PART II

INTERPRETATION OF ROTATIONAL SPECTRA OBSERVED FROM MOLECULAR CLOUDS
CHAPTER I

Introduction
In this part of the thesis we have dealt with the interpretation of the rotational spectra obtained from interstellar molecular clouds. Clouds in the earth's atmosphere with which we are familiar are discrete physical entities with well defined boundaries containing matter clearly distinguishable from the immediate surroundings. In interstellar space the term 'cloud' cannot be defined very precisely. One suggested definition of cloud (Verschuur 1974) is that it is an object within which the various observable properties such as density, temperature or velocity remain coherent.

The molecular clouds may be broadly divided into two types. The first of these, is called molecular dense clouds. These are associated with active phenomena—bright O to B stars, HII regions, infrared emission or continuum radio emission. They exhibit broad spectral lines corresponding to velocities of 4 - 40 Km/s. In contrast, dark clouds are not associated with such activity but are quiescent with line breadths indicative of only 1 Km/s internal velocities. Further, dense clouds have higher kinetic temperatures, larger sizes and are more massive than the dark clouds. For both the types of clouds molecular hydrogen is the most abundant species though other molecules of greater complexity are also found. In molecular clouds the formation of stars may be in progress.

The dark clouds have densities of the order of $10^3$ hydrogen molecules per c.c. and temperatures are generally between 5 and 10K. Among the molecular spectra they exhibit are the centimetre lines of OH and $H_2CO$ as well as the 2.6 mm CO line.

For dense molecular clouds the spectra are more intense and rich. It is from such clouds that the sizeable body of molecular disco-
veries have been made. Their large sizes and masses dwarf even
the giant HII regions often associated with them. Due to these
features those clouds may be more appropriately described as 'giant
molecular clouds'.

The first attempt to make a systematic survey of such clouds
was undertaken by Liszt (1973). The $J = 1-0$ line emission from the
two most abundant isotopic species of CO, viz. $^{12}\text{CO}$ and $^{13}\text{CO}$ in
twenty one molecular clouds associated with HII regions as well as 4
OH sources were studied by millimeter lines. However, since then,
there has been a dramatic increase in the number of molecules
identified in the interstellar medium. The molecular spectra are very
useful sources for obtaining information about the physical condi­
tions existent in the cloud. The molecules identified range from
simple diatomics like $\text{H}_2$ to 11-atomics like $\text{HC}_3\text{N}$. In addition to
neutral molecules, molecular ions like $\text{CH}^+$, $\text{HCO}^+$, $\text{DCO}^+$, $\text{N}_2\text{H}^+$ etc.
have also been detected. A list of interstellar molecules detected
till September 1979 has been given by Mann and Williams (1980).

We shall now briefly describe the observational technique for the
spectra. In radioastronomy, the incident energy is coherently
amplified i.e., the phase of the incident wave is preserved in the
process. The device used to intercept and coherently add such an:
incident electromagnetic field is called an antenna. The most
generally used antenna and the one which most nearly resembles its
optical counterpart is the parabolic reflector. The terminals of the
receiver are located at the focal point, where the field in the
aperture is coherently added.
Before going into the details of observations and their interpretations we define a few terms frequently used in this connection.

a. **Antenna temperature \( (T_A) \):**

This is defined as the power per unit bandwidth received at the antenna terminal divided by Boltzmann constant. This is an intensity which corresponds to a thermodynamic temperature in the Rayleigh-Jeans limit. Radioastronomy observations are simply the measurements of antenna temperature as a function of angle and frequency.

b. **Brightness temperature \( (T_B) \):**

This is defined as the physical temperature of a perfect absorber with the same angular dimensions as the object which would produce the observed antenna temperature \( T_A \). Thus the brightness temperature is an equivalent blackbody temperature used to describe the specific intensity \( I \) of radiation by the Rayleigh-Jeans relation

\[
I = \frac{2kT_B}{\lambda^2} 
\]

where \( k \) is the Boltzmann constant and \( \lambda \) is the wavelength of the incident radiation.

c. **Excitation temperature \( (T_{ij}) \):**

The excitation temperature \( T_{ij} \) of a molecular transition \( i-j \) is defined by the Boltzmann equation,

\[
\frac{n_i}{n_j} = \frac{g_i}{g_j} \exp \left[- \frac{(E_i - E_j)}{kT_{ij}} \right] 
\]

where \( n_i \) is the number of molecules with energy \( E_i \) and \( g_i \) is the
degeneracy of the $i$th level. If the molecules are in local thermal equilibrium (L.T.E) with their surroundings, then the entire ensemble of energy levels is described by the same $T_{ij}$ i.e., the excitation temperature between all pairs of level will be $T_{ij}$ and $T_{ij} = T_k$, where $T_k$ is the kinetic temperature of the environment. In most astrophysical conditions deviations from L.T.E. occur because of the low densities, resulting in collision rates too small relative to the radiative transition rates to provide sufficient population in the higher energy levels.

2. Observations.

We shall briefly describe the important observations on some molecules and ions from interstellar sources which are likely to play important role in obtaining information about physical conditions existing therein.

a. CO

Interstellar CO was discovered by Wilson, Jefferts and Penzias (1970) who observed the intense line emission from $J = 1-0$ (2.6 mm) transition of $^{12}$C $^{16}$O species in nine galactic sources and found a velocity width (full width at half-maximum) of 6.2 km/s of the line spectrum from Orion A. Following this Penzias et al (1971) investigated a number of representative sources and detected $J = 1-0$ lines of $^{13}$C $^{16}$O and $^{12}$C $^{18}$O along with CO from W51, Sgr A and Sgr B2. They also reported brightness temperatures and line widths of $J = 1-0$ lines of CO detected from a number of other sources. Later, Penzias et al (1972) in their observations of 1-0 lines of CO from twelve sources...
and $^{13}$CO from four of these found that the $^{13}$CO line intensities were approximately one-third of those of $^{12}$CO. By calculating optical depth they showed that the 1-0 line of CO is optically thick and so is expected to be thermalized and hence suggested that the observed line intensities can be used to obtain kinetic temperatures.

