriate to the observations of this source. For definitions of $T_{\text{wing}}$, $T_R$, $x$, $x_{\text{est}}$, $n_{\text{H}_2}$, $n_{\text{H}_2}$ (thin) and $r_{31}$, see text.
Figure 5.16 M17(SW), CO J=1-0 and J=3-2 transition only, otherwise same as Fig. 12.
intensity at the central velocity, but an enhancement in the red wing, by a factor of 1.8 over the J=2-1 transition. The central intensities are quite consistent with Levreault's quoted cloud density of 2x10^3 cm^{-3} for the lower velocity gas, if the cloud temperature is in the range 10-15K. However, the enhancement of the J=3-2 line wing is inconsistent with gas at temperatures of 10K. Inspection of Levreault's Figure 4 suggests that a more appropriate source size for the red wing may be 1 arc minute. This would give roughly equal corrected intensities in the J=1-0, J=2-1 and J=3-2 transitions, which would in turn imply the presence of dense clumps (n_H2 > 4x10^4 cm^{-3}).

5.7 Discussion

The results of the LVG modelling are presented in Table 5.3. Included in this Table and on Figure 5.17 and 5.18 (discussed below), are results for S255 derived in Chapter 6. As well as values of x and n_H2, the models also yield the optical depth and excitation temperature for each transition. The general features of the results are as follows.

5.7.1 x, the molecular abundance ratio per unit velocity gradient.

We compare the derived values of x with the value, x_{est}, that might be expected if the value of X in the outflow were the same as that found for dark clouds 8x10^{-5} (Dickman 1978). As a typical local velocity gradient, we take ΔV/R, where ΔV is the observed velocity half width and R is the estimated radius of the outflow. For most of the cases where x can be estimated independently from the LVG modelling, we find that it is less than x_{est}, typically by an order of magnitude. This may be an indication that, as found by Wootten et al. (1978), the relative abundance of CO in comparatively hot and dense regions is considerably less than the values appropriate in
dark clouds, possibly due to destruction of molecules by UV photons from embedded early-type stars (Bernes and Sandqvist 1977). The result may alternatively reflect the fact that the determination of $x$, unlike densities, depends on the absolute derived values of $T_{\text{wing}}$, rather than the ratios between different transitions. If, in a particular source, we have underestimated $T_{\text{wing}}$ by a constant factor in each line, then the true value of $x$ will be higher. For example, for an outflow of density $10^4 \text{ cm}^{-3}$ and $x = 10^{-7}$, at a kinetic temperature of 30K, (e.g. DR21), a dilution factor of 0.5 in each transition would allow an equally good fit to the data at a similar density, but at a value of $x$ which was greater by an order of magnitude. Such a dilution could occur if there had been an overestimate in source size (for sources whose angular extents are less than the beam sizes), or, perhaps more importantly, if there was an appreciable degree of clumping within the assumed extent of the source.

5.7.2 Optical depths and excitation temperatures

For many of the sources, the CO J=2-1 wing intensity ($T_{\text{wing}}$) is enhanced over that of the CO J=1-0 transition, and is also significantly greater than that of the J=3-2 line. A possible explanation for this is that the lowest two lines are sufficiently optically thin and thermalised to give the J=2-1 enhancement, but the density is not high enough to thermalise the J=3-2 transition. This combination of circumstances is reflected in the derived values of $T_{\text{ex}}$ and $\tau$ for the 3 transitions. These show that the frequently made assumptions of thermalisation and optical thinness are often valid for the J=1-0 transition, but not necessarily for the J=3-2 line.

We find in general that the optical depth in the CO J=1-0 line is $< 1$. This is due in part to the fact that the transition tends in this physical regime to be superthermally excited ($T_{\text{ex}} \ J=1-0 > T_K$,
see Table 5.3), as discussed by Leung and Liszt (1976). The implication is that the integrated intensity of the CO J=1-0 emission in the wings provides quite a good measure of the CO column density. (However, the fact that our values of $T_{\text{wing}}$ may be underestimates could have resulted in our underestimating the J=1-0 optical depth. The optically thin approximation could then lead to underestimates in column density of up to ~ 40%).

The optical depths derived from our analysis are lower than those deduced by Plambeck, Snell, and Loren (1983) for those sources common to the 2 studies, the discrepancy being greatest for GL490, GL961 and DR21; also, our ratios of J=2-1 to J=1-0 optical depths are greater than theirs, typically by a factor of 1.6. This is because, for the less dense sources, a relatively low value of the ratio $T_{\text{wing}}$ (J=2-1)/$T_{\text{wing}}$ (J=1-0) is partly interpreted in our model as due to incomplete thermalisation of the upper level rather than simply to high optical depth.

For sources such as Orion, where all 3 lines are thermalised, it is not possible uniquely to derive $\chi$ and $n_{\text{H}_2}$ - the latter quantity can be increased by an arbitrary ratio provided the former is decreased by the same ratio. A more precise determination of $n_{\text{H}_2}$ can only be made from observations of other lines, either higher lines of CO or lines of other molecules with higher dipole moments.

5.7.3 Masses and densities

For most sources we find densities in the range log ($n_{\text{H}_2}$ cm$^{-3}$ = $4.0 \pm 0.5$. For the denser sources, the derived values of $n_{\text{H}_2}$ are lower limits only, due to thermalisation of all three transitions.

For the reasons discussed above, over derived densities, being for the most part determined from intensity ratios rather than
absolute values, are more accurate than the values of x. As well as
determining densities from the LVG model, we can also fix absolute
lower limits from the ratio R_{31}, since, in the optically thin limit,
the ratio determines a unique n_{H_2} (for an assumed kinetic tempera-
ture) which is independent of x; we call this n_{H_2} (thin).

It is interesting to note that even this lower limits yields
hydrogen densities for some sources which are higher, by an order of
magnitude or more, than those derived by Bally and Lada (1983) from
J=1-0 data alone. Even allowing for considerable errors in the
assumed beam efficiencies, the fact that we have detected J=3-2 wings
at all in H7-11, T Tau, L1551 and GL961 is sufficient to raise
appreciably the densities derived from J=1-0 data. This highlights
the usefulness of the CO J=3-2 line for investigating outflows: its
degree of excitation (and hence its intensity) varies appreciably
over densities which are high enough to thermalise the J=1-0 trans-
ition but which are too low to give easily observable emission in
less abundant and less easily excited species such as CS, HCN and
HCO^+.

From their mass and velocity estimates, Bally and Lada (1983)
have calculated the mechanical luminosity in these sources, and
hence have estimated the time it would take the outflow sources to
supply enough energy to account for the present mean turbulent
velocity of the molecular hydrogen in the galaxy. They find that
this is likely to exceed the time scale for gravitational collapse
of the galactic material by over an order of magnitude. If this were
the case, these sources would not be energetic enough to inhibit
gravitational collapse of molecular clouds. Our CO - derived den-
sities tend to increase the energy available, and render more likely
the inhibition of gravitational collapse.
The estimated hydrogen densities may be used in conjunction with
the velocity widths and source sizes to derive a number of properties
of the outflows, such as their total mass, kinetic energy, momentum,
force and rate of mass loss (Bally and Lada 1983). A difficulty with
this (apart from the large errors already discussed) is that selection
effects may be important. Contamination of low velocity outflow
emission by the ambient cloud material may artificially reduce the
apparent range of outflow velocities, and the difficulty of defining
precisely the velocity widths and source sizes may lead to illusory
correlations between derived properties.

Such correlations as have been found remain far from clear cut,
although there does seem to be a significant negative correlation
between source extent and velocity width (Bally and Lada 1983), which
for bipolar sources would be to some extent expected from purely
geometrical considerations. Our revised estimates of source density
could be used to rederive outflow masses. Since, however, these are
sensitive to the assumed size and geometry (neither of which is known
with great precision) we omit such a calculation here. It is clear,
however, that the fairly narrow range of $n_{H_2}$ that we find, for
sources of widely differing sizes, implies that the total derived
mass of the outflow will increase with assumed source size.

It is relevant here to point out, in view of the possibility of
beam dilution discussed above, that any assumption of clumping would
reduce the estimates of outflow mass, in addition to bringing derived
average densities into closer agreement with the average values quoted
by Bally and Lada (1983). The degree of possible beam dilution is
however limited by the fact that values of $T_{\text{wing}}$ usually peak at an
appreciable fraction (typically ~ 0.5) of the assumed outflow kinetic
temperature. Allowing for some dilution could therefore only reduce...
the estimates of total mass for most sources by about half an order
of magnitude.

We prefer here to concentrate on more directly observed quanti-
ties, and first consider the ratio $R_{31}$, which provides some measure of
the degree of thermalisation and hence the density of the outflow.
This appears to be negatively correlated with source size (Figure
5.17). For the 6 sources of size $< 0.5$ pc the average value of $R_{31}$
is 2.6, while for the 6 largest sources the average is 1.0.

Figure 15.18 shows a logarithmic plot of derived density against
source size. Again, some evidence of a negative correlation is seen
but the scatter is large. Nevertheless, for 4 of the smallest
sources; OriA, NGC2024, Elias 1-12, and L1551, the large values of $R_{31}$
(which imply high levels of J=3-2 thermalisation) suggest that even
higher densities may be present in them. Moreover, the assumptions
made in correcting for beam efficiency have mainly been such as to
underestimate the real J=3-2 enhancement. Thus, the real correlation
may be more pronounced than indicated on the diagram.

If we assume a power law for the variation of $n_{H_2}$ with source
diameter $D$, we conclude that

$$n_{H_2} = kD^{-\alpha},$$

(5.4)

where $k$ is a constant and $\alpha > 0.7$.

The extent to which self-gravity is important in the motion of
the outflow may be examined by calculating the ratio $R$ of kinetic
energy per unit mass to gravitational potential for material at the
edge of the outflow. This is given by
Figure 5.17  \( R_{31} \) (see text for definition) plotted against source size (parsecs).
Figure 5.18 Log $n_{H_2}$ plotted against log (source size/pc)
\[
R = \frac{3\Delta V^2}{8 \pi \gamma n \nu H_2 \nu H_2 D^2} = 6.0 \times 10^2 \frac{(\Delta V / \text{kms}^{-1})^2}{(n_{H_2} / \text{cm}^{-3})(D / \text{pc})^2}
\]  

(5.5)

where \(\Delta V\) and \(D\) are the full velocity width and diameter respectively of the outflow. This quantity (see Table 5.3) is found to be \(> 10^{2.2}\) for the small sources but \(< 10^{1.7}\) for most of the larger ones, although the dependence on \(\Delta V^2, D^2\) and the degree of clumping make the values subject to order of magnitude errors.

The above features of the data are consistent with a model in which a violent wind from a protostellar object sweeps up an expanding shell of the ambient molecular gas. Alternatively, the energy could be provided by an expanding magnetic bubble (Draine 1983) or a centrifugally driven wind (Pudritz and Norman 1983). The compressed gas initially attains high densities (e.g. Orion KL) but as it expands the density drops to nearer that of the quiescent cloud, and the outflow velocity decreases, while the effect of self gravity becomes important. In these later stages, it becomes more difficult to distinguish an outflow with certainty from the ordinary surrounding molecular cloud.

5.8 Conclusions

We have observed 13 high velocity wing sources in the CO J=3-2 transition.

1. We find that local densities derived using observations of this transition in combination with the lower lines can be considerably higher than those derived purely from mapping in the CO J=1-0 transition, in some cases (HH7-11, L1551, GL961 and T Tau) by over an order of magnitude. This general conclusion, which is fairly
insensitive to errors associated with beam efficiencies and uncertain source sizes, tends to increase the likelihood that the outflows are capable of supporting clouds against free-fall gravitational collapse.

2. The apparent value of $x$ in many of the sources is less by a factor of 10 or more than that which would be expected from consideration of typical relative CO abundances, measured velocity widths and source sizes. The result is tentative because of its dependence on absolute values of $T_{\text{wing}}$, but it would indicate a depletion of the relative CO abundance in the outflow region, or dilution due to the existence of clumps, or both.

3. The ratio $R_{31}$ tends to be higher for smaller sources ($D < 0.5$ pc), indicating a higher degree of thermalisation within them.

4. There are indications of a negative correlation between outflow density and source size, and for the smaller sources our derived densities are lower limits. There is a need to observe the more compact sources in a variety of high excitation lines with small beam sizes.

5. LVG modelling indicates that, for many of the regions, optical depths in the CO $J=1-0$ line are $< 1$, while those in the CO $J=3-2$ transition are $> 1$. The former transition is usually thermalised but the latter may not be, a situation which has the effect of depressing the observed CO $J=3-2$ intensity below its thermalised value, and which makes the CO $J=3-2$ line a useful density probe for the outflows.
CHAPTER 5

REFERENCES

CHAPTER 6

SUBMILLIMETRE AND CONTINUUM OBSERVATIONS OF
THE S255 MOLECULAR CLOUD

6.1. Summary

The S255 molecular cloud has been observed using both continuum and spectral line techniques at several submillimetre and millimetre wavelengths. From photometry at 350, 760 and 1070 microns, the dust is estimated to have a central temperature of 44K and an emissivity which varies as $\lambda^{-1}$. Spectral mapping of the source has been carried out in the CO J=2-1, CO J=3-2 and HCN J=4-3 molecular lines, and central spectra obtained in the transitions HCO$^+$ J=4-3 and $^{13}$HCO$^+$ J=4-3. Many features of the line observations can be modelled by assuming that the cloud is centrally condensed (with a central $H_2 + He$ density of $\sim 5 \times 10^5$ cm$^{-3}$) and undergoing large scale gravitational collapse. Mapping at 350$\mu$m has revealed an elongated central structure, also suggested by the HCN mapping, in which 2 clumps are separated by 1 arc minute along a north-south line. The intensity ratios between the pairs of transitions CO J=3-2, CO J=2-1 and HCO$^+$ J=4-3, $^{13}$HCO$^+$ J=4-3, suggest that fragmentation has occurred in the cloud. An optically thin, high velocity component is detected in the CO J=3-2 line, for which a density of $n(H_2+He) \sim 4-7 \times 10^4$ cm$^{-3}$ and
a size of ~ 0.7′ are deduced. This component is hotter than the ambient cloud material and may originate from a high velocity molecular outflow. Additional evidence for this hypothesis is provided by our detection towards S255-IRS1 of emission in the 2.12 μm v = 1-0 S(1) line of shocked molecular hydrogen, at a surface brightness of ~ 10^{-11} Wcm^{-2} sterad^{-1}.

6.2 Introduction

S255 is a relatively isolated molecular cloud associated with a group of optical HII regions (S255, S257 and S256), which exhibits several of the characteristic features of star formation. These include intense thermal molecular line emission, e.g. in CO and CS (Evans, Blair and Beckwith 1977; Linke and Goldsmith 1980), multiple compact infrared sources (Beichman, Becklin and Wynn-Williams 1979), submillimetre thermal continuum emission (Cunningham 1982; Sargent et al. 1981) and H2O maser emission (Blair, Davis and Dickinson 1978; Turner 1971; Lo and Burke 1973; White and Macdonald 1979).

As in the Orion-KL source, the continuum radio emission associated with the embedded infrared objects is much weaker (in this case by a factor of several hundred; Beichman, Becklin and Wynn-Williams 1979) than that which would be expected were the observed far-infrared emission produced by early-type ZAMS stars (Israel 1976; Habing and Israel 1979). This observational result has been interpreted as indicating that the infrared objects in the cloud are in a pre-main sequence stage of evolution (Beichman, Becklin and Wynn-Williams 1979; Sargent et al. 1981). In addition, lunar occultation measurements (Schloerb and Scoville 1980) have suggested the existence of compact "hot spots" which may be similar to the BN and KL objects.

