Astrophysical Exercises: Excitation and Emission of a Molecular Cloud

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1. Physical Background

In the interstellar medium one finds a variety of regions with densities higher than the surroundings. In these ”clouds” the gas is mainly in molecular state. The molecules possess a number of rotational and vibrational energy states, transitions between which are caused by collisions with other molecules and by absorption and emission of photons of the ambient radiation field. This radiation field is partly due to external sources — such as stars — but also affected by the absorption and emission of the molecules themselves. Thus the state of excitation of the molecules is the result of the interaction of radiation and matter, which has to be solved consistently. Once one knows how many molecules are in each energy level, one can compute the spectrum emitted by the cloud.

We shall consider a simple model of a spherically symmetric cloud composed of H_2 and CO, the most abundant molecules. The excitation of the rotational energy levels of CO molecules at the centre of the cloud are to be computed by taking into account all collisional and radiation processes. In principle, the population of the energy levels and the radiation field depend on the position in the cloud, e.g. near the outer rim the radiation field is more like the external one, and the excitation could be higher than near the centre, where the external radiation has been attenuated by absorption of the outer layers. We shall not attempt to solve this, as it would be very time consuming. We rather assume that the state of the molecules at the centre is more or less representative for the whole cloud. Then the computation of the radiation field at the centre becomes rather simple. Then the solution of the level populations consistent with the radiation field can be done within reasonable time.

Our aim is to investigate how the CO's level populations depend on the basic parameters of the external radiation field and of the clouds, i.e. the gas density and the cloud radius. In particular we look for maser effects, and find those conditions under which there are population inversions in the CO molecule. To do this, one is not so deeply interested in details, say the exact shape of the emission line profiles, but one must to be able to search through parameter space reasonably quickly. This is why we limit ourselves to a rather unsophisticated model.

2. The Equations

2.1 The Level Populations

The molecule's energy levels shall be numbered 1, 2, 3, ... with the energies E_1, E_2, E_3, ... Then let n_i be the number per unit volume of those molecules that are in state i.

To compute the level populations $\{n_i\}$ we first consider how the number of molecules in a level i is changed by the processes that change the molecule's state from i to k. Let the rate R_{ik} be the number of these transitions per unit time. Then $n_i R_{ik}$ is the number of transitions $i \to k$ per unit time and volume, which cause a de-population of the level i. But likewise, this is the populations rate of level k. Summation over all levels k gives the total rate of change:

$$\frac{dn_i}{dt} = \sum_{k \neq i} n_k R_{ki} - n_i \sum_{k \neq i} R_{ik} \tag{1}$$

where the first sum is over all populating transitions and the second over all de-populating processes.

If we look for the equilibrium solution — i.e. we assume that all parameters of the model do not change within the typical timescale of any of the transitions: R_{ik} is the inverse timescale for the process $i \to k$ — we demand that for all levels the population is constant $dn_i/dt = 0$ for all i. Then the system of rate equations (Eq. 1) is a homogeneous system of linear equations for the number densities, which would have an infinite number of solutions. The constraint that the total number of CO molecules in all levels must be constant, as for a given chemical abundance ϵ_{CO} and a (total) gas density n_{gas}, supplies the missing equation. If one substitutes any single rate equation by the conservation of numbers equation

$$\sum_i n_i = n(CO) = \epsilon_{CO} n_{gas} \tag{2}$$

one now has a set of n equations for the n unknown level populations, which yields a single solution.

2.2 The Rate Coefficients

The rate coefficient for excitation ($i < k$) is the sum of the absorption rate in the line $i \to k$ and of excitation by collisions with other particles (here these are H_2 molecules):

$$R_{ik} = B_{ik} J_{ik} + C_{ik} \tag{3}$$

Processes that lead to deexcitation ($i > k$):

$$R_{ik} = A_{ik} + B_{ik} J_{ik} + C_{ik} \tag{4}$$

are: Spontaneous (A) and stimulated (B) emission of a line photon, and collisional de-excitation (C).