A survey of 1-0 emission line of CO in a wide variety of galactic objects was made by Wilson et al (1974). Phillips et al (1973) reported the observations of 2-1 (1.3 mm) lines of $^{12}$CO and $^{13}$CO from Orion A. They plotted the corrected antenna temperatures ($T_A^*$) against right ascension (R.A.), declination and velocity with respect to the local standard of rest. The peak brightness temperature of the 2-1 line of $^{12}$CO was observed to be 76K which is very close to that of 1-0 line (75K). Also, the 2-1 line was found to be more opaque than the 1-0 line implying that both the lines of $^{12}$CO in Orion A are thermalized. Later, Phillips et al (1974) reported more accurate data ($T_A^*$ Vs R.A. curve) on 2-1 line of CO from Orion A which shows an oscillatory structure. They suggested that this oscillatory nature indicates gravitational instabilities in the molecular cloud on the scale of light years.

Wannier et al (1976) have reported more refined observations of 1-0 transition of $^{12}$CO, $^{13}$CO and $^{18}$O observed from fourteen molecular clouds. The data for 1-0 transitions for $^{13}$C $^{18}$O, $^{13}$C $^{17}$O, $^{13}$CN, $^{15}$CN, H$_2$CO and H$_2^{13}$CO from a few sources have also been reported. Using these data they studied the abundance ratios of carbon and oxygen isotopes in dense molecular clouds and obtained a value of $^{12}$C/$^{13}$C $\approx$ 40. In Orion A, they made a comparison of 1-0 and 2-1 lines of CO to provide experimental verification of the thermalization of these lines.
Encrenaz et al (1973) observed the spectra of 1-0 transition of \(^{17}\)C\(^{18}\)O and \(^{18}\)O from the two molecular clouds, Orion A and P Ophiuchi. From the line intensity ratio they studied the \(^{17}\)O/\(^{18}\)O abundance ratios for both the clouds and obtained a value close to the terrestrial value of 0.186. Later Wannier et al (1976) presented the same but more refined spectral data observed from eight dense molecular clouds including the two mentioned above. They obtained a value of 0.24 for the ratio \(^{17}\)O/\(^{18}\)O which is significantly higher than the corresponding terrestrial value.

Goldsmith et al (1975) observed the 2-1 rotational transitions of \(^{12}\)CO and \(^{13}\)CO in Orion A and other five dense molecular clouds and obtained close agreement with the line intensities and linewidths as reported earlier for 2-1 and 1-0 lines of \(^{12}\)CO. They argued that \(^{13}\)CO (2-1) line is optically thick in these sources. Subsequently, Plambeck et al (1977) reported the observations of 2-1 and 1-0 transitions of CO in eight molecular clouds, including several dark clouds and obtained similarities in intensities and line profiles for both the transitions as obtained from the different clouds.

More accurate spectra and strip maps (\(T_A^*\) vs. R.A.) of 2-1 lines of \(^{12}\)CO, \(^{13}\)CO and \(^{18}\)O for a variety of molecular clouds have been reported and compared with the equivalent CO(1-0) spectra and strip maps by Phillips et al (1979). They have discussed the behaviour of line widths and spatial extents as a function of line opacity.

The features evident in the observations of CO may be summarised as follows:

i) It extends over a wide region in each source selected.
ii) The lines have widths of several km/s and the peak brightness temperature varies from about 20 to 80K.

iii) In most clouds CO lines are optically thick. The peak brightness temperature of $^{13}$CO is generally found to be one-third of that of CO line.

iv) The central maxima of $^{13}$CO and CO coincide and their spatial variations are similar.

v) $^{13}$CO lines are centred at the same velocities as those of CO lines and generally have linewidths between 1/2 and 2/3 of those of the latter.

b. CS

With the detection of emission from $J = 3-2$ (2.0 mm) transition of $^{12}$C$^{32}$S species in the sources Orion A, W51, DR21 and IRC+10216 Penzias et al (1971) discovered interstellar CS. With this discovery CS is the first molecule containing sulphur that has been detected in interstellar space. The observations on CS from Orion A are most extensive. From a study on these observations they argued that 3-2 transition of CS implies a high excitation rate which can be used to obtain hydrogen densities ($n(H_2)$) for the central regions of the clouds. They obtained $n(H_2)$ values equal to $4.3 \times 10^5$ cm$^{-3}$ for Orion A and $3.5 \times 10^5$ for W51.

Turner et al (1973) first observed that 1-0 (5.1mm) and 2-1 (3.1mm) transitions of $^{12}$C$^{32}$S and its isotopic species $^{12}$C$^{33}$S and $^{12}$C$^{34}$S in a number of interstellar sources which includes Orion A and W3. From a study on these observations they suggested that CS should be one of the best interstellar molecules for probing exci-
tation conditions in interstellar clouds. This is due to its simple and fairly compact energy level structure and numerous detectable isotopic species.

A survey of 1-0 and 2-1 lines of CS with nearly equal beam sizes and high velocity resolution in 32 molecular sources including a variety of source types was made by Linke and Goldsmith (1980).

c. HCN, HCO\(^+\) and \(N_2H^+\):

The first detection of interstellar hydrogen cyanide (HCN) is the observation of its 1-0 (3.4mm) transition from Orion A and other five interstellar sources made by Snyder and Buhl (1971). The 1-0 transition of its isotope H\(^{13}\)CN was also detected in Orion A and Sgr\(^{\prime}\)A(NH\(_3\)). However, the quadrupole hyperfine components could not be resolved which they were able to do in a subsequent observation (Snyder and Buhl 1973) from the central region of Orion A. From the later observations they concluded that 1-0 line profile is dominated by an unsaturated component. Gottlieb et al (1975) reported better quality 1-0 H\(^{12}\)CN and H\(^{13}\)CN line profiles from Orion A, M17, NGC 2264 and NGC 1333. The values for the ratios of the hyperfine-split intensities were given. Theoretical studies with different cloud models were done to explain the observed line brightness temperatures and anomalous ratios of hyperfine-split components.