Evans, Blair and Beckwith (1977) have remarked upon the suit-
ability of this cloud for detailed investigation of phenomena associated with star formation, in view of its relatively simple appearance. There are, however, serious gaps in the body of published observational data on it, especially far-infrared data, which could help determine the emissivity variation towards long wavelengths of the dust in the source and also molecular line spectra and mapping, which would elucidate the structure and kinematics of the cloud. The observations described below were carried out with a view to filling in some of these gaps.

6.3 Observations

The molecular line data were obtained in the periods 29 November to 10 December 1982 and 1 to 12 September 1983, with the 3.8 m United Kingdom Infrared Telescope (UKIRT) on Mauna Kea, Hawaii. The receiver used was the Queen Mary College submillimetre heterodyne system. Details of the system performance and calibration during these periods are given in White, Phillips and Watt (1981) and Chapter 4 and 5 and will not be repeated here. The measured beam width (FWHM) was 55 arc seconds at 345 GHz and 1.4 arc minutes at 230 GHz. The telescope pointing was checked at approximately 20 minute intervals against nearby SAO stars and is believed to be good to 5 arc seconds. The total system noise temperature was typically 200-400 K, depending on frequency. All intensities are expressed as $T_R^*$ as defined by Kutner and Ulich (1981) where, for UKIRT, $n_{fss} = 0.9$. On this scale, the peak intensities of Orion A in the observed CO lines are $T_R^*(J=2-1) = 65K$ and $T_R^*(J=3-2) = 80K$. These values are consistent with earlier measurements (e.g. Plambeck and Williams 1979) when beamwidths and efficiencies are taken into account.

The continuum observations were made on 6 and 7 May 1983 at the
Table 6.1

The observational parameters and peak fluxes for S255 (measured at \( \alpha (1950) = 06^h 09^m 59^s, \delta(1950)= +18^\circ 00' 15'' \)).

<table>
<thead>
<tr>
<th>Effective wavelength (( \mu m ))</th>
<th>Half-power width(( \mu m ))</th>
<th>Beam size (FWHM(''))</th>
<th>Flux (Jy)</th>
<th>Statistical error (Jy (1( \sigma )))</th>
<th>Flux of OMC1 (Jy)</th>
</tr>
</thead>
<tbody>
<tr>
<td>350</td>
<td>100</td>
<td>40</td>
<td>230</td>
<td>9</td>
<td>3800</td>
</tr>
<tr>
<td>370</td>
<td>180</td>
<td>40</td>
<td>180</td>
<td>2</td>
<td>2900</td>
</tr>
<tr>
<td>370</td>
<td>180</td>
<td>55</td>
<td>380</td>
<td>6</td>
<td>5600</td>
</tr>
<tr>
<td>760</td>
<td>260</td>
<td>58</td>
<td>36</td>
<td>2</td>
<td>630</td>
</tr>
<tr>
<td>1070</td>
<td>290</td>
<td>64</td>
<td>17</td>
<td>1</td>
<td>300</td>
</tr>
</tbody>
</table>
The results of the 350 µm scan in declination through the position given in the caption to Table 1.

<table>
<thead>
<tr>
<th>Declination (°)</th>
<th>350 µm flux (Jy)</th>
<th>Statistical error (Jy)</th>
</tr>
</thead>
<tbody>
<tr>
<td>+120</td>
<td>&lt;8</td>
<td>(3σ)</td>
</tr>
<tr>
<td>+105</td>
<td>63</td>
<td>5</td>
</tr>
<tr>
<td>+75</td>
<td>200</td>
<td>5</td>
</tr>
<tr>
<td>+60</td>
<td>250</td>
<td>4</td>
</tr>
<tr>
<td>+45</td>
<td>240</td>
<td>12</td>
</tr>
<tr>
<td>+30</td>
<td>170</td>
<td>5</td>
</tr>
<tr>
<td>+15</td>
<td>220</td>
<td>4</td>
</tr>
<tr>
<td>0</td>
<td>230</td>
<td>9</td>
</tr>
<tr>
<td>-15</td>
<td>180</td>
<td>3</td>
</tr>
<tr>
<td>-30</td>
<td>100</td>
<td>4</td>
</tr>
<tr>
<td>-45</td>
<td>65</td>
<td>3</td>
</tr>
<tr>
<td>-60</td>
<td>51</td>
<td>9</td>
</tr>
</tbody>
</table>
f/35 Cassegrain focus of UKIRT, with the Queen Mary College/University of Oregon \(^3\)He-cooled submillimetre photometer. This instrument is described in detail in Ade et al. (1984). The observational parameters and measured fluxes are given in Table 6.1. The secondary was chopped at a frequency of 10 Hz and gave a beam separation of 150\(''\) (EW). Orion A was used as a calibration source; this in turn had been calibrated against planets on several previous occasions, and its fluxes at the relevant wavelengths are given in Table 6.1. The results of a 350 \(\mu\)m scan in declination are given in Table 6.2 and Figure 6.3, which also shows the UKIRT beam profile normalised to the flux measured at the S255 IRS1 position. For each measurement in Tables 6.1 and 6.2 atmospheric correction and calibration fluxes is estimated to be \(-15\%\).

Observations at the wavelength 2.12 \(\mu\)m of the \(v = 1-0\) S(1) line of molecular hydrogen were made on 16 April 1984, using the UKIRT cooled grating spectrometer (CGS2) (Wade 1983). The aperture used was 5.4 arc seconds and calibration was achieved by ratioing the spectra with that of a nearby standard star K Gem, which has a K magnitude of 1.46, a spectral type of G8, and a featureless spectrum over the wavelength range of interest.

### 6.4 The continuum data

The fluxes for a 60\(''\) beam given in Table 6.1 are in good agreement with the earlier measurements of Cunningham (1982), and are plotted in Figure 6.1, together with previously published data at other wavelengths which were taken with similar beam sizes (Beichmann 1980; Wright et al. 1981). The best fit to the data is achieved with a \(\nu B(\nu, T)\) function, with \(T = 44K\); such a curve would be obtained for emission by dust grains having an emissivity variation of \(Q_\nu \propto \nu\). The
Figure 6.1 The 50 µm to 1 mm spectrum of S255. Data points: x Wright et al. (1981); ▼ Beichman (1980); ▲ this work. The error bars represent the total error. The solid line represents a νB(ν, 44K) spectrum. (Courtesy of G.Cee).
### Table 6.3

The parameters derived for S255 and S255N

<table>
<thead>
<tr>
<th>Source</th>
<th>$350\mu m$ flux (Jy)</th>
<th>$350\mu m$ size (&quot;)</th>
<th>$T_d$(K)</th>
<th>$\tau_{350}$</th>
<th>$N$(H$_2$) ($10^{22}$cm$^{-2}$)</th>
<th>Peak n(H$_2$) ($10^4$cm$^{-3}$)</th>
<th>Mass ($M_\odot$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S255</td>
<td>200</td>
<td>53</td>
<td>44</td>
<td>0.018</td>
<td>8.1</td>
<td>3.8</td>
<td>840</td>
</tr>
<tr>
<td>S255N</td>
<td>210</td>
<td>41</td>
<td>35$^a$</td>
<td>0.032</td>
<td>15</td>
<td>9.2</td>
<td>920</td>
</tr>
</tbody>
</table>

$^a$ Jaffe et al. (1984)
deduced dust temperature is in excellent agreement with the 60 - 100 µm colour temperature given by Jaffe et al. (1984).

The scan in declination at 350 µm (Figure 6.2) shows 2 distinct submillimetre peaks, in agreement with Jaffe et al. (1984). The more northerly of these, S255N, is situated -1' due north of the S255 - IRS1 position. The deconvolved source fluxes and sizes, obtained by assuming that the sources have Gaussian intensity distributions at this wavelength, are presented in Table 6.3, together with other derived quantities. Again, the results are in good agreement with Jaffe et al. (1984), except for the size of S255N, for which we deduce a value of 41" (FWHM). This discrepancy can probably be attributed to the uncertainty entailed in the deconvolution of data from a source which is only partially resolved. (Note also that the derived parameters listed by Jaffe et al. are averaged over a 48" beam, while our results have been corrected for beam effects).

6.5 The molecular line data

In the transitions CO J=2-1, CO J=3-2 and HCN J=4-3 we have obtained spectra towards different positions on the source, which are shown in Figures 6.3, 6.4a and 6.5. The data are also displayed in the form of position - velocity diagrams in Figures 6.6a-d. All offsets are expressed with respect to the position of S255-IRS1, i.e. α(1950) = 06h09m59s, δ(1950) = +18°00'15".

The CO J=2-1 data consist of spectra taken at 1 arc minute spacings along the EW and NS directions, extending 3 arc minutes to the north, south and west, but 5 arc minutes to the east, of IRS1. The peak intensities follow a qualitatively similar pattern to the CO J=1-0 map of Evans, Blair and Beckwith (1977), the peak antenna temperature (T_R^*) falling off more rapidly to the west and north than to
S255
CO J = 2-1

Central position:
$\alpha = 06^h 09^m 59^s$, $\delta = +18^\circ 00' 15''$

Figure 6.3 CO J=2-1 spectra of S255
Figure 6.4 (a)

CO J=3–2 spectra of S255, on a 30" grid. Overlaid on the positions (0", 0"), (-60", 0") and (+60", 0") are the corresponding CO J=2–1 spectra (broken lines).

Central position as in Figure 3.
Figure 5.4(b) Ratioed spectra for central position.
the south and east. There appears to be a weak wing feature which is red shifted with respect to the central LSR velocity of 7.0 km s\(^{-1}\). The peak central TR\(^*\) is 22 K; this contrasts with the value of 40 K found by other observers (Israel 1983, private communication; Wannier, Lichten and Morris 1983) who used a smaller beamwidth of 30 arcsec (FWHM), and suggests that small scale structure is present which is diluted by our beam.

Spectral mapping in the CO J=3-2 transition was carried out at 30 arc sec spacing over a 1x1 arc minute grid, together with extensions to 1 arc minute east and 1.5 arc minute west of the central position. These spectra are shown in Figure 6.4a, with the CO J=2-1 spectra superimposed for the 3 positions for which data in both transitions were obtained.

Across the core of the line (i.e. 5 km s\(^{-1}\) to 9 km s\(^{-1}\)) the value of TR\(^*\) for the J=3-2 transition differs from that of the lower line by less than 30%; however, in the range 11 km s\(^{-1}\) to 14 km s\(^{-1}\) the ratio R\(_{32}\), defined by

\[
R_{32}(v) = \frac{R*_{(J=3-2)}}{R*_{(J=2-1)}}
\]  

has an average value of 2.8 (Figure 6.4b). The J=3-2 intensity over this range is also enhanced over that in the J=1-0 line (R\(_{31}\) > 3.0; Evans, private communication). We will refer to this emission, which is < 1 arc minute in diameter, as the high velocity component.

In Figure 6.5 are shown HCN spectra for positions along a NS line and drift scans along the EW direction through S255-IRS1 and a point 30" due north. The observed source diameter along the EW line is 1.25 arc minutes (FWHM). Along the NS line, the HCN J=4-3 emission is more
Figure 6.5

HCN J=4-3 spectra (along a north-south line) and EW drift scans across S255. Central position as in Fig. 6.3.
extended; in particular, the integrated intensity across the line appears to peak around the position of the northern source (S255N) observed in the 350 \( \mu \text{m} \) continuum. The shape of the spectrum changes appreciably over angular distances of \( \sim 30'' \), suggesting that the central cloud region contains smaller scale clumping, with the fragments having a range of line-of-sight velocities. The combined spatial and velocity information is displayed in Figure 6.6d.

Deep spectra towards the central position were taken in the transitions \( \text{HCO}^+ \, J=4-3 \) and \( \text{H}^{13}\text{CO}^+ \, J=4-3 \) and are presented in Figure 6.7. The ratio of the integrated intensities is 6.9, much less than usually assumed isotopic abundance ratios (\( \gtrsim 40 \)). Modelling and further discussion of these and other lines observed from the low velocity gas are presented in Section 6.6.

6.6 Modelling and discussion

We consider separately (a) the emission from the line cores, in all the observed transitions, and (b) the high velocity CO emission, defined above as having \( \text{lsr} \) velocities from 11 to 14 \( \text{km s}^{-1} \).

6.6.1 The emission from the line core

The problems of determining the kinematical states of molecular clouds from molecular line data were discussed in Chapter 3. We now need to confront these for the case of this particular object.

S255 is a typical hot-centred cloud in which both FIR continuum and line data strongly suggest an enhancement of density towards the centre. Moreover, the shorter wavelength data (e.g. at 20 \( \mu \text{m} \)) and lunar occultation measurements indicate the presence of compact, obscured regions at higher temperatures than the bulk of the cloud.

As discussed in chapter 3, a general characteristic of micro-
Figure 6.6(a)

Velocity-position (RA) map of S255 in the CO J=2-1 transition. Contour levels $T_R^{\mathrm{mb}}$ 1 to 22.5 in intervals of 3.5K. Central position as in Figure 6.3.
Figure 6.6(b)

Velocity - position (dec) map of S255 in the CO J=2-1 transition. Contour levels (T_{R}^*) 1 to 22.5 in intervals of 3.5K. Central position as in Figure 6.3.
Velocity-position (RA) map of S255 in the CO J=3-2 transition. Contour levels (T_advanced) 1, 2 and 4 to 25K in intervals of 3K. Central position as in Figure 6.3.
Velocity-position map of S255. HCN J = 4-3 NS (Contour levels 0.25 K to 1.75 K in steps of 0.25 K). Central position as in Figure 6.3.
turbulent models in which the excitation temperature increases towards the cloud centre is that they predict self absorbed spectra in optically thick transitions. Of the transitions we have observed, CO J=2-1, CO J=3-2 and HCO⁺ J=4-3 are clearly optically thick. They also become thermalised over different density ranges, but in none of their spectra have we observed self reversal. Spectra predicted from models combining both microturbulence and large scale velocity gradients are not always obviously self reversed, but do tend to be asymmetric and to peak at different velocities for different lines, in contrast with observations presented here.

The qualitative features of the present data can, however, be reproduced by LVG models (e.g. Goldreich and Kwan 1974; de Jong, Chu and Dalgarno 1975), or by ones which assume the material to consist of clumps smaller than the telescope beam. A clumpy model was investigated by Snell et al. (1984) who, however, employed an LVG program together with derived filling factors in their analysis. Another was developed by Martin, Sanders and Hills (1984) who, to obtain an analytical solution, assumed constant excitation temperatures both within and between clumps. In applying their model to CO data, they also assumed identical fragments. Although these assumptions are often reasonable for CO, they are unsatisfactory here, since the linewidths and sources sizes in the HCO⁺ and HCN transitions strongly suggest that local excitation temperatures increase towards the cloud centre. As pointed out by the last-named authors, the inclusion of a distribution of clump properties leads to a much increased number of free parameters. LVG models are more tractable in this respect, and we have therefore attempted initially to fit our data to such a case.