Between the three radiative rate coefficients the well-known Einstein relations exist, which are purely atomic constants and independent of the physical conditions which the molecules are subjected to. For $i > k$:

$$g_i B_{ik} = g_k B_{ki} \tag{5}$$

$$A_{ki} = \frac{2h\nu_{ik}^3}{c^2} B_{ki} \tag{6}$$

Because of this, we need to know only the spontaneous transition rate A for all the lines (see below). Here, g_i is the statistical weight of level i, e.g. for a rotational quantum number J one has $g = 2J + 1$. ν_{ik} is the centre frequency of the line, with an energy $h\nu_{ik} = E_k - E_i$. This apparently inconsistent designation is chosen, as a negative frequency does not make sense physically. The other quantity J_{ik} is the mean intensity of the line $i \rightarrow k$, integrated over the all frequencies, i.e. over the line profile (see below). Naturally, we have $J_{ik} = J_{ki}$.

For the collisional rate coefficients there is a generally valid relation:

$$g_i C_{ik} = g_k C_{ki} \exp(-\frac{h\nu_{ik}}{kT_{kin}}) \tag{7}$$

which involves the kinetic temperature of the colliding particles which is the mean kinetic energy of the H_2 molecules. In interstellar clouds one has $T_{kin} = 10...100$K.

2.3 The Collisional Deexcitation Rate

To compute all collisional rates, we only need to know the deexcitation rate C_{ki} for $i < k$. This is either computed from a quantum mechanical treatment of the collision of a CO and a H_2 molecule, or measured experimentally. We shall make a very crude approximation, which is not too far from the truth: $C_{ki} \approx N\sigma v$. Here N is the number density of the H_2 molecules, σ is the collision cross section, and v the relative velocity between CO and H_2 particles.

The cross section will be of the order of the geometrical cross section: $\sigma \approx (1\text{Å})^2 = 10^{-20}\text{m}^2$ for **all** transitions.

The relative velocity is about the thermal velocity $v = \sqrt{2kT_{kin}/m}$, where m is the mass of a H_2 molecule.

2.4 Energy Levels and Molecular Data

The differences between the energies of successive levels having rotational quantum numbers J and $J + 1$ ($J = 0, 1, 2, 3, ...$) are computed from

$$E_{J+1} - E_J = h\nu_{J,J+1} = 2hB_0(J + 1) \tag{8}$$

using the rotational constant $B_0 = 5.78975\,10^{10}$ Hz of the CO molecule. The Einstein A-value, or spontaneous emission rate for this transition one gets from:

$$\begin{aligned} A_{J+1,J} =& \frac{(J+1)^4}{2J+3}\frac{128}{3}\frac{\pi^3}{hc^3\epsilon_0}\mu^2 B_0^3 \\ =& \frac{(J+1)^4}{2J+3} 1.046\,10^{21}\ \nu_{J+1,J}^3\ \mu^2 \end{aligned} \tag{9}$$

using the electrical dipole moment $\mu = 0.112\,\mathrm{Debye} = 0.112\ 3.333\,10^{-30}\mathrm{Cbm}$ of the CO molecule. All other transitions (e.g. $J+2 \rightarrow J$) are forbidden for electrical dipole radiation, and the A-values for magnetic dipole or electric quadrupole radiation are smaller by many orders of magnitude. We shall neglect them here.

2.5 Mean Intensities

Assuming an homogeneous and isotropic spherical cloud, the mean intensity at the centre of the cloud is

$$J_{ik} = I_{ik}^0 \exp(-\tau_{ik}) + S_{ik}(1 - \exp(-\tau_{ik})) \tag{10}$$

where I_{ik}^0 is the intensity of the external radiation which we assume to hit the clouds surface from all directions. This could be equal to the cosmic background radiation $B_\nu(\nu_{ik}, T_{BG})$ with $T_{BG} = 3\mathrm{K}$. $\tau_{ik} = \kappa_{ik} R$ is the optical depth of the cloud in the line $i \rightarrow k$, as measured from the surface to the centre. $S_{ik} = j_{ik}/\kappa_{ik}$ is the source function of the line.