Turner and Thaddeus (1977) made a survey of the emission lines of \(N_2H^+\) and HCO\(^+\) from 73 sources, including detailed maps of four sources (Orion A, OMC-2, DR21(OH) and NGC6334). They combined the data of \(N_2H^+\) and HCO\(^+\) with the data of HCN and CN available by that
time and made a detailed study of the spatial relationship of these four species. They studied abundance ratios and their spatial variations in terms of ion-molecular formation and destruction processes. They suggested that the degree of ionization of the Orion A may be significantly different from that of other molecular clouds. They concluded that HCN is usually optically thick and HCO\(^+\) is probably intermediate while \(\text{N}_2\text{H}^+\) and CN are probably optically thin in most sources.

Huggins et al (1979) reported the first measurements of the 3-2 lines of HCN (1.1 mm), HNC, and HCO\(^+\) in the Orion molecular cloud. Comparing these lines with the equivalent 1-0 lines in the extended cloud they suggested that fractional abundances for those molecular species are in the range \(10^{-10}\) to \(10^{-9}\) and a molecular hydrogen density \(\approx 3 \times 10^5\) cm\(^{-3}\).

**Cloud Models.**

In the construction of a model of interstellar clouds, the most important point is the fact that the molecular lines have widths of several kilometres per second. At a first glance, one may suggest that the linewidths are due to purely thermal motions of the gas molecules. This can however, be readily discarded due to its following consequences. For example, let us take the \(^{12}\text{CO}\) line from Orion A the linewidth of which is of the order of 7 km\(\text{s}^{-1}\). The thermal velocity component along any direction is given by,

\[
\overline{v}_{\text{th}} = (kT/m)^{1/2}
\]

In the case of a uniform cloud in thermal equilibrium, \(m\) is taken
as the mass of $^{12}$CO and $v_{th}$ is 0.08 kms\(^{-1}\) at 20K. In the case of inhomogeneous cloud the estimated value of $v_{th}$ is 0.3 kms\(^{-1}\). Thus, purely thermal velocities cannot explain the observed line-widths. This conclusion is also true for other molecules. Therefore, to explain the experimental data two different models for the clouds have been suggested viz. (1) collapse model with large scale systematic velocity gradient and (2) turbulent model involving velocity variations comparable to the total observed velocity differences which occur on scales much smaller than the dimensions of the cloud. We shall briefly describe the two models mentioned above.

1) **Collapse Model**.

In this model the cloud is assumed as a pressure-free sphere collapsing radially towards its centre due to its self-gravity. If $\rho(r)$ be the density at a radial distance $r$ from the centre, then the mass of the cloud is

$$M(r) = 4\pi \int_0^r \rho(u) u^2 du.$$  \hspace{1cm} (4)

and the infall velocity will be

$$v(r) = -\sqrt{\frac{2GM(r)}{r}} \frac{1}{2}.$$  \hspace{1cm} (5)

where $G$ is the gravitational constant. Now, we consider the following cases.

i) For the case of a uniform density

$$\rho(r) = \rho_0 \text{ (constant)}; \quad \ldots \text{(6)}$$

$$M(r) = 4\pi \rho_0 \int_0^r u^2 du.$$  \hspace{1cm} \ldots \text{(7)}

$$= \frac{4}{3} \pi \rho_0 r^3.$$  \hspace{1cm} \ldots \text{(7)}
and
\[ v(r) = -\left( \frac{8\pi G \rho_o}{3} \right)^{1/2} r \] ... (8)

Therefore,
\[ v(r) \propto r \] ... (9)

We need not consider the case of density increasing with radius because observations on optically thin lines excluded such a model.

So, we next consider the case
\[ \rho(r) = \frac{\rho_o}{r} \] ... (10)

In that case
\[ M(r) = 4\pi \rho_o \int_0^r u \, du = 2\pi \rho_o r^2 \] ... (11)

and
\[ v(r) = -\left( \frac{4\pi G \rho_o r^2}{r} \right)^{1/2} \] ... (12)

Thus
\[ v(r) \propto r^{1/2} \] ... (13)

In this choice, both the density and velocity are varying with \( r \); the former decreases and the latter increases as \( r \) increases.

We have tried to incorporate this choice with some modification in velocity variation in chapter II to structure the innermost portion of Orion A from the observation on \(^{12}\)CO and HCN.

The third case is
\[ \rho(r) = \frac{\rho_o}{r^2} \] ... (14)

whence
\[ M(r) = 4\pi \rho_o r \] ... (15)

and
\[ v(r) = -\left( \frac{8\pi G \rho_o r}{r} \right)^{1/2} \] ... (16)

so that
\[ v(r) = \text{constant} \] ... (17)
If the cloud is divided into a number of concentric spherical shells, then with this choice of density, the rate of flow of mass through each spherical shell is the same, i.e. the density distribution is stable. This constant velocity model has the difficulty that it leads to rather unphysical looking line shapes.

If a cloud is more centrally condensed than $\rho \propto r^{-2}$, then the velocity increases toward the centre. In that case the wings of the observed line would be formed toward the centre of the cloud while the line centre would be formed at the boundaries. But in any consistent model of a cloud, the observed intensity peaks at the centre of the map and centre of the line must correspond. This correspondence between velocity and position is a key feature of systematic velocity models.

2) **Turbulent model**.