Despite the asymmetric appearances of the central HCN map and, for example, the CO J=1-0 map of Evans, Blair and Beckwith (1977),
Figure 6.7

$T_R^*$ vs $V_{LSR}$ (kms$^{-1}$)

- HCO$^+$ J=4-3 and H$^{13}$CO$^+$ J=4-3 spectra towards the central position of S255.
- The H$^{13}$CO$^+$ intensity has been multiplied by 10.
one can hope to gain insight into the principal features of the cloud structure by using a spherically symmetric model. We consider a cloud which has a core of density \( n(H_2+He) = 5 \times 10^5 \text{ cm}^{-3} \), and of diameter ~ 0.6 arc minute at the assumed distance of 2.5 kpc. We take the central dust temperature to be 44K, derived from the continuum photometry. Outside this, the dust temperature variation is assumed to satisfy \( T_{\text{dust}} \propto r^{-0.4} \), which is the expected variation for optically thin dust whose emissivity varies as \( \lambda^{-1} \) and which is heated by a central source (Scoville and Kwan 1976).

The various contributions to the heating and cooling of the gas have been considered in detail by several authors (e.g. Scoville and Kwan 1976; Goldsmith and Langer 1978; Gilden 1984). For computational simplicity, though, we use the following formulae to deduce the variation of the gas temperature, \( T_g \), in the cloud, given the dust temperature and gas density:

\[
\Lambda_g = \Gamma_{gg} + \Gamma_{cr}
\]

where,

\[
\Lambda_g = 2 \times 10^{-27} T_g^3
g_{gg} = 2.4 \times 10^{-33} T_g^{0.5} (T_{\text{dust}} - T_g) n^2(H_2+He)
\]

and,

\[
\Gamma_{cr} = 6.4 \times 10^{-28} n(H_2+He)
\]

The \( \Gamma \) terms represent the gas heating rates due to grain-gas collisions, and cosmic rays (Goldsmith and Langer 1978). The term \( \Lambda_g \) uses a simple formula for the gas cooling rate (Scoville and Solomon 1974), which gives qualitatively similar results to those of Goldsmith and Langer (1978). For 100 radial points in the cloud, the equations of statistical equilibrium and radiative transfer were solved for the lowest 11 rotational levels of each molecule using LVG kinematics, with collisional rates from Green and Thaddeus (1976), Green and Chapman (1978) and Green and Thaddeus (1974). Hence, emergent spectra could be determined for each transition, together with pre-
dicted drift scans across the cloud centre. Fuller details of the parameters used in the cloud model are given in Table 6.4.

The predicted spectrum and scan for each line have been convolved with a Gaussian beam corresponding to the relevant telescope and frequency. The beams are those of UKIRT at the CO J=2-1, CO J=3-2 and HCN J=4-3 frequencies, NRAO at the CO J=1-0 frequency, and OVRO for the CO J=2-1 line. The outputs from the modelling are shown in Table 6.5 and Figure 6.8.

The model provides a good fit to many of the main features of the data; for example, the relative peak temperatures of all lines (including the difference in CO J=2-1 intensities observed with respective beamwidths of 30" and 1.4'), the linewidths, and their shapes. The predicted source sizes (after convolution with the appropriate beams) also reproduce the observed data within the limits of error due to the non-sphericity of the actual cloud. The form of the assumed density variation \( n_H_2 \propto r^{-1} \) was chosen to correspond with the empirically chosen gravitational collapse law \( v \propto r^{0.5} \).

Difficult to reconcile with the predictions of a pure LVG model is the observation that, towards the line wings (apart from the spatially compact high velocity component discussed below), the CO J=2-1 and J=3-2 line intensities remain quite similar, while their absolute intensities drop. A similar feature was also observed towards M17 by Martin, Sanders and Hills (1984). It implies that the local \( H_2 \) densities throughout the cloud are high enough \( (> 10^4 \text{ cm}^{-3}) \) to thermalise both transitions. Towards the cloud edge, the cosmic ray term in (6.2) prevents the gas temperature from dropping below ~15K and thus precludes an explanation of the intensity variation simply in terms of a radially decreasing gas kinetic temperature. Hence, in order to reproduce the line shapes out into the wings, it
Table 6.4
Cloud model (excluding high velocity components)

(a) Variation in parameters

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Outside Core</th>
<th>Inside Core</th>
</tr>
</thead>
<tbody>
<tr>
<td>Collapse velocity</td>
<td>$V = V_{\text{core}} \left( \frac{r}{r_{\text{core}}} \right)^{-\alpha}$</td>
<td>$V = V_{\text{core}} \left( \frac{r}{r_{\text{core}}} \right)$</td>
</tr>
<tr>
<td>Density</td>
<td>$n = n_{\text{core}} \left( \frac{r}{r_{\text{core}}} \right)^{-\beta}$</td>
<td>$n = n_{\text{core}}$</td>
</tr>
<tr>
<td>Dust temperature</td>
<td>$T_{\text{dust}} = T_{\text{dcore}} \left( \frac{r}{r_{\text{core}}} \right)^{-\gamma}$</td>
<td>$T_{\text{dust}} = T_{\text{dcore}}$</td>
</tr>
<tr>
<td>Dust emissivity</td>
<td>$\varepsilon \propto \lambda^{-q}$</td>
<td></td>
</tr>
<tr>
<td>Volume filling factor for clumps</td>
<td>$W = \left( \frac{r}{3 \text{pc}} \right)^{-1}$, $r &gt; 3 \text{pc}$; = 1 elsewhere</td>
<td></td>
</tr>
</tbody>
</table>

(For assumed source distance of 2.5 kpc, angular and linear distances are related through $\theta$ (arcmin) = 0.73 $\times$ r (pc)).

(b) Numerical values used in model

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value</th>
<th>Ref (or source of information if from this work)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$q$</td>
<td>1</td>
<td>This work (continuum photometry)</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>0.4</td>
<td>&quot; (optically thin variation for $q=1$)</td>
</tr>
<tr>
<td>$r_{\text{core}}$</td>
<td>0.2 pc</td>
<td>&quot; (HCN and continuum mapping)</td>
</tr>
<tr>
<td>Cloud radius</td>
<td>10 pc</td>
<td>Evans, Blair and Beckwith (1977)</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>0.5</td>
<td>This work (to give correct relative velocity widths for HCN and CO.)</td>
</tr>
<tr>
<td>$\beta$</td>
<td>1</td>
<td>&quot; (Free fall value for $\alpha = 0.5$)</td>
</tr>
<tr>
<td>Core dust temp</td>
<td>44K</td>
<td>&quot; (continuum photometry)</td>
</tr>
<tr>
<td>Core density</td>
<td>$5 \times 10^5 \text{cm}^{-3}$</td>
<td>Free parameter</td>
</tr>
<tr>
<td>Cloud collapse velocity at edge</td>
<td>$5 \text{kms}^{-1}$</td>
<td>Chosen to give observed CO line widths</td>
</tr>
<tr>
<td>[CO]/[H$_2$+He]</td>
<td>$2 \times 10^{-5}$</td>
<td>Gerola and Glassgold (1978).</td>
</tr>
<tr>
<td>[HCN]/[H$_2$+He]</td>
<td>$5 \times 10^{-11}$</td>
<td>Wootten et al. (1978).</td>
</tr>
</tbody>
</table>
Table 6.5  
Comparison between model and observations

<table>
<thead>
<tr>
<th>Line</th>
<th>Beam (FWHM)</th>
<th>Peak $T^*_R$ (K)</th>
<th>Line width (FWHM) km s$^{-1}$</th>
<th>Source size (FWHM) arc min</th>
<th>References for observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO 1-0</td>
<td>64&quot; (Spectrum - ref 2)</td>
<td>obs.model</td>
<td>obs.model</td>
<td>obs.model</td>
<td>1,2</td>
</tr>
<tr>
<td></td>
<td>2.3' (Map - ref 1)</td>
<td>35</td>
<td>32</td>
<td>3.4 4.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>~9 9.0</td>
<td></td>
</tr>
<tr>
<td>CO 2-1</td>
<td>30&quot;</td>
<td>40</td>
<td>37</td>
<td>4.0 3.4</td>
<td>3,4</td>
</tr>
<tr>
<td>CO 2-1</td>
<td>1.4'</td>
<td>22</td>
<td>27</td>
<td>4.0 4.0</td>
<td>This work</td>
</tr>
<tr>
<td>CO 3-2</td>
<td>55&quot;</td>
<td>24</td>
<td>29</td>
<td>7.0 3.5</td>
<td>This work</td>
</tr>
<tr>
<td>HCN 4-3</td>
<td>55&quot;</td>
<td>1.6</td>
<td>1.4</td>
<td>~4±2 1.8</td>
<td>This work</td>
</tr>
</tbody>
</table>

a  Observed spectrum broadened by high velocity compact source  
b  Very approximate results due to existence of small scale structure

REFERENCES:--  
(1) Evans, Blair and Beckwith (1977).  
(2) Evans (1983 private communication).  
(4) Israel (1983, private communication).
Figure 6.8 (a) - (c)

Results of the modelling for S255 (line core component). In each case, the observed data (histogram) are superimposed on the predicted model spectrum (smooth curve) for the same position on the source.

(a) CO J=2-1. Central position.
Figure 6.8(b)

S255 (2 arc min from centre)

CO J = 2-1

\[ \text{Observations (NSE average)} \]

\[ \text{Model} \]

CO J = 2-1. 2 arc minutes displacement from the centre. (The observational data plotted are averages of the positions 2 arc minutes east, south and north).
Figure 6.8(c)

CO J=3-2. Central position. (The high velocity component shows up as an enhancement over the predicted intensity).
Figure 6.8 (d)

S255 (30 arc sec E)

CO J = 3-2 Observations

Model

V_{LSR} (km s^{-1})

0 - 5 10 15 20 25

T^*_R

32 28 24 20 16 12 8 4 0

CO J=3-2, 30 arc sec east of the central position.
was necessary to assume that the material further than 3pc from the centre was clumped, thus giving a dilution in the absolute predicted line temperatures. The volume dilution function used was \( W_{\text{dil}} = (r/3\text{pc})^{-1} \). This additional factor means that in the outer parts of the cloud, the average density in the model is proportional to \( r^{-2} \). Note, however, that its incorporation into the model does not affect any of the predictions in Table 6.5, except for a slight effect on the predicted CO J=1-0 source size.

Since our mapping is mainly concentrated within 2pc of the cloud centre the observations provide limited information on the density structure of the outer parts of the cloud, and cannot be used reliably to deduce, for example, its total mass. However, within a distance of 3pc from the cloud centre, our model gives a total mass of \( \sim 2.7 \times 10^5 \, M_\odot \). This volume is similar in extent to the region within the \( T_R^* \) J=1-0=10K contour used by Evans, Blair and Beckwith (1977); and their method of deducing mass from the \(^{13}\text{CO} \) J=1-0 transition, with an assumed \( X^{13}\text{CO} = 2.4 \times 10^{-8} \) (Wootten et al. 1978), would give a mass of \( 1.3 \times 10^5 \, M_\odot \). These values are of the same order of magnitude, and are both much larger than the virial mass of \( 5 \times 10^3 \, M_\odot \) (Evans, Blair & Beckwith 1977).

The presence of clumping in the cloud is suggested both by the divergence of the CO observations from LVG predictions, and by the structure revealed by the mapping at 350 \( \mu \text{m} \) and in the HCN J=4-3 transition. Using the HCO\(^+\) observations, we now assess further the likelihood of small scale fragmentation in the cloud core.

Characteristic length scales likely to fragment in a cloud of molecular hydrogen are given by the Jeans length

\[
l_J = 0.27 \ (T/10K)^{0.5} \ (n_{H_2}/10^4 \text{ cm}^{-3})^{-0.5} \text{ pc}
\]

(6.3)
(Silk 1980). Substituting a central density of $5 \times 10^5$ cm$^{-3}$ and a temperature of 44K into (6.3), we find $l_J = 8 \times 10^{-2}$ pc which, at an assumed source distance of 2.5 kpc, gives ~ 0.1 arc minute. This suggests, not only that the observed condensations comparable in size to our arc minute beam are unstable to gravitational collapse, but also that fragmentation may be occurring on smaller scales than this, although the inhibiting effects of clump rotation and magnetic fields are unknown.

From the spectra of the transitions HCO$^+$ $J=4-3$ and H$^{13}$CO$^+$ $J=4-3$ we derive an integrated intensity ratio

$$ R_{\text{int}} = \frac{\int T_R^* (\text{HCO}^+ \ J=4-3) \ dv}{\int T_R^* (\text{H}^{13}\text{CO}^+ \ J=4-3) \ dv} = 6.9 \quad (6.4) $$

This (beam independent) ratio contrasts markedly with commonly assumed isotopic abundance ratios of 89 (terrestrial) and 40 (Dickman 1978) and implies either that the H$^{12}$CO$^+$ transition is optically thick, or that isotopic fractionation has occurred.

Guélin, Langer and Wilson (1982) have shown that the maximum enhancement factor for the H$^{13}$CO$^+$/HCO$^+$ abundance ratio relative to $^{13}$CO/$^{12}$CO is obtained in the limit of low electron density and is $\exp (17/T)$, which for $T = 44$K gives ~ 1.5. Probably a better estimate comes from substituting an electron density of $N_e = 4.9 \times 10^{-8}$ relative to H$_2$ + He (Wootten, Snell and Glassgold 1979) and a CO relative abundance of $X_{\text{CO}} = 2 \times 10^{-5}$ into equation B4 of Guélin, Langer and Wilson (1982), using rate constants from Prasad and Huntress (1980). This gives an enhancement factor of 1.2. Fractionation, therefore, is probably not an important effect here.

The observed $R_{\text{int}}$ may be used in conjunction with a value for
$X_{\text{HCO}^+}$ to estimate the local $H_2$ densities within the core region. We first derive a value for $X_{\text{HCO}^+}$ from the integrated intensity in the optically thin $H^{13}C_\text{O}^+ J=4-3$ line. Assuming as a first approximation that this transition is also thermalised, we have

$$N_{H^{13}C\text{O}^+} = 5.7 \times 10^{10} \frac{\int T^*_R (J=4-3)(dv/\text{kms}^{-1}) \exp(25.7/T)}{n_c(1') (1 - \exp(-17.1/T))} \text{ cm}^{-2} \quad (6.5)$$

where the diameter of the emitting region is assumed to be 1 arc minute. Substituting $T = 44K$ and $n_c(1') = 0.6$ we find $N_{H^{13}C\text{O}^+} = 6.5 \times 10^{11}$ cm$^{-2}$ and (using the value for $N(H_2)$ from Table 6.3) $X_{H^{13}C\text{O}^+} = 8 \times 10^{-12}$. For an isotopic abundance ratio of 40, we obtain $X_{\text{HCO}^+} = 3.2 \times 10^{-10}$. Taking $dv/dr$ for the core to be $\sim 3.5$ kms$^{-1}$ pc$^{-1}$, we have used an LVG model to estimate the density required to give the observed $R_{\text{int}}$, and obtained $\sim 10^6$ cm$^{-3}$. Since, however, the predicted excitation temperature in the $H^{13}C\text{O}^+$ line was $\sim 15K$, some iteration of the above procedure was carried out. This gave revisions of the above estimate to

$$X_{\text{HCO}^+} = 4.7 \times 10^{-10}$$

and

$$n_{H_2} = 9 \times 10^5 \text{ cm}^{-3}$$

The value of $X_{\text{HCO}^+}$ thus derived is similar to those found for comparable sources by Wootten, Loren and Snell (1982) but is a factor of $\sim 100$ larger than the earlier value for this source given by Wootten, Snell and Evans (1980). We have essentially assumed that the region of 350 $\mu$m emission is the same as that of $H^{13}C\text{O}^+$ emission. In addition, our determination of $N(H_2)$ may be uncertain to a factor
- 225 -

~ 3 (Hildebrand 1983). Nonetheless, our estimate has been derived from optically thin radiation and therefore should not be much affected by the complex radiative transfer effects which can plague determinations of relative molecular abundance derived from lines of higher opacity.