Apart from the collapse model which has been described earlier, there is the possibility for supporting the cloud by supersonic turbulence in which the cloud is modelled as largely empty and containing small emitting elements moving at high velocities. In the context of millimeter line observations it is necessary to define the term turbulence.

In hydrodynamics, turbulence is defined as state of motion with high Reynolds number in which the inertial terms in the equations of motion dominate the viscous dissipation. The velocity field is characterized by fluctuations which though still being governed by the Navier-Stokes equation can be considered as random. In radiative transfer, the term turbulence may be identical with hydrodynamic
turbulence but it may also be a field of acoustic or shock waves or even a velocity field of more regular structure (Treving 1975).

In radiative transfer theory to describe turbulence two important scale lengths have to be considered viz. the photon mean free path \( l \) and the correlation length \( L \) of the velocity field (the characteristic of a typical turbulent element). The turbulent motions may be classified into three categories, viz. (a) microturbulence (b) macroturbulence and (c) mesoturbulence.

Microturbulence implies that the correlation length \( L \) is small compared with the photon mean free path \( l \) \((l/l \rightarrow 0)\). With respect to line formation, the turbulent motions of individual atoms and molecules are uncorrelated and are treated as thermal Doppler shifts which produce a change in thermal velocity. This means that the turbulent velocity enters the calculations in essentially the same manner as thermal velocity.

Macroturbulence implies that the scale length of the turbulent fluctuations is large compared with mean free path of photons \((l/l \rightarrow \infty)\). The consequence is that random and global Doppler shift of the whole line is produced. The result is a broadening of the mean profile with no change in the equivalent width. For a particular correlation length the macroturbulent model is valid only in the limit of very high optical depth and thus not applicable to most of the interstellar molecular turbulence.

The microturbulent and macroturbulent models represent two limiting cases. In reality turbulent fluctuations tend to extend over a wide range of wave numbers and photon mean free paths also
vary widely over the line profile. These conditions produce finite values of \( \frac{L}{l} \) and are represented by a model known as mesoturbulent. The emergent profiles for mesoturbulent models fall between those given by micro- and macroturbulent models.

Till now the actual calculations on spectral line intensities have been confined to microturbulent models. Leung and Liszt (1976) and Liszt and Leung (1977) have performed the calculations on CO and CS.

The most serious objection to the turbulent model is the question whether turbulence can persist the molecular clouds. Arons and Max (1975) have suggested a possible mechanism for support involving hydromagnetic waves. The difficulty of this concept is that the outward pressure due to the magnetic field must be balanced by gravitational forces to keep the condensation stable (Penzias 1975). The density and the diameter of the cloud required to produce the gravitational field needed are too high to be physically realistic.

However, if we assume the existence of turbulence, it is possible with appropriate choice of parameters to fit the main requirements with a turbulent model. It allows the observer to 'see' the centre of the cloud, self absorption can be avoided and the desired linewidth is formed by the velocity distribution of the elements. Arguments in favour of the turbulent were put forwarded. Among those Zuckerman and Evans (1974) have pointed out that there is general agreement between formaldehyde absorption and CO emission velocities in a number of clouds. If the source of continuum radiation
(HII region) were generally in the centre of the collapsing cloud, then the formaldehyde would only absorb in the proximal half of the cloud and exhibit a higher average velocity than the CO which originates from the cloud as a whole. However, Penzias (1975) has given counter arguments against that given above and has concluded that on balance the collapse model is better than the turbulent model. Phillips et al (1979) have also discussed the superiority of the collapse model over the turbulent model in the interpretation of 2-1 lines of CO.

Leung (1978) has discussed in detail the line formation in both the models and the ranges of their validity when both turbulent and systematic velocities are present. He has suggested that under certain conditions both the cloud models may be simultaneously applicable to a cloud. It may be mentioned that Kwan (1978) has constructed a model with microturbulence at the centre and a collapsing mantle on the outside. But in a subsequent study with a large number of clouds, Phillips et al (1979) have found that such a model may be possible only for two sources, M17 and NGC 2024.

In view of the position explained above we have confined our work presented in this thesis to the large systematic velocity gradient collapse model.
Theory of Radiative Transfer:

To use the spectral data for obtaining information about the physical conditions existent in the interstellar cloud it is necessary to have a reliable theory of line formation. We shall describe below briefly the outline of the radiative transfer theory with a large velocity gradient existent in the cloud. Such a theory has been first proposed by Sobolev (1960) and extended further by Castor (1970) and Lucy (1971).

The starting point in the analysis of any spectral line is always the equation of radiative transfer. For this, we consider a spherical cloud and because of its spherical symmetry we need to consider only radiations in a particular direction. We choose this direction as the vector $\hat{z}$ which makes an angle $\cos^{-1} \mu$ with the radius vector $r$ to the point $P$ where we consider the transfer of radiation. Let $I(\nu, r, \mu)$ be the specific intensity defined such that

$$I(\nu, r, \mu) \, d\nu \, d\omega \, dA \, dt$$

is the total energy in a frequency interval $d\nu$ about $\nu$ passing through a solid angle $d\omega$ subtended about an area $dA$ located at position $z$ in a time interval $dt$. The elementary area is perpendicular to the photon direction $\hat{z}$. Then the equation of radiative transfer which specifies the positive or negative alteration of $I(\nu, r, \mu)$ due to the interaction of photons with matter along some path $dz$, is

$$\frac{dI(\nu, r, \mu)}{dz} = -k(\nu, r, \mu) \, I(\nu, r, \mu) + j(\nu, r, \mu)$$

(18)

where $j(\nu, r, \mu)$ and $k(\nu, r, \mu)$ are emission and absorption coefficients.
in units of erg sec\(^{-1}\) cm\(^{-3}\) ster\(^{-1}\) Hz\(^{-1}\) and cm\(^{-1}\) respectively. These are given by

\[ j(v, r, \mu) = j_0(r, \mu) \varepsilon(v) \]  

(19)

and

\[ k(v, r, \mu) = k_0(r, \mu) \phi(v) \]  

(20)

where \(\varepsilon(v)\) and \(\phi(v)\) are respectively the line profiles for emission and absorption normalized to unity and \(j_0\) and \(k_0\), the emission and absorption coefficients at the centre of the line \((v = v_0)\). If complete redistribution of frequencies is assumed,

\[ \varepsilon(v) = \phi(v) \]  

(21)

The transfer eqn. (18) may be rewritten as

\[ \frac{dI(v, r, \mu)}{dz} = k(v, r, \mu) \left[ S(v, r, \mu) - I(v, r, \mu) \right] \]  

(22)

where \(S(v, r, \mu)\) is the line source function defined by

\[ S(v, r, \mu) = \frac{j(v, r, \mu)}{k(v, r, \mu)} \]  

(23)

Eqn. (22) has to be solved subject to the boundary condition that outside the cloud, the mean radiation field integrated over line profile and averaged over angle, i.e.

\[ \langle J \rangle = \int_{4\pi} \frac{d\Omega}{4\pi} \int_{-\infty}^{\infty} dv \phi(v) I(v, r, \mu), \]  

(24)

is equal to the Planck function \(B(v, T_{BB})\) evaluated at the cosmic blackbody temperature \(T_{BB} = 2.7\) K. Integrating eqn. (22), we obtain
\[ I(v, r, \mu) = \exp \left( - \int k(v, r, \mu) \, dz \right) \left[ \int s(v, r, \mu) \ exp \left( \int k(v, r, \mu) \, dz' \right) \ K(v, r, M) \, dz' + C \right] \tag{25} \]

where \( C \) is the constant of integration.

Equation (24) has to be evaluated with the expression for the specific intensity (eqn. 25). This task is exceedingly difficult when the medium of the cloud is stationary or moving without a velocity gradient. Because in that case photons created in the interior of the medium must undergo a large number of scattering before emerging. Hence, the quality of radiation at any point will depend on what happens at the other points. In general, each point is coupled to all other points through the radiative field.

The problem is however, considerably simplified when a macroscopic velocity field with a velocity gradient much larger than the thermal velocities of the molecules exists in the cloud (Sobolev 1960). In this case, because of the Doppler effect, photons can escape from the interior of the medium. Thus, in a spherically symmetric cloud with a large velocity gradient, photons emitted at a certain point are either absorbed within a small distance \( d \sim v_t R / v \) (\( v_t \) being thermal velocity, \( v \) the macroscopic velocity at \( r = R \), the radius of the cloud) or not at all. This is due to the fact that a photon cannot be absorbed by molecules which are more than a Doppler width away in frequency, provided \( v(r) \) is a monotonic function of \( r \). Therefore, with large velocity gradient (LVG) radiative transfer model, the situation at a given point inside the cloud depends little on what happens at other points so
that the transfer of radiation depends only on the local properties.

With the assumption of the large velocity gradient and the assumption of the complete redistribution of frequencies, the source function can be taken out of the integral (23) and mean intensity is obtained as (Castor 1970)

$$\langle J_{ij}(r) \rangle = \left[1 - \beta_{ij}(r)\right] S_{ij}(r) + \beta_{ij}(r) B_{ij}(r) T_{BB}$$  \hspace{1cm} (26)

where $\beta_{ij}(r)$ is the escape probability of a photon in the transition from level $i$ to level $j$ at the radial distance $r$ and $S_{ij}(r)$ is the local source function for the corresponding transition. It is apparent from eqn. (26) that if all photons escape, $\beta_{ij} = 1$ and $\langle J_{ij}(r) \rangle$ is the blackbody radiation field; if none escapes $\langle J_{ij}(r) \rangle$ is the local source function $S_{ij}(r)$.

The source function $S_{ij}(r)$ can be expressed in terms of the Einstein A, B coefficients for spontaneous and stimulated emissions and level populations $n_i(r)$ at the point of radial distance $r$. The expressions for $j_0(r)$ and $k_0(r)$ in terms of these quantities are

$$j_0(r) = \frac{h\nu_0}{4\pi} n_i(r) A_{ij} \hspace{1cm} \text{(27)}$$

$$k_0(r) = \frac{h\nu_0}{4\pi} \left[ n_j(r) B_{ji} - n_i(r) B_{ij} \right] \hspace{1cm} \text{(28)}$$

where $\nu_0$ is the frequency at the centre of the line. Using these eqns. for $j_0(r)$ and $k_0(r)$ and eqn. (21), we get from eqn. (23)

$$S_{ij}(r) = \frac{j_0(r)}{k_0(r)} = \frac{n_i(r) A_{ij}}{[n_j(r) B_{ji} - n_i(r) B_{ij}]} \hspace{1cm} \text{(29)}$$
Use of the relation between A, B coefficients

\[ A_{ij} \mathrel{=} \frac{2\hbar
u^3}{c^2} B_{ij} \tag{30} \]

\[ g_i B_{ij} = g_j B_{ji} \tag{31} \]

where \( g_i \) and \( g_j \) are the statistical weights of levels i and j respectively, gives

\[ S_{ij}(r) = \frac{2\hbar
u^3}{c^2} \left[ \frac{n_i(r)g_i}{n_j(r)g_j} - 1 \right]^{-1} \tag{32} \]

To obtain an expression for the escape probability \( \beta_{ij}(r) \), we introduce a dimensionless parameter, the optical depth \( t(\nu,r,\mu) \) at the point P at frequency \( \nu \) obtained by integrating from P to the boundary of the spherical cloud along the z direction. Then

\[ t(\nu,r,\mu) = \int k_0(z, r, \mu) \phi [\nu - \nu_0 + \frac{\nu_o z}{c} \frac{dv}{dz}] \, dz \tag{33} \]

where it is assumed that the velocity gradient is constant over the range z that contributes significantly to the integral.