We note that for the above-derived conditions, the HCO$^+$ line (but not H$^{13}$CO$^+$) is thermalised by the combination of density and radiative trapping. The dilution factor (within a 1 arc minute diameter region) required to give the observed absolute H$^{12}$CO$^+$ J=4-3 intensity is ~ 0.07, suggesting that the material is indeed clumped. The assumption that the emission came from a single clump would imply a diameter of ~ 0.2 pc. If, however, many clumps are present, the derived factor will consist of a combination of dilutions in both velocity and physical space which it is not possible to separate without further assumptions.

6.6.2 The high velocity emission

When Schloerb and Scoville (1980) performed lunar occultation observations of this source, they interpreted their results as suggesting the presence of a Kleinmann Low-type object, of diameter ~ 40" ± 7" and peak temperature 65 K. Since KL is a prominent molecular outflow source, exhibiting high velocity wings in a variety of molecular transitions (see Genzel and Downes 1981, for a summary), our detection of a CO wing towards the centre of S255 lends additional support to their hypothesis.

It is possible to deduce a value for the H$_2$ column density in an outflow from a single molecular transition (Bally and Lada 1983), but it is in practice necessary to assume a molecular abundance relative to CO, and that the transition is optically thin and thermalised.
The adoption of these assumptions can give rise to large errors as discussed in Chapter 5 (Richardson et al. 1985).

Here we use the ratio $R_{32}$ defined in Section 6.5, which, however, has not yet been corrected for coupling on to the source. This poses a problem: the CO $J=3-2$ emission in this range is spatially compact (it has reduced to about half its central intensity at positions 30" W, 30" E and 30" S but is more extended to the north) and efficiencies of different telescope beams often diverge strongly for small source sizes. To estimate a value for the radiation temperature $T_R$ which would be observed with infinite spatial resolution we should need to divide $T_R^*$ by a beam coupling efficiency $n_c$. (All these quantities are as defined by Kutner and Ulich 1981). To correct $R_{32}$ for coupling on to the source distribution, the ratio

$$n_{32} = \frac{n_c (CO J=3-2)}{n_c (CO J=2-1)} \quad (6.6)$$

was calculated as a function of diameter, for a uniform disc source, using a computer program which describes the optics of the QMC heterodyne system on UKIRT (Lesurf 1981). This ratio rises from 1.7 to 2.2 as the assumed source size varies from 1 arc minute to zero (Figure 4.2). As a check on this procedure, we also obtained, on each occasion when S255 was observed, a spectrum of the Orion A high velocity source, which has a measured diameter of about 0.7 arc minutes (Phillips, White and Watt 1982; Erickson et al. 1982). After correcting the CO $J=2-1$ and CO $J=3-2$ wing intensities by our calculated beam coupling efficiencies, we find the intensities in the two transitions to be consistent to within about 20% with previous measurements (Erickson et al. 1982; Plambeck, Snell and Loren 1983;
Richardson et al. 1985). (Although calculated values of \( n_{32} \) depend on the source geometry, we have found that, over the assumed range of source sizes, the values for a uniform disc of diameter \( D \) differ by < 10% from those for a Gaussian of FWHM = \( D \).)

The corrected ratio \( R_{32}/n_{32} \) therefore gives an observationally determined estimate which may be compared against the theoretically predicted quantity

\[
R_{32} = \frac{T_R (J=3-2)}{T_R (J=2-1)} 
\]

For all assumed source diameters we find values of \( R_{32}/n_{32} > 1 \), which are symptomatic of optically thin gas in which both transitions are at least partially thermalised. Since, at low optical depths, predicted values of \( T_R \) become insensitive to the assumed kinematics, we have for convenience used a simple LVG model to interpret the data (see Chapter 2). For various assumed gas temperatures \( T \), contours of \( r_{32} \) and \( T_R \) (CO J=2-1) were plotted on grids of \( n_{H_2} \) and \( X_{CO}/(dv/dr) \). The data which the model is required to fit are the ratio \( R_{32} \), the absolute intensity \( T_R^* \) (CO J=3-2) and the upper limit on the HCO\(^+\) J=4-3 intensity over the velocity range 11-14 km s\(^{-1}\). Within the possible range of \( r_{32} \), the combination of density and optical depth must be sufficient to give an appreciable absolute intensity in the CO lines, but cannot be so high that observable wing emission would be predicted in the HCO\(^+\) J=4-3 transition. The free parameters are the kinetic temperature and the source diameter. Three values of temperature were investigated: 44K (the derived dust temperature), 65K (Schloerb and Scoville 1980) and 80K (similar to the Orion outflow). We estimate \( T_R^* \) (CO J=3-2) = 9 ± 3K for this velocity range. For each of a set of assumed source diameters < 1.2 arc minutes, \( R_{32}/n_{32} \) and \( T_R^*/n_3 \) were estimated, which resulted in a range of
allowed solutions (shown in Figure 6.9 for T = 80K). In addition, from the observed upper limit of T\(_R^*\) (HCO\(^+\) J=4-3) < 0.5 K, and using \(X_{\text{HCO}^+} = 4.7 \times 10^{-10}\) and \(dv/dr = 14 \text{ km s}^{-1} \text{ pc}^{-1}\), we computed the value of \(n_{\text{H}_2}\) required for \(T_R\) to exceed \((0.5/n_3)K\). This gave an excluded region on the plot. No solutions were found for \(T = 44\) K. For \(T = 65\) K a best fit was found at \(n_{\text{H}_2} = 7 \times 10^4 \text{ cm}^{-3}\) and \(X_{\text{CO}}/(dv/dr) = 6 \times 10^{-8}\), while for \(T = 80\) K the respective values were \(4 \times 10^4 \text{ cm}^{-3}\) and \(1 \times 10^{-7}\). These results imply that \(X_{\text{CO}} \sim 1 \times 10^{-6}\) i.e. that CO is depleted in the outflow. However, higher temperatures, which would give a higher \(X_{\text{CO}}\), cannot be excluded. Bearing in mind that of the observed data \(R_{32}\) is the least dependent on the assumed spatial intensity variation, we note that the allowed contours of \(R_{32}\) define an absolute lower limit on \(n_{\text{H}_2}\) in the limit of low optical depth (see Figure 10). This is \(n_{\text{H}_2} \geq 1.3 \times 10^4 \text{ cm}^{-3}\) for \(T = 80\) K and \(n_{\text{H}_2} \geq 1.7 \times 10^4 \text{ cm}^{-3}\) for \(T = 65\) K.

What is the nature and kinematic state of this high velocity gas? The range of solutions defined by Figure 6.9 (and corresponding ones for other temperatures) do not enable the mass of gas in this component to be calculated very accurately. From the integrated intensity \(\int T_{R^*} (J=3-2) \text{ dv}\) and other parameters estimated from the LVG modelling, we estimate for this component, a mass of \(\sim 300 \text{ M}_\odot\), a kinetic energy of \(\sim 10^{40}\) J, and a ratio of kinetic to gravitational potential energy of \(\sim 10\). This ratio suggests that the gas may be an outflow, although the many sources of error make the above estimates uncertain to a factor of \(\sim 3\) in either direction and we cannot unequivocally exclude either gravitational collapse or turbulent motions within a gas in virial equilibrium, on the basis of these data alone.

In order to investigate the physical mechanism responsible for
Results of the modelling for the high velocity component ($T = 80K$). The dotted contours are for different values of $r_{32}$. The contour levels from left to right are 1.2, 1.3 (0.3), 1.4 (0.6), 1.5 (0.8), 1.6 (0.95) and 1.7 (1.1), where the numbers in brackets are the source diameters which would give $R_{32}/n_{32}$ for each contour. The solid contours are for values of $T_R (\text{CO } J=3-2) = T^*/n_3$, where $T^* = 6K$, 9K, 12K and $n_3$ is given by the correspondence between $r_{32}$ and source size. The hatched line shows the excluded region $T_R (\text{HCO}^+ J=4-3) > 0.5/n_3$. The horizontal arrow indicates the allowed values of $r_{32}$ as the assumed source diameter varies from 0 to 1.1 arc minutes.
the high velocity wing, we observed S255-IRS1 at 2.12 μm, the wavelength of the ν = 1-0 S(1) line of molecular hydrogen. Observations of S255 in this line have previously been made by Simon and Joyce (1983), who made weak detections of \( \sim 4 \times 10^{-20} \text{Wcm}^{-2} \) at positions 20 arcsec S, 30 arcsec E, and 30 arcsec S, 35 arcsec E of IRS1, in a 35 arcsec aperture, and upper limits (3σ = 7 \times 10^{-20} \text{Wcm}^{-2}) at several surrounding positions. They avoided the position of IRS1 because of their relatively low spectral resolution.

The 2 positions we observed were that of S255 IRS1 itself, which our CO line observations indicate may be associated with a molecular outflow, and a point 45 arc seconds north of IRS1, situated on the edge of the more northerly 350μm continuum peak and where the HCN line profile shows rapid spatial variation. The reason for looking at the latter position was that, if the emission was due to collisions between dense clumps in a central turbulent region, a positive detection might be expected here also; however, no emission was seen (1σ = 7.3 \times 10^{-22} \text{Wcm}^{-2}). At the former position, however the line was detected and is shown in Figure 6.10. The flux in the resolution element around 2.12 μm (Δλ = 3.5 \times 10^{-3} μm) was 1.1 \times 10^{-20} \text{Wcm}^{-2} (1σ = 1.8 \times 10^{-21} \text{Wcm}^{-2}), half of which is attributable to continuum. These measurements of the S(1) line (which show a surface brightness towards IRS1 which is 2 orders of magnitude greater than those measured by Simon and Joyce (1983)) provide additional circumstantial evidence that S255-IRS1 is associated with an outflow.

The intensity of 5.5 \times 10^{-21} \text{Wcm}^{-2} attributable to H₂ emission from IRS1 will have been subject to extinction, of an unknown amount. However, one may obtain a crude estimate of this from our value of 0.018 for the optical depth at 350μm, if we assume that it is due to dust grains whose emissivity variation of λ⁻¹ extends down to 2.12 μm,
and that IRS1 is situated at an optical depth which is half that through the whole cloud. We then have ~3 magnitudes of extinction at 2.12 μm, and an estimated corrected surface brightness $I_{2.12}$, averaged over the 5.4" aperture, of $\sim 5 \times 10^{-11}$ W cm$^{-2}$ sterad$^{-1}$.

Since the molecular line spectra peak around 7 kms$^{-1}$ and the CO J=3-2 emission extends to $\sim 20$ kms$^{-1}$ at the position of IRS1, we take 13 kms$^{-1}$ as an estimate of the shock velocity. A shock with this velocity gives the observed surface brightness for preshock densities $n_0 = n_{H_2} \sim 10^5$ cm$^{-3}$ (Kwan 1977), similar to the cloud core densities derived from our molecular line modelling. For $T = 80$K, the shock has a Mach number of $\sim 20$; if it is isothermal, the predicted postshock density is $\sim n_0 n^2 \sim 5 \times 10^7$ cm$^{-3}$, and the pressure required to push the shock is given by

$$P_{\text{shock}} = n_0 \mu m_{H_2} v^2 = 6.5 \times 10^{-8} n m^{-2}$$

where $\mu$ is the average molecular weight (assumed = 2.33). If the shocked region is assumed to be a spherical shell, of radius 0.35 arc min on the sky, then the integrated pressure acting on the shell is $4\pi R^2 P_{\text{shock}} = 5 \times 10^{25} N \approx 0.8 M_\odot$ kms$^{-1}$ yr$^{-1}$. These order of magnitude estimates would also be appropriate for the case of colliding clumps in the centre producing the shock, since the working surface area would still be of the order of the square of the size of the affected region. The mechanical luminosity = integrated pressure x velocity $= 6 \times 10^{29}$ W ($\sim 1700 L_\odot$).

To relate these estimated parameters of the molecular outflow to the corresponding ones for the stellar wind requires an assumption about whether the flow is momentum or energy driven (Königl 1982; Dyson 1984). For a unique specification of the wind outflow velocity and mass loss rate, further information is needed, and Dyson (1984) has suggested that this can be provided by measurement of the radio
Figure 6.10 Spectrum of the $v = 1-0$ S (1) line of H$_2$ at 2.12 microns towards S255-IRS1. The points are spaced at intervals of half the resolution element of $3.5 \times 10^{-3}$ μm. The error bars represent ± 1σ.
continuum flux, which is assumed to originate in an ionised stellar wind. Beichman, Becklin and Wynn-Williams (1979) observed the region at 5 GHz and detected no emission towards S255-IRS1 (< 1.6 mJy) but weak, extended emission (~ 6 mJy over a region ~ 3" in diameter) around S255-IRS2, as also found by Israel (1976). Assuming that this originates from the wind responsible for driving the CO outflow, we may use the method described by Dyson (1984) to estimate the wind parameters. However, in view of the inhomogenous structure of the region, which could have an important influence on the outflow (Königl 1982), we stress that any estimate will be very approximate. Substituting S5 = 6 mJy, D = 2.5 kpc, M⊙ = 300 M⊙ and R⊙ = 0.25 pc into his equations (29) and (30) we obtain, for the constant density case, a wind velocity of ~ 800 km/s and a mass loss rate of ~ 3.5 x 10^-5 M⊙ yr^-1. The derived wind velocity is consistent with an energy driven flow (Dyson 1984, equation (8)). The wind momentum flux of ~ 3 x 10^-2 M⊙ km/s (a factor of ~ 30 smaller than that in the molecular flow) and the wind mechanical luminosity of ~ 9 x 10^3 L⊙ are readily explicable in terms either of a magnetic bubble model of the outflow (Draine 1983) or of a centrifugally-driven wind (Hartmann and Mac-Gregor 1982; Pudritz and Norman 1983). We speculate that IRS2 is the centre of the outflow and is situated towards the front of the dense core of S255. The redshifted CO wing emission would then come from a swept up shell of molecular hydrogen which was being driven towards the interior of a relatively dense region, while the shocked H2 emission from S225-IRS1 could be due to a dense clump at this position which provides a sufficiently high preshock density. The complexity of the region, though, is such that a thorough investigation of these suggestions will have to await more detailed mapping of the region in the H2 lines. High velocity resolution
would be needed but with apertures large enough to enable the whole central square arc minute to be covered. Subsequent small scale mapping might then reveal clumpy structure in the molecular hydrogen emission.

6.7 Conclusions

We have observed the S255 molecular cloud at several submillimetre line and continuum wavelengths, and drawn the following conclusions on conditions within it:

(i) The line shapes and central velocities are consistent with a cloud undergoing gravitational collapse in which the large velocity gradient approximation is valid. The line intensities, widths and map sizes in different transitions have been modelled using a spherically symmetric LVG model. However, to match the observed intensities in the line wings of the CO transitions it appears necessary to postulate the existence of fragmentation in the outer parts of the cloud. Mapping in the 350\mu m continuum and in the J=4-3 line of HCN indicate a density enhancement (~ 5 \times 10^5 \text{ cm}^{-3}) at the cloud centre, of observed diameter ~ 2 arc minutes. Evidence of inhomogeneity is also seen; both continuum and line mapping reveal two peaks, situated along a north-south line and separated by about 1 arc minute.