If the velocity gradient is large, \( \phi \) is strongly peaked at \( z = 0 \) and then \( k_0 \) can be taken out of the integral. Thus

\[ t(\nu,r,\mu) = k_0(r) \int_0^\infty \phi (\nu - \nu_0 + \frac{\nu_o z}{c} \frac{dv}{dz}) \, dz \tag{34} \]

With the transformation \( x = \nu - \nu_0 \) and \( x' = -x + \frac{\nu_o z}{c} \frac{dv}{dz} \) evaluated at \( z = 0 \), we obtain.
\[ t(x, r, \mu) = k_0(r) \frac{c}{\alpha_0 \nu_0} \int_{-x}^{x} \phi(x') \, dx' \quad \ldots (35) \]

The escape probability in the line, averaged over all angles, is

\[ \beta(r) = \int_{4\pi} \frac{d\Omega}{4\pi} \int_{-\infty}^{\infty} dx \, \phi(x) \exp \left[-t(x, r, \mu)\right] \quad \ldots (36) \]

Introducing the function, \( y \), defined by

\[ y(x) = \int_{-\infty}^{x} \phi(x') \, dx' \quad \ldots (37) \]

with the normalization condition

\[ y(\infty) = 1 \quad \ldots (38) \]

we obtain

\[ \beta(r) = \frac{1}{2} \int_{-1}^{1} d\mu \left\{ 1 - \exp \left[ -\frac{\tau(r, \mu)}{\alpha_0(r, \mu)} \right] \right\} \quad \ldots (39) \]

where

\[ \tau(r, \mu) = k_0(r) \alpha_0(r, \mu) \quad \ldots (40) \]

Using the expression (28) for \( k_0(r) \), \( \tau(r, \mu) \) can be written in terms of the Einstein \( A \) - coefficient and \( n_i \) as

\[ \tau_{ij}(r, \mu) = A_{ij} \frac{n_i^3(r)}{8\pi \nu_{ij}^3} \left[ \frac{n_j(r) g_i}{n_i(r) g_j} - 1 \right] \frac{dv_z}{dz} \quad \ldots (41) \]

In spherical geometry,

\[ \frac{dv_z(r, \mu)}{dz} = \mu^2 \frac{dv(r)}{dr} + (1 - \mu^2) \frac{v(r)}{r} \quad \ldots (42) \]
The excess (above cosmic background) intensity of radiation for the transition \(i \rightarrow j\) is obtained as

\[
\mathcal{J}_{ij}(r, \mu) = \left[ 1 - \exp \left\{ - \tau_{ij}(r, \mu) \right\} \right] [S_{ij}(r) - B(\nu_{ij}, T_{BB})] \quad \text{... (43)}
\]

In order to relate with the observations, a quantity called the brightness temperature, \(T_B(i \rightarrow j)\) for the transition \(i \rightarrow j\) (defined earlier) has been introduced. Using Rayleigh-Jeans formula, the expression for the brightness temperature is obtained as

\[
T_B(i \rightarrow j) = \frac{\lambda_{ij}^2}{2k} \left[ 1 - \exp \left( - \tau_{ij} \right) \right] [S_{ij}(r) - B(\nu_{ij}, T_{BB})] \quad \text{... (44)}
\]

Substituting \(S_{ij}(r)\) from (32) and

\[
B(\nu_{ij}, T_{BB}) = \frac{2\nu_{ij}^3}{c^2} \left[ \exp \left( \frac{\nu_{ij}}{kT_{BB}} \right) - 1 \right]^{-1} \quad \text{... (45)}
\]

we get

\[
T_B(i \rightarrow j) = (\nu_{ij}/k) \left[ 1 - \exp \left( - \tau_{ij} \right) \right] \left[ \frac{n_j(r) g_i}{n_i(r) g_j} - 1 \right]^{-1}
\]

\[
- \left[ \exp \left( \frac{\nu_{ij}}{kT_{BB}} \right) - 1 \right]^{-1}\] \quad \text{... (46)}

In terms of excitation temperature \(T_{ij}\) (eqn. 2) eqn. (46) can be written as (Penzias 1975, Chaisson 1976)

\[
T_B(i \rightarrow j) = (\nu_{ij}/k) \left[ 1 - \exp \left( - \tau_{ij} \right) \right] \left[ \exp \left( \frac{\nu_{ij}}{kT_{ij}} \right) - 1 \right]^{-1}
\]

\[
- \left[ \exp \left( \frac{\nu_{ij}}{kT_{BB}} - 1 \right) \right]^{-1}\] \quad \text{... (47)}

Thus, in order to calculate the brightness temperatures for different rotational transitions at a given point in the cloud,
the populations of various rotational levels at that point have to be obtained. For this, generally radiative and collision-induced transitions are simultaneously considered. \( n_i(r) \) can then be obtained by solving the equation of statistical equilibrium:

\[
\sum_{j=0}^{N-1} P_{ij}(r) = \sum_{j=0}^{N-1} n_j(r) P_{ji}(r)
\]

... (48)

where \( N \) is the total number of levels significantly populated and \( P_{ij} \) is the total probability that can be written as

\[
P_{ij}(r) = A_{ij} + B_{ij} \langle J_{ij}(r) \rangle + C_{ij} \quad (i > j)
\]

\[
= B_{ij} \langle J_{ij}(r) \rangle + C_{ij} \quad (i < j)
\]

... (49)

\( C_{ij} \) being the collision-induced transition probability. Since in molecular cloud the most abundant molecule is hydrogen, collisions of the molecule whose spectra is under study, with \( \text{H}_2 \) are generally considered. In that case

\[
C_{ij} = n(\text{H}_2) R_{ij}
\]

... (50)

where \( n(\text{H}_2) \) is hydrogen molecules per \( \text{cm}^3 \) and \( R_{ij} \) are collision rate coefficients corresponding to the transition \( i \rightarrow j \).

The Einstein \( A, B \) coefficients for the rotational transitions
\( J + 1 \) to \( J \) are given by

\[
A_{J + 1, J} = 16 \ h \ B_0^3 \ c \ (J + 1)^3 \ B_{J + 1, J} \quad \ldots \ (51)
\]

and

\[
B_{J + 1, J} = \frac{32 \ \pi^4 D^2}{3c} \ \frac{J + 1}{2J + 3} \quad \ldots \ (52)
\]

where \( B \) and \( D \) are respectively the rotational constant in cm\(^{-1}\) and the dipole moment in c.g.s. e.s.u. of the molecule. \( B_J, J + 1 \) can be obtained by using the relation (31).

It is evident that the statistical equilibrium equation (48) is a coupled equation for \( n_1 \) and an initial value of it is needed for its numerical evaluation under non-LTE condition. Usually, the initial value which is taken is the thermal population distribution at the particular kinetic temperature. It is also seen from eqn. (49) and (50) that \( n_1 \) values are dependent on the rate coefficients for rotational transitions specially under non-LTE conditions.
A brief Review of previous work:

During the last several years a number of attempts have been made to interpret the spectral lines obtained from interstellar molecular clouds. For this purpose, usually spherical collapse model or microturbulent model, or a hybrid of the two i.e., central microturbulence with a collapsing mantle, for the cloud is chosen. However, till now most of the calculations have been confined to the spherical collapse model. Although some progress have been made on the determination of the physical parameters of interstellar clouds from the spectral data, the situation is yet far from satisfactory. This is mainly due to lack of adequate knowledge about the physical conditions existent in the cloud and also about the uncertainly of the physical processes to be considered for a proper interpretation of the spectral data.

The calculations with the collapse model are comparatively simple and those are based on the radiative transfer theory of Sobolev (large-velocity-gradient model, hereafter LVG model, which represents the actual state of a dense molecular cloud satisfying Jean's criteria. On the other hand, turbulent model has some serious difficulties which cannot be avoided. So much work has been done with collapse model.

Goldsmith (1972) first studied the effects of various collisional processes on the spectral intensity of CO. He included in his calculations radiative transitions. However, radiative trapping process which is important for optically thick clouds was not considered. Only some general conclusions could be drawn from his results.
Putting arguments in favour of the gravitational collapse of molecular clouds Goldreich and Kwan (1974) have studied the formation of molecular lines in a spherically collapsing cloud with a uniform density. Using the LVG radiative transfer model they calculated $T_B$'s and energy loss rates for various rotational transitions of CO, CS and SiO and showed that the most of the observed lines of CS and SiO and stronger lines of CO are optically thick. The rate of energy radiation in the CO lines was found to exceed the rate of work done by the adiabatic compression of the collapsing gas which, in turn, requires an energy source inside the cloud to maintain the temperature of the gas against the cooling. One source suggested by them is the collisions between gas molecules and warm dust grains, the latter being heated by radiation from HII regions and protostars in the centre of the cloud. Using the same radiative transfer model Scoville and Solomon (1974) also studied excitation of CO and CS lines with a plane-parallel cloud geometry of constant density. They noticed that even when the spontaneous decay rates ($\Lambda$) are greater than collision rates ($C$) and $\tau > 1$, the excitation temperature is dependent on $n(H_2)$ and totally independent of $\Lambda$. Lucas (1974) solved radiative transfer and statistical equilibrium equations in the case of a static slab, with uniform temperature, density and velocity dispersion. Clark et al (1974) first attempted to model the innermost portion of the Orion A cloud by using the observations of HCN. But as they considered a static model and lines from only one molecule, their results are somewhat uncertain.
Gerola and Sofia (1975) first attempted to determine the structure of Orion A cloud on a realistic basis. They considered 1-0 and 2-1 lines of CO (Phillips et al. 1973) and 1-0 line of HCN (Snyder and Buhl 1973). By considering the simultaneous existence of a velocity field increasing outward and density increasing inward they tried to interpret the above lines of CO and HCN. They were, however, moderately successful in obtaining a model for the Orion A cloud which could explain the experimental data available at that time. Gerola and Sofia (1975) had the additional difficulty as at that time no reliable data for the collisions rate coefficients were available an accurate knowledge of which is important.

de Jong et al. (1975) used an interesting approach to study the sensitivity of spectral line intensities to the density and velocity distributions in the cloud. They constructed a constant velocity model with density varying as the inverse square of the distance and compared its results with the model of constant density with velocity varying directly with the distance. They studied with the data of 1-0 and 2-1 lines of CO. The $H_2$- CO collision rates calculated by Green and Thaddeus (1976) were used in the calculations with an extrapolation to high j-levels. From their study they concluded that with the collapsing models in which both density and velocity gradients simultaneously occur the observed CO lines can be interpreted. They found that the ratio of the intensities of 2-1 and 1-0 CO lines in Orion A is consistent with such models.

The observations of 2-1 and 1-0 lines from Orion A reported by Wannier et al. (1976) show that the brightness temperatures of the
two lines are almost equal so that their ratio is close to unity almost throughout the cloud. The model proposed by Gerola and Sofia (1975) cannot explain this experimental observation. In chapter II of this thesis we have attempted to obtain a structure of Orion A based on the spherical collapse model which may explain the observations.