(ii) The ratio of the intensities of the HCO$^+$ J=4-3 to the H$^{13}$CO$^+$ J=4-3 line, together with their absolute values, suggests that even higher densities ($n_{\text{H}_2} \sim 10^6 \text{ cm}^{-3}$) may be present within the cloud core, with fragmentation occurring on a smaller scale than is resolved by the UKIRT 1 arc minute beam. A relative abundance of $X_{\text{HCO}^+}$ of ~ 4.7 \times 10^{-10} is estimated.

(iii) A high velocity component to the molecular emission is seen, in which the CO J=3-2 emission is enhanced over the CO J=2-1 intensity...
(even after correction for beam size). To model the line ratio $R_{32}$, the absolute CO intensities and the non-detection of HCO$^+$ $J=4-3$ wings, it is necessary to postulate that this gas is hotter than the derived dust temperature of 44K. For an assumed $T = 80$K we estimate a gas density $\sim 4 \times 10^4$ cm$^{-3}$, a source diameter of $\sim 0.7'$ and a relative CO abundance of $X_{CO} \sim 10^{-6}$. These data, together with the detection of the 2.12 $\mu$m H$_2$ line towards S225-IRS1 suggest that this component originates in a molecular outflow. The flow may be centred at or near S255-IRS2 and be responsible for driving a shock into the front face of a dense clump at the position of S255-IRS1.
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CHAPTER 7

THE STRUCTURE AND KINEMATICS OF THE DR21 REGION

7.1 Summary

Observations of the DR21/DR21(OH) region have been made in the molecular lines CO J=2-1, CO J=3-2, HCN J=4-3, HCO+ J=4-3, H13CO+ J=4-3 and CS J=7-6, supplemented by continuum observations of DR21 and DR21(OH) at 350 μm and a 20 μm map of DR21. The CO observations show a high velocity wing region around DR21, which is blue shifted with respect to the -3 kms⁻¹ central velocity of the source, has an observed diameter of ~ 1 arc minute NS, ~ 3-4 arc minutes EW, and may be due to an outflow. The 11 kms⁻¹ component associated with W75N is in evidence over much of the region as foreground material of density ~ 10³ cm⁻³. The kinematics of the CO emitting region are discussed; a simple LVG model would appear to be inadequate. DR21 and DR21(OH) show up as compact (~ 1 arc minute diameter) regions of high intensity in the submillimetre continuum and the HCN, HCO⁺ and CS lines, and their masses are deduced to be ≈ 5.7 x 10³ M☉ and 7.9 x 10³ M☉ respectively. The central square arc minute of DR21 is discussed in detail.

The CS, HCN, HCO⁺ and H13CO⁺ intensities, spatial extents and line profiles, in addition to the self absorptions seen in some CO lines, can be understood on the basis of a simple 2 component model...
similar to that of Norman and Silk (1980) and consisting of dense 
\((10^5 - 10^6 \text{ cm}^{-3})\) clumps surrounded by a less dense \((\sim 10^3 \text{ cm}^{-3})\) interclump gas of higher temperature. A combined spatial and velocity dilution factor of \(\sim 0.1\) is derived for the clumps. The value of \(X_{\text{HCO}^+}\) is constrained to be between \(10^{-9}\) and \(10^{-8}\), the exact value depending on the assumed clump sizes and velocity widths. The high excitation transitions we have observed are less contaminated by absorption and emission in the interclump medium than the HCN, H$_2$CO and NH$_3$ lines in which the source has previously been observed at higher resolution and we discuss the feasibility of detecting the clumps directly in these submillimetre transitions.

7.2 Introduction

The observations presented and discussed below concern the condensations of gas and dust DR21 and DR21(OH) (a.k.a. W750H) situated in the Cygnus X region.

The wider region, having long been recognised as a site of star formation, has been the subject of several large scale surveys at various wavelengths in both the continuum (e.g. Downes and Rinehart 1966; Campbell et al. 1982) and in atomic and molecular lines (e.g. Dickel and Wendker 1978; Cong 1977). Higher resolution mapping over smaller spatial extents has been carried out in the CO J=1-0 and $^{13}$CO J=1-0 lines (Dickel, Dickel and Wilson 1978; Harris 1981) in the radio continuum (e.g. Harris 1973; Dickel et al. 1983) and in the infrared continuum (e.g. Harvey, Campbell and Hoffmann 1977; Thronson and Harper 1979). Data in higher excitation molecular lines, such as the rotational transitions of HCN, CS, HCO$^+$ and NH$_3$, have been acquired by many observers (e.g. Matsakis et al. 1981; White et al. 1982; Nyman 1983; Dickel et al. 1983; Dickel, Ho and Wright 1985),
and have shown that the sources contain cores of high density \( n_{H_2} > 10^5 \text{ cm}^{-3} \). In addition, the region around DR21/DR21(OH) exhibits many of the characteristics associated with continuing star formation, including maser emission (e.g. Harvey et al. 1974), evidence for a molecular outflow (e.g. Bally and Lada 1983; see also Chapter 5), shocked \( \text{H}_2 \) emission (Fischer, Righini-Cohen and Simon 1980; Garden et al. 1985), as well as compact HII regions. (The above represents only a small fraction of the published material on these sources; for other work, see the references therein, and also the collation of data on the Cygnus X region by Goudis (1976)).

Despite the plethora of published data concerning the DR21/W75 region and its environs, attempts to understand its detailed structure and kinematics have been hindered by the confused aspect which it presents to us. Since it is situated in a local spiral arm viewed tangentially, spatially separated features are superimposed along the same line of sight. Furthermore, kinematic distance determinations at galactic longitudes near \( \pm 90^\circ \) are highly unreliable.

Molecular line observations have offered the prospect of disentangling the emission due to the different gas components; different radial velocities give different points on a line profile and these can to some extent be analysed independently. Unfortunately, however, these profiles (especially in CO transitions) are often subject to self absorption, and the general complexity of the region tends to thwart attempts to allow for this in any unique way in models taking radiative transfer into account. Also, there is the perennial problem, discussed in Chapter 4, of comparing data from different telescopes which have dissimilar beam characteristics. Recent high resolution observations have provided valuable additional information on the small scale structure of DR21... They have included VLA observations
of H$_2$CO absorption against the ratio continuum source (Forster et al. 1985; Dickel et al. 1983) and observations in the J=1-0 lines of HCN and HCO$^+$ (Dickel, Ho and Wright 1985; Nyman 1983). Nyman (1983) has suggested that the densest condensations may be surrounded by lower density absorbing gas which may lead to error in derivations of molecular cloud parameters from emission spectra.

Recently estimated values of HCN and HCO$^+$ abundances relative to H$_2$ in hot centred clouds have fallen in the range 10$^{-9}$ to 10$^{-8}$ (e.g. Nyman 1983; Vogel et al. 1984; Dickel, Ho and Wright 1985). At such relative abundances the J=1-0 transitions are likely to be optically thick for n$_{H_2}$ > 10$^3$ cm$^{-3}$. For n$_{H_2}$ > 5 x 10$^3$ cm$^{-3}$ they may also emit appreciably because of the effect of radiative trapping on their excitation temperatures. Another complicating factor is the possible variations in molecular abundances relative to H$_2$ between regions of different density. Forster et al. (1981), who studied H$_2$CO in absorption against the background radio continuum source in DR21, pointed out that the denser regions could actually have lower optical depths than the less dense ones if X$_{H_2CO}$ decreased faster than n$_{H_2}^{-1}$. It is therefore desirable to observe the region in transitions which are less prone to such effects.

In the submillimetre region, there exists a number of lines of common interstellar molecular species, radiating in the 340-350 GHz range which, since they require higher H$_2$ densities to excite them, are likely to pick out selectively the densest regions. These include the rotational transitions HCN J=4-3, HCO$^+$ J=4-3, CS J=7-6 and their isotopes. They, together with the CO J=3-2 transition at 345 GHz, have the additional advantage of being observable on the same telescope with almost identical beamwidths. Observations of these lines, together with the CO J=2-1 transition, towards the DR21/DR21(OH)
region are presented and discussed below, along with continuum data at 20 µm and 370 µm.

7.3 Observations

All the data were obtained with the 3.8 metre United Kingdom Infra Red Telescope (UKIRT). The majority of the line observations were carried out during the period 1 to 12 September 1983. Combined with these were data from the periods 26 to 30 June 1982 and 28 November to 6 December 1982. In the most recent two runs, the instrument used was the Queen Mary College indium antimonide hot electron bolometer (White, Phillips and Watt 1981); in the earliest we used the UKIRT indium antimonide bolometer heterodyne system (System B). In both cases, the instrument was used at the f/9 Cassegrain focus of UKIRT. Calibration was carried out every ~ 20 minutes by the standard chopper wheel method, using ambient temperature loads and off-source sky positions (Kutner and Ulich 1981). The off position used was α(1950) = 20h 45m 13s, δ(1950) = +42º 38' 52" which, according to the mapping of Cong (1977), has no CO J=1-0 emission, but other off positions were also tried in order to verify this. Telescope pointing was checked by frequent (~ 15-20 minutes) observations of nearby stars, and was found to be correct to within a few arc seconds. The beamwidths (FWHM) at 345 GHz and 230 GHz were 55 arc seconds and 1.4 arc minutes respectively.

The 350 µm continuum observations were made at the f/35 Cassegrain focus of UKIRT with the Queen Mary College/University of Oregon 3He-cooled submillimetre photometer (Ade et al. 1984). The secondary was chopped at a frequency of 10 Hz and the chop throw was 140" (EW). The 20 µm map of DR21 was obtained on 2-3 June 1984 using the UKIRT 16 channel SiAs array (IRASFU). The area was mapped from west to east...
### Table 7.1 Positions in the DR21 region

<table>
<thead>
<tr>
<th></th>
<th>$\alpha$(1950)</th>
<th>$\delta$(1950)</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>DR21</td>
<td>20h 37m 13s</td>
<td>+42° 08' 59''</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>20h 37m 13s</td>
<td>+42° 08' 50''</td>
<td>2</td>
</tr>
<tr>
<td>DR21(CO)</td>
<td>20h 37m 09.9s</td>
<td>+42° 09' 00''</td>
<td>3</td>
</tr>
<tr>
<td>DR21(OH)</td>
<td>20h 37m 14s</td>
<td>+42° 12' 00''</td>
<td>1</td>
</tr>
</tbody>
</table>

REFERENCES:

1. Dickel, Dickel and Wilson (1978)
2. Bally and Lada (1983)
with a grid spacing of 2" in the EW direction and 4" NS. The chop throw was 70" EW.

7.4 Data

There is some disparity in the literature between positions used for DR21. We will use the name DR21 to refer to the position of Dickel, Dickel and Wilson (1978). For our arc minute beam this is also essentially similar to that used by Bally and Lada (1983) and to the point 3 arc minutes south of DR21(0H). It is where the maximum signal is detected in the HCN, HCO+ and CS transitions, as well as in the 350 μm continuum. Plambeck, Snell and Loren (1983), however, used a position 35″ west of DR21, which is where the self reversal is seen in the CO J=3-2 spectrum. We shall refer to this position as DR21(CO). The various positions used are listed in Table 7.1.

The CO data, in both the J=2-1 and the J=3-2 transitions, are presented in the form both of spectra and velocity-position diagrams in Figures 7.1 and 7.2. The CO J=2-1 data (Figure 7.1a) show that, in addition to the main component of the emission which peaks at ~ 0 to ~ 3 kms⁻¹, a less intense component peaking at around 11 kms⁻¹ is present over the the whole of the region mapped. This was found also for the J=1-0 transition by Dickel, Dickel and Wilson (1978) who showed it to be associated with the source W75N situated 18 arc minutes to the north of DR21. The 11 kms⁻¹ component is most distinct along the NS line passing 1' to the west of DR21(CO); for these positions the shapes of the J=3-2 profiles around 11 kms⁻¹ are shown superimposed upon Figure 7.1a. The emission in this velocity range is somewhat less intense in the J=3-2 transition.

In both transitions there is evidence of line broadening around
CO J=2-1 spectra of the DR21 region (reference position $\alpha(1950) = 20^h 37^m 09.9^s$, $\delta(1950) = 42^\circ 09' 00''$). The grid spacing is 1 arc minute. The dotted lines superimposed on positions west of the reference position show the shape of the CO J=3-2 profiles.
Figure 7.1b

CO J=2-1 position-velocity map (NS) through DR21(CO). Contour levels $T_R^* )$ from 2 to 22K in steps of 2.5K.
Figure 7.2a

CO J=3-2 spectra (NS) from 3 arc minutes S (bottom) to 5 arc minutes N (top) of the DR21 position.
Figure 7.2b

CO J=3-2 position-velocity map (NS) through DR21. DR21 and DR21(OH) are marked by crosses. Contour levels $T_R^*$ = 4 to 21.5 in steps of 3.5K.
Figure 7.2(c)

CO J=3-2 spectra (EW) from 3W bottom to 3E (top) of DR21(CO).
Figure 7.2d

CO J=3-2 position-velocity map (EW) through DR21(CO). Contour levels $T_R^* = 2, 5, 8, 11, 14, 16, 19$ K.
DR21(CO). This may be due to an outflow (see Chapter 5). On the red side of the spectra, any outflow emission would be obscured and confused by the 11 kms\(^{-1}\) component. On the blue side (velocity range \(-28\) kms\(^{-1}\) to \(-12\) kms\(^{-1}\)) the high velocity gas is more prominent, especially in the higher spatial resolution CO J=3-2 data. This emission is relatively extended (FWHM = 4 arc min; see Figure 7.2d) along the EW direction but more compact (FWHM = 1.5 arc min; see Figure 7.2b) along the NS line. The latter diagram represents a line very close (11" W) to that used for the velocity position diagram of Fischer (1981) in the CO J=1-0 transition and observed with a similar beamwidth to that of UKIRT. The two diagrams are very similar to one another in appearance, both showing considerable broadening at the DR21 position and very slight broadening at the position of DR21(OH). The size, shape and orientation of the wing region as observed in the CO J=3-2 line also agree well with the mapping of Garden et al. (1985) in the \(v = 1\)-0 \(S(1)\) line of molecular hydrogen.

Over much of the region mapped, the J=2-1 and J=3-2 profiles are quite similar both in shape and peak intensity. However, there are two exceptions to this:

(i) At positions to the west of DR21(CO) there is some indication that the J=2-1 emission peaks at a higher LSR velocity (~ 0 kms\(^{-1}\)) than that of the J=3-2 peak (~ -3 kms\(^{-1}\)). This may be because low (~ 10\(^3\) cm\(^{-3}\)) density foreground gas in the 11 kms\(^{-1}\) component (associated with W75N) is absorbing the J=3-2 line;

(ii) The J=3-2 spectrum towards DR21(CO) is self reversed - this is still apparent when the frequency resolution is degraded to that used for the J=2-1 spectrum which shows no such feature. This qualitative difference between the two line profiles has been noted by Phillips et al. (1981).
Figure 7.3a

HCO\(^+\) J=4-3 spectra around the DR21 position, extending from 1 arc minute S to 5 arc minute N of DR21.
Figure 7.3b

Superimposed HCO\(^+\) and H\(^{13}\)C\(^+\) J=4-3 spectra towards DR21. The H\(^{13}\)C\(^+\) intensity has been multiplied by 5.
Figure 7.4a

HCN J=4-3 spectra around DR21(OH).