From a study on the observations of lowest three rotational transitions of CS with the spherical collapsing model Liszt and Linke (1975) calculated the limiting values of $n(H_2)$ in Orion A, DR21 and W51. With the same cloud model Phillips and Huggins (1977) calculated $n(H_2)$ near the centres of the same three clouds from the observations of CO. They obtained $n(H_2)$ values much lower than those estimated by Liszt and Linke (1975) from the data of CS. Particularly, for Orion A the deviation is remarkable. One of the reasons for this discrepancy suggested by them is the influence of electron-molecule collisions in addition to that with H$_2$ on the spectral intensity. The magnitude of this influence is dependent on the dipole moment of the molecule and the concentrations of electrons with respect to H$_2$ ($X_e$). As the dipole moment of CS is much higher (about 20 times) than that of CO, it gives a higher value of $n(H_2)$ if the effect of electrons is neglected. They also pointed out that clouds having hot centres are often associated with highly reddened IR sources which may be associated with internal sources of ionizing radiation such as Orion A. This may be the reason for the largest discrepancy found in the case of Orion A. Considering the influence of electrons they estimated a value of
\[ S \times 10^{-4} \] for \( X_e \) near the centre of Orion A. Recently Plambeck and Williams (1979) calculated average densities of \( H_2 \) in a number of molecular clouds from the observations of the very weak polar molecule CO and its isotopes. They also found that the densities determined from CO are much lower than those estimated from the strongly polar molecules. Hydrogen densities in molecular clouds from the data on strongly polar molecules have also been estimated by Turner and Gammon (1975), Gottlieb et al (1975), Evans et al (1975), Wotten et al (1978), Huggins et al (1979) and Linke and Goldsmith (1980). Their estimated values are also found to be much higher than those obtained from CO (Chapter III, Section B). From the above discussions it is clear that a systematic investigation on the effect of electron-molecule collisions on the spectral lines obtained from molecular clouds is necessary. This study may help in the explanation of a number of anomalies and discrepancies which exist in the interpretation of spectral data.

Dickinson et al (1977) have investigated in some detail the effect of electron-molecule collisions on the spectral data of HCN. For simplicity of the calculations they have considered only the optically thin case. They have considered the effect of electron-molecule collisions on the intensity ratio of 1-0 and 2-1 lines of HCN as function of electron abundance and hydrogen density. The results show that the ratio increases due to electron-molecule collisions. However, in many cases, the spectral lines of HCN are optically thick (Turner and Thaddeus, 1977) so that it is necessary to assess the effect of electron-molecule collisions in optically thick clouds. This has been attempted in Chapter III.
The rate coefficient for electron-molecule collisions is dependent on the density of electrons so that a knowledge of the latter is necessary. Although a few attempts have been made to estimate the densities of electrons in molecular clouds, the estimates made by different workers vary widely amongst themselves. Oppenheimer and Dalgarno (1974) have estimated the value of $X_e \approx 10^{-6}$ whereas on the basis of deuterium enhancement of the interstellar molecules and gasphase ion-molecule reactions some workers (e.g. Watson et al 1978; Guelin et al 1977, Wootten et al 1979) have estimated the upper limit of it in a number of molecular clouds as $10^{-8}$ to $10^{-7}$. Chaisson (1973) has estimated an upper limit of $8 \times 10^{-4}$ in Orion nebula. Phillips and Huggins (1977) have also suggested a comparatively high value of $X_e$ near the centre of Orion A.

Since, for polar molecules the effect of electron may be significant in some clouds, the observations on these molecules can be used to estimate electron density in such clouds provided hydrogen density can be obtained from another source, e.g. from the observations on weakly polar molecules. An attempt to estimate $X_e$ by following the procedure described above has been made in Chapter III (Section B).

Studies on the interpretation of the spectral lines have also been started with the turbulent model. Leung and Liszt (1976) dealt rigorously the excitation and radiative transfer of CO in a microturbulent, spherical medium. They constructed theoretical models for giant molecular clouds associated with HII regions and for simple dark dust clouds, using static, spherical models and a microturbulent velocity field and compared their results with the
available observations. The agreement of their results with many general features of CO implies that turbulent gas motion could be an important mechanism for line broadening but, as they concluded, this does not rule out the possibility of the existence of systematic velocity gradients. Later, they (Liszt and Leung 1977) performed a similar study of CS and estimated fractional abundance and central densities lying in the ranges $2 \times 10^{-10} \lesssim X_{CS} \lesssim 2 \times 10^{-9}$ and $5 \times 10^{4} \lesssim n(H_{2}) \lesssim 2 \times 10^{5}$ respectively. Following Zuckerman and Evans (1974), Baker (1976) studied CO lines from massive molecular clouds in large-scale turbulent (macroturbulent model) with the assumption of spherical shape of the clouds. He suggested that magnetic pressure probably supports the cloud and the slow contraction of the cloud due to neutral particle drift through the magnetic field can be the source of turbulent energy.

Molecular line formations have also been studied with the simultaneous existence of both systematic and turbulent velocities. Lucas (1976) studied CO line formation by considering simultaneously both microturbulence and a small velocity gradient. He presented CO line profiles for model parameters.

Kwan (1978) in his study on the line profiles of CO, $^{13}CO$ and CS from M17 and Kleinmann-Low Nebula noticed that these observations can be best reproduced by a cloud model having a turbulent core with a collapsing mantle, i.e. turbulence dominates the central part and collapse at the outer part. According to him, the $^{12}CO$ lines observed from such a cloud will be blueshifted because of the absorption of the redshifted side of the emission from the core by
the near-side cold collapsing gas. Later, in search of the possibility of the existence of different velocity structures in molecular clouds, Phillips et al (1979) made a systematic study on the observations of CO from a number of clouds. From the variation of line shape and mapsizes with CO line opacity they found a monotonic increase of linewidths and mapsizes with opacity which they have taken as evidence for central condensation. The hybrid model of Kwan (1978) although found to be possible for the case of two sources, M17 and NGC 2024, cannot be taken as universally applicable.

Though the systematic velocity gradient and turbulent models are basically different, White (1977) in his study on CO lines in both the models with same parameters showed that CO line intensities calculated by these two models had little difference. A similar conclusion has also been drawn by Linke and Goldsmith (1980) in their study of CS. They found that the two models give more or less the same antenna temperature for the three lowest transitions.