HCN J=4-3 spectra around DR21(OH).
Map of DR21(OH) in the HCN J=4-3 transition ($v_{\text{LSR}} = -3 \text{ km s}^{-1}$). The crosses show the positions of the HCN spectra in Figure 7.4a.
Superimposed HCO$^+$ J=4-3 and HCN J=4-3 spectra towards DR21.
Superimposed $\text{HCO}^+ J=4-3$, HCN $J=4-3$ and CS $J=7-6$ spectra towards DR21(OH).
Mapping and spectra in the $J=4\rightarrow3$ transitions of HCO$^+$, H$^{13}$CO$^+$ and HCN, and in the $J=7\rightarrow6$ transition of CS, are shown in Figures 7.3, 7.4 and 7.5. In the HCN and HCO$^+$ lines, DR21 and DR21(OH) show up as positions of peak intensity and are only partially resolved by our 55" beam. The HCN map of DR21(OH) gives an observed size of $\sim 2$ arc minutes (FWHM) and the HCO$^+$ mapping suggests similar sizes in this transition for DR21 and DR21(OH). These would give deconvolved source sizes of $\sim 1.5 \pm 0.5$ arc minutes for each source. The peak intensities of HCO$^+$ $J=4\rightarrow3$ towards DR21 and DR21(OH), and that of CS $J=7\rightarrow6$ towards DR21(OH), are all equal to within $\sim 10\%$; the peak intensities of the HCN line are $\sim 70\%$ of these values. The similarity in line shapes between the different transitions is also noticeable (although the CS $J=7\rightarrow6$ spectrum towards DR21(OH) appears skewed in the opposite sense to the others). This is particularly significant for the HCO$^+$ $J=4\rightarrow3$ and H$^{13}$CO$^+$ $J=4\rightarrow3$ spectra shown superimposed in Figure 7.3b. The ratio of their integrated intensities is 5.3, which is significantly less than any likely isotopic abundance ratio (Guelin, Langer and Wilson 1982) and implies that the HCO$^+$ transition is optically thick, as also found for the core of S255 (see Chapter 6). Nevertheless, the H$^{13}$CO$^+$ line has the same width as, and a similar shape to, the HCO$^+$ profile. We also obtained an H$^{13}$CO$^+$ spectrum of DR21(OH) which suffered from relatively poor signal to noise and baseline and is not presented here. This, however, suggests that a similar phenomenon is present towards DR21(OH) as well, and we estimate an integrated line intensity ratio $< 9.9$.

The 350 $\mu$m continuum observations consisted of determinations of the flux densities (in a 40" beam) and source sizes of DR21 and DR21(OH). The results are given in Table 7.2. The fluxes and sizes for the two sources are approximately similar, and the spatial extents
Table 7.2  350 micron fluxes and source sizes

<table>
<thead>
<tr>
<th></th>
<th>Flux (Jy)</th>
<th>Source Size (FWHM)(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DR21</td>
<td>870 ± 90</td>
<td>53 ± 5</td>
</tr>
<tr>
<td>DR21(OH)</td>
<td>1290 ± 200</td>
<td>50 ± 5</td>
</tr>
</tbody>
</table>

\(^a\) Derived assuming Gaussian source and beam profiles
Figure 7.6

20 µm map of DR21 taken with a 4'' aperture. The crosses mark the positions of the continuum peaks A, B, C and D at the 5 GHz map of Harris (1973), from which the shape of the lowest contour (392K) is also superimposed (dotted line). Contour levels: 1, 2, 3, 4, 6, 12.5, 18.75, 25, 32.25 Jy/beam. (1σ = 0.5 Jy).
are also roughly the same as those measured in the HCN and HCO$^+$ lines.

The 20 $\mu$m map of DR21 is shown in Figure 7.6, with the main features of the 5 GHz continuum map of Harris (1973) superimposed. In addition to the three sources DR21(N), DR21(S) and W75-IRS2 observed by Wynn-Williams, Becklin and Neugebauer (1974), further small scale structure is evident which will be discussed further in Section 7.5.

7.5 Discussion

The data tend to fall naturally into 3 categories: (a) the CO emission, observed over the whole region; (b) the submillimetre continuum data; and (c) the 20 $\mu$m continuum and other molecular line data. The last two categories concern the compact (∼ 1 arc minute diameter) condensations in DR21 and DR21(OH).

7.5.1. The results from CO mapping

The complexity of this region makes it difficult to represent by a single, unified model, without either introducing intolerable oversimplifications or allowing an unmanageably large number of free parameters. This is especially true for the CO data. Firstly, there appear to be 3 components in the CO emitting gas: (i) the high velocity wings discussed in Chapter 5 (ii) the bulk of the gas around $V_{\text{LSR}} ∼ - 3$ kms$^{-1}$ centred around DR21 and DR21(OH); and (iii) the gas with velocities near $V_{\text{LSR}} = 11$ kms$^{-1}$, which is particularly prominent around W75N but is in evidence all over the region. These components are not easily separable and may be interacting in complex ways. Secondly, high optical depths in CO transitions are in many circumstances likely to lead to absorption effects which hinder the unique interpretation of data.
Dickel, Dickel and Wilson (1978) attempted to model their CO J=1-0 and $^{13}$CO J=1-0 data with a large velocity gradient (LVG) model (Goldreich and Kwan 1974), having argued that the line wings over the DR21/DR21(OH) region are due to gravitational collapse in the outer parts of the cloud. They found that it was possible to fit quite well the observed J=1-0 spectra at the central DR21 position but that the fits were not so good at other observed positions on the cloud. Their model involved a collapsing cloud in which the collapse velocity variation with radial distance satisfied $v(r) \propto r$, and the gas density $n_{\text{H}_2}$ varied as $r^{-2}$.

Without any quantitative analysis it is clear that such a model cannot reproduce the reversed spectra observed towards DR21(CO) in the CO J=3-2 (this work) and CO J=4-3 (White et al. 1985, work in preparation) lines. It also fails to reproduce the observed line-widths of the different CO transitions. We have run an LVG program for a spherical cloud using the parameters of Dickel, Dickel and Wilson (1978), convolving the predicted spectra with Gaussian beams corresponding to the actual observations. For the central DR21 position, the predicted full widths at half intensity for the CO transitions were 12 kms$^{-1}$ (J=1-0), 10 kms$^{-1}$ (J=2-1) and 6 kms$^{-1}$ (J=3-2). The reason for the narrower predicted CO J=3-2 linewidth is that the density towards the cloud edge in the model is too low to populate the J=3 level sufficiently. There is, however, no evidence for this from the data, in which the line-widths over the region appear fairly similar between transitions. This is true even up to the J=4-3 transition. A similar phenomenon was observed for M17 by Martin, Sanders and Hills (1984), who interpreted it in terms of a cloud consisting of thermalised clumps. For similar reasons, the predicted (LVG) linewidth for the HCN J=4-3 line is 2 kms$^{-1}$, in
contrast to the observed values of $\Delta V$ (FWHM) = 7.5 kms$^{-1}$ towards DR21(OH) and $\Delta V$ (FWHM) = 14 kms$^{-1}$ towards DR21.

The general similarity in intensity, qualitative appearance and shape of many maps and spectra presented here and elsewhere (e.g. Plambeck, Snell and Loren 1983; Fischer 1981) in the lowest 3 CO transitions implies that they are thermalised and optically thick in the $-3$ kms$^{-1}$ gas component around DR21/DR21(OH). For likely CO relative abundances ($X_{\text{CO}} > 10^{-5}$), thermalisation of the J=3-2 transition requires local densities of $n_{\text{H}_2} \gtrsim 10^4$ cm$^{-3}$, and these are presumably present along the NS line from DR21(OH) to DR21. However, along an east-west line through DR21, comparison of a drift scan in the J=3-2 line at a velocity of $-3$ kms$^{-1}$ with the CO J=1-0 data of Dickel, Dickel and Wilson (1978) suggests that between 2 and 4 arc minutes from DR21, the ratio of intensities drops from $\sim 0.8$ to $0.2$. For LVG kinematics and an assumed $X_{\text{CO}}/(dv/dr) = 10^{-5}$ pc km$^{-1}$s, this would occur as the gas density decreased from $\sim 5 \times 10^3$ to $\sim 4 \times 10^2$ cm$^{-3}$. It is difficult to assess the changes in velocity width of the emission from the ambient cloud material because of contamination by the high velocity wings, although the appearance of Figures 7.2c and 7.2d suggests a radial decrease. It is probable that the gross features of the CO data could be described by some model which combined large scale velocity gradients with small scale clumping, with both the space density of clumps and the local densities present within them decreasing with radial distance. Closer constraints on such a model than can be placed here might be possible from detailed high resolution mapping (in e.g. $^{13}$CO or C$^{18}$O) over a small selected region situated away from the central density peaks.

We now consider possible explanations for the self reversals observed towards DR21(CO) in the CO J=3-2 and CO J=4-3 transitions,
but not in the J=1-0 or J=2-1 lines. As described in Chapter 3, such features are often predicted by microturbulent models (Leung 1978); also, by modified LVG models with collapse laws such as \( v \propto r^{-0.5} \). Here we adopt a simpler, 2 component model similar to those investigated by Phillips et al. (1981) and Loren et al. (1981), in which radiation from a background cloud of temperature \( T_{BG} \) passes through foreground material of excitation temperature \( T_K \). It is easy, using such a model, to obtain self reversals either in all transitions, or in all transitions except J=1-0. What is not so easy to reproduce is a non-reversed CO J=2-1 line in a case where higher transitions are reversed. It is true that our relatively large beam size in the J=2-1 line might obscure any self reversal which was present, but it is significant that J=2-1 spectra taken with a similar beamsize to our own J=3-2 observations (e.g. Plambeck, Snell & Loren 1983) are not self reversed either. This point was mentioned by Phillips et al. (1981) who then concluded that, despite its appearance, the J=1-0 line must also be strongly absorbed, but did not give model fits for the velocities corresponding to the peaks of the J=3-2 intensity, nor an explanation for the profile shapes.

We will assume that the background material is both optically thick and thermalised (to a kinetic temperature \( T_{BG} \)) at least up to the CO J=4-3 transition. The observed radiation temperature \( T_R \) is then related to \( T_{BG} \), for a non-absorbed line, by

\[
T_R(J,J-1) = (2hBJ/k)[(\exp(2hBJ/kT_{BG})-1)^{-1}-(\exp(2hBJ/2.7k)-1)^{-1}].
\]

(7.1)

In the presence of foreground absorbing material the observed radiation temperature would fall below that given by (7.1) by an
amount $\Delta T$ where

$$\Delta T = (1-e^{-\tau})\frac{2\hbar B J}{k}\left[\left(\exp\left(\frac{2\hbar B J}{kT_{BG}}\right)-1\right)^{-1} - \left(\exp\left(\frac{2\hbar B J}{kT_{ex}}\right)-1\right)^{-1}\right].$$  

(7.2)

($T_{ex}$ is the excitation temperature and $\tau$ is the optical depth of the absorbing gas). From the (assumed) non-absorbed lines CO $J=1-0$ and $J=2-1$, we estimate $T_{BG} = 28K$. The observed values of $\Delta T$ are 0K ($J=2-1$), 6K ($J=3-2$) and 10K ($J=4-3$). Since we have made no correction for differing beam efficiencies and are dependent on a small number of velocity channels to define $\Delta T$, these values may be in some error, and we have therefore also considered deviations of $\Delta T$ by $\pm 3K$ from the above values. Since we are ignorant of the detailed structure of any foreground material we have for computational convenience used an LVG program and examined the consequences of the material having kinetic temperatures of $T_K = 18K$, 28K and 38K in turn. Grids of models were run in which $\Delta T$ for each transition was computed as a function of $X_{CO}/(dv/dr)$ and $n_{H_2}$, these symbols having their usual meanings in LVG terminology (Chapter 2). The resulting plots are shown in Figure 7.7. We find that only for the case where $T_K > T_{BG}$ can the observations be fitted. This eventuality was not considered by either Phillips et al. (1981) or Loren et al. (1981), who assumed that the absorbing material would be cooler; however this latter assumption tends to predict self absorptions in all transitions (see Figure 7.7a). The reason why a hot absorbing layer can match the observations is that it is sufficiently hot to emit appreciably in the $J=2-1$ line, but not dense enough to thermalise the $J=3-2$ transition, with the result that it absorbs the higher frequency radiation. We stress that the temperatures chosen in Figure 7.7c are merely illustrative; it is likely that many combinations of temperature in
Figures 7.7a-d

Models of the depth of self absorption ($\Delta T$) in the CO transitions for various choices of background ($T_{BG}$) and foreground ($T_K$) temperatures. See text for further details.
Figure 7.7(b)
which $T_K > T_B$ could account for the observations (e.g. see Figure 7.7d). For example, the true temperature of the background material could be nearer to the 47K derived for the dust temperature, but be beam diluted to $\sim 28$K. Figure 7.8c does not fix a unique pair of values for $n_{H_2}$ and $X_{CO}/(dv/dr)$, but to fit the J=4-3 observations it appears necessary that $X_{CO}/(dv/dr) > 5 \times 10^{-7}$. The derived $n_{H_2}$ then depends on the value used for $X_{CO}/(dv/dr)$. If, for example, we take $X_{CO}/(dv/dr) = 10^{-5}$, we estimate a density for the hot absorbing gas of $n_{H_2} = 2 \times 10^3$ cm$^{-3}$; if $X_{CO}/(dv/dr) = 10^{-4}$, we get $n_{H_2} = 6 \times 10^2$ cm$^{-3}$.

Where could the absorbing gas be situated? Young et al. (1982) have shown for the dark cloud B5 that grain photoelectric heating, in addition to cosmic ray heating, may be sufficient to raise the gas temperature to $\sim 40$K in the outer cloud regions (as compared with $\sim 10$ to $15$K in the centre), while Keene et al. (1980) have considered the heating in the surface layers of B335 by the interstellar radiation field. In contrast, the densities present in the DR21 cloud may not everywhere be sufficiently high to couple the kinetic temperature of the gas to the values of $\sim 40$-50 K deduced for the dust from continuum data (Harvey, Campbell and Hoffman 1977; Thronson and Harper 1979).

But if the self absorption does take place in the outer layers of the cloud, it is difficult to understand why the region of self absorption should be so compact ($\sim 1$ arc min diameter round DR21(CO), with a marginal self absorption round DR21(OH)). An alternative explanation could be that the absorbing gas is situated in the cloud core. A feature of the observations which supports this is that the self absorptions seem only to occur towards the positions where there is a strong HCO$^+$ J=4-3 detection (see Fig 7.3a) and with a similar velocity width. (The maximum velocity width of the HCO$^+$ line occurs...
at the DR21 position, so the suggestion would now be that in the CO J=3–2 spectrum at DR21 in Figure 7.2a, the self absorption is so broad as to cut off completely the double peaked appearance seen towards DR21 (CO)).

We argue below that the HCO+ J=4–3 and H13CO+ J=4–3 data can be understood in terms of a clumpy central region in the DR21 cloud (and also possibly in DR21(OH)). The CO self reversals might then be interpreted as occurring in a relatively hot and rarefied interclump medium, possibly associated with the outflows emanating from pre-main sequence objects. Such an interclump medium could also be responsible for the fact that over some or all of their profiles, intensities in the HCO+ J=1–0 transition are for many sources lower than in the HCO+ J=3–2 line (Sandqvist et al. 1982; Loren and Wootten 1980; Wootten et al. 1984) or the HCO+ J=4–3 line (Padman et al. 1982; this work). Plots of ΔT similar to those described above for CO are presented in Figure 7.8, for the likely range of values of XHCO+//(dv/dr). These show that for the likely density range of the interclump medium, the J=1–0 transition of HCO+ is self absorbed but the J=4–3 transition is not.

7.5.2 The results from submillimetre continuum photometry

From the results presented in Table 7.2 it is possible to make estimates of column densities and masses, which will be used in the interpretation of the high excitation molecular line spectra to be discussed in Section 7.5.3.

The column density of H2 molecules can be estimated from the continuum flux Sν at ν GHz using the equation

\[ N(H_2) = 6 \times 10^{24} \left( \frac{750}{\nu/\text{GHz}} \right)^2 \nu \text{ cm}^{-2} \]  

(7.3)
Figure 7.8

Same as Figure 7.7, for HCO⁺.
(Hildebrand 1983) where the optical depth, \( \tau_\nu \), is given by

\[
\tau_\nu = 5.42 \times 10^{10} \frac{\Theta_S^2 + \Theta_B^2}{\Theta_S^2 - \Theta_B^2} \frac{S_\nu}{B_\nu(T)}
\]  

(7.4)

(Jaffe et al. 1984). Here, \( \Theta_S \) and \( \Theta_B \) are the source diameter and beamwidth (FWHM) expressed in arc sec. From the photometry of Harvey, Campbell and Hoffman (1977) we assume a temperature of 47K.

Hence we obtain, for DR21,

\[
\tau_{350\mu m} = 0.08
\]

and

\[
N(H_2) = 3.9 \times 10^{23} \text{ cm}^{-2}.
\]

Taking the observed source size as an estimate of the linear extent through the source we obtain an average density \( \bar{n}(H_2) \) given by

\[
\bar{n}(H_2) = 1.6 \times 10^5 \text{ cm}^{-3}
\]

For DR21(OH), the corresponding results are

\[
\tau_{350\mu m} = 0.12
\]

\[
N(H_2) = 6.0 \times 10^{23} \text{ cm}^{-2}
\]

\[
\bar{n}(H_2) = 2.7 \times 10^5 \text{ cm}^{-3}
\]

The estimated total masses for DR21 and DR21(OH) are respectively 5.7 \( \times 10^3 \) \( M_\odot \) and 7.9 \( \times 10^3 \) \( M_\odot \).

The chop throw employed for these observations was 140 arc seconds. In view of the relatively small sizes observed for the two sources, it is unlikely that the above derived quantities have been seriously underestimated on account of the finite chopping amplitude.

7.5.3. The results from molecular species other than CO

The HCO\(^+\) \( J=4-3 \) and \( H^{13}CO^+ \) \( J=4-3 \) spectra towards both DR21 and
DR21(OH) seem to offer the best chance of penetrating into the innermost cloud structure. The shortcomings of CO data in this respect have already been referred to. Also, many previous observations of HCN and HCO⁺, though having higher spatial resolution than the data presented here (e.g. Dickel, Ho and Wright 1985; Nyman 1983), have been carried out in the J=1-0 transition. These lines may not provide a good probe of the densest regions because they suffer from absorption in any surrounding, lower density gas (Wootten et al. 1984; Nyman 1983). By contrast, since in much of the outer part of the cloud the gas density is almost certainly not high enough to thermalise the J=3 level of HCO⁺ appreciably, self absorption should be a much less serious problem in the J=4-3 transition.

A few results from the data suggest themselves without any quantitative analysis. The low ratio of 5.3 between the HCO⁺ and H₁³CO⁺ integrated line intensities towards DR21 shows that the HCO⁺ line at least is optically thick. The similarity of the line profiles would then tend to exclude a homogeneous kinematic model in which the linewidth was produced by small scale "microturbulent" motions; most such models would predict qualitatively different profile shapes for the two transitions and would be quite likely to give a self reversed HCO⁺ profile (Chapter 3). A constant density LVG model could fit the observed line shapes and intensities, as also could one in which the densest material was clumped, and where the total linewidth was due to the dispersion between clump LSR velocities. The fact that the H₁³CO⁺ line is detected at all implies that it must be at least partially thermalised, and the higher optical depth in the H₁²CO⁺ J=4-3 transition, which would enhance the degree of radiative trapping, raises the possibility that this transition may be totally thermalised. Consistent with this is the similarity of both the peak and
integrated intensities in the CS J=7-6, HCO\(^+\) J=4-3 and HCN J=4-3 lines (Figures 7.5a, 7.5b), but their low absolute values strongly suggest that the emission region(s) are beam diluted. Since, however, the source diameters in both the HCN J=4-3 and HCO\(^+\) J=4-3 lines are > 1 arc minute (see Figures 7.3a and 7.4a), a model involving many small clumps would appear to be more appropriate for this central region than one with a single dense core. The 20 \(\mu\)m map of DR21 also provides indirect evidence for such a model; but not conclusively, since the intensity peaks will be heavily weighted towards points of high temperature rather than high density, and these will not necessarily be coincident.

### 7.6 A clumpy model for DR21

Clumpy models for molecular cloud cores have been considered by e.g. Little et al. (1980); Martin, Sanders and Hills (1984); and Matthews et al. (1984). Here we describe such a model for the core of DR21.

Consider a spherical volume containing \(N\) identical dense homogeneous clumps of radius \(r\), which are assumed small compared with the radius \(R\) of the emitting region. We will allow more than one clump to exist along the same line of sight, but not at a similar LSR velocity, so that emission from one clump is not reabsorbed by another. The integrated intensity in a molecular line (assumed observed with a beamsize > the extent of the emitting region) is given by

\[
\int T_R^* \, dv = T_{ex} \, (1 - e^{-\tau}) \, \Delta v \, N_c \, n_c(H) \, r^2 / R^2
\]

(7.5)

where \(T_{ex}\) is the excitation temperature, \(\tau\) is the average optical depth through a clump (= 0.75 \(\times\) the optical depth through its dia-
meter) and $\Delta v_c$ is the linewidth (in units of velocity) from an individual clump. The quantity $n_c(R)$ is the beam coupling efficiency onto the clumpy region (Kutner and Ulich 1981) and the beam is assumed to be uniform within this, so that $r^2/R^2$ represents the further dilution factor for one clump in the beam. In reality, the clumps are unlikely to be homogeneous, but will in general possess structure; a rigorous analysis would then require $T_{ex}$ and $\tau$ to be replaced by integral expressions. However, we ignore such complications here and regard $T_{ex}$ and $\tau$ as average values.

The predicted ratio $R_{int}$ of integrated intensities in, for example, the $J=4-3$ transitions of HCO$^+$ and $^3$HCO$^+$ is then given by

$$R_{int} = \frac{1 - \exp (-\tau_{12})}{1 - \exp (-\tau_{13})} \frac{\Delta v_c^{12}}{\Delta v_c^{13}} \frac{T_{ex}^{12}}{T_{ex}^{13}}$$ \hspace{1cm} (7.6)

where the meanings of the terms on the right hand side are self-evident. For thermalised lines, $T_{ex}^{12} = T_{ex}^{13}$ and $\tau_{12}/\tau_{13}$ is simply equal to the isotopic abundance ratio, here assumed to be 40. If we assume further that $\Delta v_c^{13} = \Delta v_c^{12}$, then from the observed $R_{int} = 5.3$ we derive $\tau_{13} = 0.2$ and $\tau_{12} = 8.4$. Since, in these circumstances, the $^3$HCO$^+$ line is optically thin, we can then estimate a column density $N_{^3}$HCO$^+$ from

$$N_{^3}$HCO$^+ = 9.4 \times 10^{11} \left( \frac{\int T_R^*(HCO^+ J=4-3)dv(kms^{-1}) \exp (25.7/T)}{n_c(R) (\mu/debye)^2 (1-\exp(-17.1/T))} \right) \hspace{1cm} \text{cm}^{-2}$$ \hspace{1cm} (7.7)

We insert the values $n_c = 0.6$ for the coupling of the QMC system on UKIRT onto a 1 arc minute diameter uniform source (Lesurf 1981), $\mu = 4.05$ debye (Haese and Woods 1979) and $T = 47 K$ (Harvey, Campbell...
and Hoffman 1977). From the observed integrated intensity of 7 K km s\(^{-1}\) we find \(N_{H^{13}CO^+} = 3.8 \times 10^{12} \text{ cm}^{-2}\) and \(N_{HCO^+} = 1.5 \times 10^{14} \text{ cm}^{-2}\). From the \(H_2\) column density estimated in Section 7.5.2 on the basis of the 350 \(\mu\)m observations we estimate a lower limit to the \(HCO^+\) abundance relative to \(H_2\) of \(X_{HCO^+} > 4 \times 10^{-10}\). Also, we find \(X_{H^{13}CO^+} > 10^{-11}\), (c.f. the estimate of \(X_{H^{13}CO^+} = 2.7 \times 10^{-12}\) derived for DR21(OH) by Wootten, Loren and Snell 1982).

However, these values may be severe underestimates. It is possible that \(T_{\text{ex}}^{12}/T_{\text{ex}}^{13}\) and \(\Delta v_c^{12}/\Delta v_c^{13}\) are both > 1, due respectively to incomplete thermalisation of the \(H^{13}CO^+\) line and saturation of the \(H^{12}CO^+\) line. In this case \(\tau_{13}\) will be correspondingly greater (e.g. for \((T_{\text{ex}}^{13} \Delta v_c^{13})/(T_{\text{ex}}^{12} \Delta v_c^{12}) = 0.5\), we have \(\tau_{13} \sim 0.5\)). The use of equation 7.7 will then underestimate the column density, in the first instance because \(T_{\text{ex}}\) is less than the kinetic temperature and in the second because of the appreciable optical depth. Also, our estimate of \(X_{H^{13}CO^+}\) implicitly assumed that the 350 \(\mu\)m emission originated from the same mass of gas as the \(H^{13}CO^+\) emission, whereas probably the continuum intensity contains a sizeable contribution from regions whose densities are too low to produce significant thermalisation in the \(H^{13}CO^+ J=4-3\) transition.

The derivation of local \(H_2\) densities within the clumps requires information about their internal kinematical structures. If the \(H^{12}CO^+ J=4-3\) line is optically thick and thermalised to 47K, then inserting the observed \(\int T_R^* d\nu = 37 \text{ K km s}^{-1}\) into equation 5.1, we find

\[
\Delta v_c N_r^2 / R^2 = 1.3 \text{ km s}^{-1}
\]

or, for the observed total linewidth \(\Delta \nu = 14 \text{ km s}^{-1}\),
which is a combined velocity and spatial dilution factor. If all the material is assumed to exist within the clumps of density $n_{H_2}$ then we also have

$$\frac{n_{H_2} \bar{n}_{H_2}}{R^3/Nr^3} = R^3/Nr^3$$

(7.9)

where the average density $\bar{n}_{H_2}$ in the clumped region has been estimated in Section 7.5.2. Lacking information on the kinematic state of an individual clump, we assume that its emergent radiation temperature $T_R$ in any line (i.e. with infinite spatial and velocity resolution) can be estimated without too much error using LVG kinematics. For any assumed clump density $n_{H_2}$ the observed value of $R_{int}$ can be used with an LVG program to define $X_{HCO^+}/(dv/dr)$ (Figure 7.9). Equations 7.8 and 7.9 can be solved for $\Delta v_c/r$, thus fixing $X_{HCO^+}$, whose derived value decreases monotonically with $n_{H_2}$. An absolute lower limit on $n_{H_2}$ is the average value of $1.6 \times 10^5 \text{ cm}^{-3}$. A severe lower limit on $X/(dv/dr)$ is obtained by taking $X_{HCO^+} > 4 \times 10^{-10}$ as above, $\Delta v_c < 14 \text{ km s}^{-1}$ (the total linewidth) and $2r > 1_j$, the Jeans length given for $T = 47 \text{ K}$ by $1_j \sim 0.6 \left( n_{H_2}/10^4 \text{ cm}^{-3} \right)^{-0.5} \text{ pc}$. These limiting values are also shown in Figure 7.9, together with the region of solutions defined by $T_R (HCO^+ J=4-3)/T_R(H^{13}CO^+ J=4-3) = 5.3 \pm 1$, and one or two relevant contours of excitation temperature and optical depth. They show that, for the $H_2$ density range $10^5$ to $10^6 \text{ cm}^{-3}$, the excitation temperatures are related by $T_{ex} (H^{13}CO^+ J=4-3)/T_{ex} (HCO^+ J=4-3) \approx 0.5$. In this regime, even the $H^{13}CO^+ J=4-3$ transition is optically thick, and the fact that the observed $R_{int}$ is $> 1$ is now accounted for by the difference in excitation temperatures (see equation 7.6) rather than optical depths.
Figure 7.9

Clumpy model of DR21: results.

The parallel solid lines show the range of allowed solutions.

Shaded lines show regions excluded (see text for details).
The derived value of $X_{\text{HCO}^+}$, obtained from Figure 7.9 and the solution of 7.8 and 7.9, is shown as a function of assumed clump density in Figure 7.10 together with the corresponding variation in $v/r$. Also plotted is the free-fall value

$$\left(\frac{v}{r}\right)_{ff} = 3.2 \left(\frac{n_{\text{H}_2}}{10^4}\right)^{0.5} \text{km s}^{-1} \text{pc}^{-1}$$

(7.10)

which would be obtained if the clumps were in a state of unimpeded gravitational collapse. It is assumed that the true value of $v/r$ cannot be greater than this, which excludes clump densities $> 10^7$ cm$^{-3}$. For high densities, the derived $X_{\text{HCO}^+}$ tends to a lower limit of $8 \times 10^{-10}$ which, in view of the uncertainties involved in correcting the absolute observed $T_R^*$ ($\text{H}_{13}\text{CO}^+$ J=4-3), is consistent with the lower limit of $\sim 4 \times 10^{-10}$ estimated earlier. The permitted range of solutions for the clump density is $\sim 1.6 \times 10^5$ cm$^{-3}$ to $10^7$ cm$^{-3}$ and a corresponding range of $X_{\text{HCO}^+}$ from $\sim 10^{-8}$ to $10^{-9}$. It is not possible to be more specific without knowledge of $v/r$. If $v/r \sim 16$ km s$^{-1}$ pc$^{-1}$ (total linewidth/total region diameter), we obtain $n_{\text{H}_2} = 1.3 \times 10^6$ cm$^{-3}$, $X_{\text{HCO}^+} = 1.8 \times 10^{-9}$. If on the other hand we take a thermal velocity width of 0.4 km s$^{-1}$ for $\Delta v_c$ and a typical Jeans length of $\sim 0.1$ pc for the clump diameter, then we get $v/r \sim 4$ km s$^{-1}$ pc$^{-1}$, $v_{\text{H}_2} = 3.5 \times 10^5$ cm$^{-3}$ and $X_{\text{HCO}^+} = 6 \times 10^{-9}$. These cases are shown on Figure 7.10 by points L and T respectively.

It is therefore of interest to know whether the individual clump extents and velocity widths for the high excitation submillimetre transitions described in this paper could be resolved, thus enabling us to pin down $n_{\text{H}_2}$ and $X_{\text{HCO}^+}$ more precisely. If the region (of diameter $2R$ and velocity width $\Delta V$) were observed with a beam size $B$
Derived relative HCO\(^+\) abundance as a function of assumed clump density. Superimposed are the values of v/r given by (i) the observed dilution factor (ii) unimpeded gravitational collapse. Points marked T and L are described in the text.
and a velocity resolution $\Delta v_{\text{res}}$, the average number of clumps in each spatial–velocity resolution element would be $N B^2 \Delta v_{\text{res}}/(4 R^2 \Delta V)$ and typical fluctuations $\Delta T/T$ in the observed intensity between resolution elements would be $\sim (2 R/B) (\Delta v/\Delta v_{\text{res}})^{0.5} N^{-0.5}$. For case T mentioned above, equation 7.8 predicts $N \sim 260$ clumps (of average mass $\sim 20 M_\odot$).

For our HCO$^+$ J=4–3 data, in which $B \sim 1$ arc minute and $\Delta v_{\text{res}} = 1 \text{ kms}^{-1}$, we obtain $\Delta T/T \sim 0.25$. A 30" beam and a 0.4 kms$^{-1}$ velocity resolution would give $\Delta T/T \sim 0.75$ with an average of $\sim 2$ clumps per resolution element. Although our present data are not quite sufficient in this respect, use of such a better resolution and observations in 2 or more isotopic lines should in this case enable constraints to be placed on the clumps' velocity widths and sizes, even if the beam size was not quite small enough to resolve them spatially.

In the foregoing analysis we have assumed the clumps to be homogeneous and that any inter-clump medium which may be present is of such low density and excitation that it neither emits nor absorbs significantly in the HCO$^+$ J=4–3 transition. However, it seems more plausible that the clumps have internal density gradients. Because different transitions thermalise over different density ranges, depending on their dipole moments and optical depths, this means that both the size and velocity width of an individual clump will vary between transitions. As a result, the values of $n_{\text{H}_2}$ derived from different transitions may also vary, because they will be characteristic of different fractions of each clump. Densities determined from a variety of molecular lines could then be used in conjunction with the derived dilution factors to arrive at a more detailed model of the clumpy structure (Martin, Sanders and Hills 1984).
7.7 Conclusions

We have mapped the DR21/DR21(OH) region in several millimetre and submillimetre molecular lines, and made further continuum observations at 350 µm and 20 µm.

Over the whole region mapped, the -3 km s\(^{-1}\) gas component observed by Dickel, Dickel and Wilson (1978) in the CO \(J=1-0\) transition is prominent also in the CO \(J=2-1\) and \(J=3-2\) lines. The 11 km s\(^{-1}\) component associated with W75N is also seen, and is more intense in \(J=2-1\) than \(J=3-2\). To the west of DR21 there are indications that gas at \(V_{\text{LSR}}\sim 11\) km s\(^{-1}\) and of density \(\sim 10^3\) cm\(^{-3}\) is absorbing emission from the red wing of the -3 km s\(^{-1}\) component, particularly in the CO \(J=3-2\) line. The relative line widths are not consistent with the LVG model of Dickel, Dickel and Wilson (1978). Gravitational collapse cannot be excluded as an explanation for the linewidths and intensities but it is probable that the material throughout the region is also clumped; higher resolution observations are needed in the outer cloud regions to check this. A high velocity wing is seen around DR21, which is compact along the NS direction but more extended (3-4 arc minutes) EW. This is probably caused by an outflow. DR21 and DR21(OH) appear as compact (\sim 1 arc minute) condensations of high intensity both at 350 µm and in the submillimetre lines of HCN and HCO\(^+\). The average \(H_2\) density over these central regions is \(\sim 10^5\) cm\(^{-3}\), but the spatial extent of the line observations, together with the observed intensity ratios \(T_R(\text{HCO}^+ J=4-3)/T_R(\text{H}^{13}\text{CO}^+ J=4-3)\) imply that the dense core regions consist of clumps of density \(\sim 10^6\) cm\(^{-3}\). The precise values depend on the unknown typical values of \(\Delta v/r\) within the clumps; if these could be specified, the clump densities could be more tightly constrained. This is true also of the relative abundance \(X_{\text{HCO}^+}\), which however must be between \(10^{-9}\) and \(10^{-8}\).
The self absorptions seen in the J=3-2 and J=4-3, but not the J=2-1 or J=1-0, transitions of CO around DR21 can be explained in terms of a simple 2 component model in which the absorbing gas has a density \( \sim 10^3 \text{ cm}^{-3} \) and is hotter than the optically thick and thermalised background gas. This absorbing material may be the interclump medium situated in the core of the cloud. The presence of this material highlights the usefulness of observing in lines higher than J=1-0 for the HCO\(^+\), HCN and other species, since the lowest transitions may be contaminated by emission and absorption from this less dense material. More direct information about the individual dense clumps should be obtainable with higher resolution (both velocity and spatial) observations in a variety of transitions, using currently available telescopes and instrumentation, and should enable close constraints to be placed on clump densities and internal structures, as well as relative molecular abundances. Derived densities might be expected to vary between transitions used, because different fractions of the gas were being sampled, but the different dilution factors found in each case would enable estimates to be made of the distribution of the gas between different densities.

The occurrence within the same square arc minute of high velocity CO emission, self absorbed CO spectra, high density clumps, HII regions, positions of relatively high dust temperature (20 \( \mu \text{m} \)) and a molecular outflow invites the speculation that all these phenomena are intimately physically connected. A particular model which appears to fit the observations is the clumpy cloud model of Norman and Silk (1980). In particular, they predict the existence of fragments of typical size > 0.1 pc, density \( \sim 10^5 \text{ cm}^{-3} \) and velocities \( \sim 1-5 \text{ km} \text{s}^{-1} \), embedded in a warmer interclump medium of density \( \sim 10^3 \text{ cm}^{-3} \). Within the context of our data, the interclump gas could be producing the CO
self absorption and the dense optically thick clumps the HCO$^+$ emission.

One question arising from this is why only some high velocity wing sources have self reversed CO spectra. In the analysis of Chapter 5, DR21 was identified as a source whose high velocity component contained relatively low gas densities ($\sim 10^4$ cm$^{-3}$). This, together with the large spatial extent of the high velocity gas put it into the category of sources in which it was difficult to distinguish an outflow from the surrounding cloud material. Such a situation might exist in the later stages of expansion of an outflow, when the total mass of swept up material had become large, and its velocity decreased to values similar to those found in the ambient cloud material. We note that most of the clouds which show reversed CO spectra are larger (e.g. Serpens, GL961, RCrA and DR21) than most of the those which do not (e.g. OriA, L1551, Elias 1-12 and S255) and in which higher local outflow densities tend to be found (see Chapter 5). This could be because the former group are more evolved and have therefore formed a greater volume of the 2 phase cool clump/warm interclump material. This would consequently be sufficiently extended, firstly not to spatially dilute any self absorption, and secondly to provide sufficient optical depth in the interclump medium (and a high enough beam filling factor for the clumps) to produce observable self absorption.
REFERENCES


This thesis has attempted to use submillimetre molecular line data to enhance our understanding of conditions in and around dense molecular cloud cores. In pursuing this end it has been necessary to undertake some reassessment of the techniques often used in data analysis, and also to address the issue of data calibration and comparability.

We have been confronted by two particular recurrent problems. The first is a theoretical one: that due to complex radiative transfer and other effects the derivation from observed data of conditions within clouds can be highly model dependent (see Chapter 3). The second is that to carry out anything more than the most superficial analysis, a variety of lines must be observed and we are thus faced with the problems of data comparability discussed in Chapter 4. Both problems are exacerbated by the apparently complex and inhomogeneous structure of cloud cores, since this both complicates the radiative transfer and introduces extra uncertainties into the estimation of beam coupling efficiencies.

We have still found it useful in many cases to perform fairly simple analyses. Often, the very failure of contrasting alternative simple models to account for observations can be more physically illuminating than a more exact fit using a relatively complex model and involving a larger number of free parameters, because the
more complex the model, the less certain can one be that the solution is unique.

A case in point is the analysis of the high velocity wing sources presented in Chapter 5. In section 5.2 we discussed two simple analyses from the literature, pointing out that their basic assumptions and conclusions were mutually contradictory. Our own analysis too was undoubtedly an oversimplification of the real situation, but it enabled us to avoid assuming optical thinness, thermalisation of the CO transitions, or a value for $X_{\text{CO}}$. Our derived values for line optical depths and excitation temperatures fell in most cases between those implied by the other two studies. Unlike them, we were also able to make estimates of local $\text{H}_2$ densities rather than spatially averaged values. Our main conclusion was that in the high velocity gas there exist local densities which are considerably higher than previously estimated average values. (These results could be partially reconciled if the density structure was inhomogeneous). Also, the local densities tended to be higher in the more compact sources (Figure 5.18).

There were, however, two specific weaknesses in this treatment. Firstly, our data were incomplete in that we had to rely mainly on single spectra towards the centre of each source. In view of the complex bipolar structure of many high velocity wing sources, this is a serious deficiency. Secondly, we had to analyse our data in conjunction with results taken by other observers at different telescopes. The dangers inherent in this were discussed in Chapter 4.

Probably the most satisfactory modelling of a wing source was that carried out for S255 (Section 6.6.2) since here we were able to combine observations in two different lines observed with the same receiver on the same telescope. Although this gave different beam-
sizes, it was possible to correct for this in a self-consistent way, as described in Chapters 4 and 6. Another advantage was that the high velocity gas component could be distinguished by the different line intensity ratio over a particular velocity range (Figure 6.4b). This may in the future prove to be a cleaner and more satisfactory criterion for the identification of outflows than is given by the visual inspection of a position-velocity map in a single transition. For example, Figure 6.6c would have been decidedly unconvincing in this respect; and in any case, models with purely gravitational collapse can also predict spatially compact high velocity wings (e.g. see Figure 3.8).

Other suggestions from our high velocity wing analysis were that CO may be depleted in the central cloud regions, and that the total mass of high velocity gas may be higher by up to an order of magnitude than was previously thought to be the case. In some instances, this weakens the evidence from kinetic energy considerations that the gas is outflowing rather than in rotational equilibrium or gravitational collapse.

Despite the calibration difficulties we have encountered, it is clear that deductions from data are sometimes possible on the basis of their qualitative aspects without having to rely on precisely calibrated absolute intensities. Two examples discussed in Chapter 3 are particularly relevant. One semi-quantitative result was the correspondence between intensity variations in frequency and physical space predicted in LVG models, which had implications for relative linewidths and source sizes. Another lay in the qualitative contrast predicted by microturbulent models between the profiles of pairs of lines such as HCO+ and H13CO+ J=4-3, which have very different optical depths. (In fact, the HCO+ J=4-3 line was often predicted to be self-
reversed). In Chapters 6 and 7 we were able from the observed similarities in profiles, together with (in Chapter 7) the spatial extent of the emission and the relative widths of different lines, to interpret the data as probably excluding an LVG or microturbulent model for dense cloud cores, but favouring one consisting of small, dense fragments. Furthermore, the pattern of self reversals in the CO spectra towards DR21 which were presented in Chapter 7 led us to the conclusion that emission from the densest core gas was passing through a hotter but less dense medium, probably also situated in the core. Again, this result depended on the mere presence or absence of self reversals, not on their precise depth.

The more extensively we employ clumpy models to explain observations, the more prone is the analysis to the uncertain details of the radiative transfer. The discussion of Section 7.6, the results from which are summarised by Figures 7.9 and 7.10, serves to emphasise how inextricably linked are values of derived molecular abundance with assumed clump densities. The same is true between derived optical depths and assumed excitation temperatures, due to the unknown extent of radiative trapping. For example, it is not even certain that the H$^{13}$CO$^+$ J=4-3 line is optically thin. Under such conditions, sub-millimetre continuum data become indispensable, since they are undoubtedly optically thin. We accordingly used continuum observations in Chapters 6 and 7 to deduce values for $X_{\text{HCO}^+}$. A great utility of these data lay in their ability to yield average $\text{H}_2$ densities; this proved to be a cornerstone in our discussions of the clump properties. We were hence able to place important constraints on clump parameters and values of $X_{\text{HCO}^+}$ (see Figure 7.10), and to assess the feasibility of narrowing these further, given higher spatial and velocity resolution. Such a synthesis of continuum and line data
should in the future yield a powerful method of measuring chemical abundances and their variations within and between cloud cores, which are essential to the testing of models of cloud chemistry.

It should be recalled that we still made use of a basic LVG program in investigating the clumpy model of DR21, despite the reservations expressed in Chapter 3. As was pointed out in Chapter 7, the dense cloud fragments are not necessarily identical and homogeneous as we assumed in our simple model, but may contain density gradients and have a spectrum of masses. The observed intensity in a molecular line might then consist of contributions from three types of region within the beam, each giving a different $T_R$. These would be (i) an unexcited region where $T_R \approx 0$; (ii) optically thick and thermalised regions where $T_R \approx T_K$, the kinetic temperature; and (iii) points where $0 < T_R < T_K$ because the gas was either optically thin or unthermalised. It is important to investigate this situation theoretically and estimate the extent to which a variety of line data can be used to determine clump density structures. A start was made in Chapter 3 on this, although there we considered gas spheres which were resolved by the beam. Research is now planned to deal with the case of large numbers of clumps individually much smaller than the telescope beam, and particularly to assess the sensitivity of the modelling to their small scale structure.

As regards future observational work, the implication of the discussions presented in this thesis is that for the satisfactory investigation of any dense star formation region at submillimetre wavelengths, a combination of three types of data is needed: (i) optically thin data; (ii) data of high spatial and velocity resolution; and (iii) data which are well calibrated in an absolute sense, with beams of accurately known characteristics, in order to ensure
comparability between lines at different frequencies.

We have seen in Chapters 6 and 7 that even observations in $^{13}$C isotope lines cannot be relied upon to be optically thin. Submillimetre continuum data, however, do satisfy condition (i) and should preferably be used in combination with line observations.

High resolution is needed for the direct detection of clumpy structure, and the determination of clump velocity widths. For example, at the distance of S255 and DR21, the 15" beam of the Millimetre Wave Telescope at 345 GHz will correspond to ~ 0.2 pc, a typical Jeans length. Such direct observations of clumps in high excitation transitions of simple linear molecules such as CS and HCO$^+$ should be relatively free of the problems of interclump and foreground absorption encountered for J=1-0 transitions, and also of the dilution of emitted energy between large numbers of transitions which occurs with less symmetric molecules. The observed qualitative profile shapes from individual clumps will be further informative of their structures.

However, the pursuit of the highest possible spatial resolution is inevitably accompanied by the increased difficulty of achieving a perfect antenna reflecting surface. In aiming for the smallest possible beamwidth, one may have to pay the price of having a significant error pattern of much larger diameter than the diffraction limited beam and containing a significant fraction of the total power (e.g. see Section 4.4; also the Nobeyama 45m antenna data in Table 4.1). For complex clumpy cloud cores especially, this could introduce formidable beam coupling uncertainties and constitute a barrier to the valid comparison of data between different telescopes. As a vital complement to such work, therefore, it will still be essential to carry out concurrent observations at lower spatial resolutions, in which the priority is accuracy of absolute intensity calibration.