2.6 Line Absorption and Emission Coefficients

As we had assumed the cloud to be homogeneous, both the absorption (κ) and emission (j) coefficients are equal throughout the cloud. We compute them at the centre of the cloud from the number densities of the CO molecule in the relevant energy levels. We make a further simplification by assuming that all lines have the same simple box-like shape, the relative width $\Delta\nu_{ik}/\nu_{ik} = b$ being the same for all ik. Then we have for $i > k$

$$\kappa_{ik} = \frac{h\nu_{ik}}{4\pi\Delta\nu_{ik}}(n_k B_{ki} - n_i B_{ik}) \tag{11}$$

and for the emissivity

$$j_{ik} = \frac{h\nu_{ik}}{4\pi\Delta\nu_{ik}} n_i A_{ik} \tag{12}$$

2.7 The Emergent Spectrum

Since the radiation emerging at the surface of the cloud — for simplicity we taken only the one line-of-sight through the centre — also has a contribution from the external radiation field entering at the other side, one gets:

$$I_{ik}^{em} = I_{ik}^{0} \exp(-2\tau_{ik}) + S_{ik}(1 - \exp(-2\tau_{ik})) \tag{13}$$

3. Method of Solution

The system of rate equations (Eq. 1) together with the conservation of particles (Eq. 2) yields a system of linear equations for the unknown number densities. This is easily solved by Gauss' method of elimination. A FORTRAN program can be provided.

Since the radiative rates depend on the population numbers, the combined system of rate equations, optical depths, and mean intensities is a non-linear system. So starting from N, R, T_{kin}, b, and ϵ_{CO} we cannot compute the population numbers straight away. We shall use a fix-point iteration, solving in succession the rate equations, then the intensities, then again the rate equation, and so on, until the level populations become sufficiently stable.

If we were to do this right away, the iteration would show a very slow convergence indeed. But since the mean intensities can be written as relatively simple expressions, one can insert the J_{ik} into the rate equations. Some terms cancel out, leaving the net-rate equations which yield the same solution as the full equations. Without derivation we note that one gets these net-rate equations by substituting

$$A_{ik} \rightarrow A_{ik} \exp(-\tau_{ik})$$

$$B_{ik} J_{ik} \rightarrow B_{ik} I_{ik}^{0} \exp(-\tau_{ik})$$

everywhere.

Despite this trick, the convergence behaviour for certain values of (N, R) is rather bad. The radius of convergence becomes rather small. Do make tests with a 2 level molecule, and study the convergence. A remedy is the application of a dampening of the solution: If one gets with the old n_i^{old} the solution n_i^{new}, then we won't take for the next step not the new values n_i^{new}, but $n_i = \sqrt{n_i^{old} n_i^{new}}$ for all i. With this technique, it should be possible to get convergence to 10^{-3} relative accuracy in the number densities within a some dozens of iterations.

3.1 Program Structure

(1) Prepare all molecular data
(2) Input and calculation of all physical parameters
(3) Make an initial guess for the $\{n_i\}$
(4) Compute the intensities, radiative rates, collisional rates. Fill the matrix of coefficients for the linear equations.

(5) Solve the system of rate equations.

(6) Checks on the iteration:
on convergence ($\sum_i |\Delta n_i/n_i| < 10^{-3}$?)
on maximum number of iterations.
If the accuracy is not good enough and the number of iterations is less than the maximum permissible number, then goto Step (4).

(7) If convergence accuracy is acceptable: Output of results, etc.

(8) In case one scans through the parameter space, now set the parameters for the next model. Goto Step (3).

4. Hints, Kinks, and Tests

4.1 General Notes on Program Design

0. Before actually writing the program, do make a flow chart diagram in order to understand the sequence of what is computed; a diagram of the program structure and the data structure to find out, how the loops and iterations are nested, which data from earlier parts you need at each section, which kind of vectors and arrays you are going to need. This may seem bureaucratic, boring or even old fashioned, but **don't start typing anything, before you are absolutely clear about what you plan to do**. Otherwise you may really end up wasting much time in trying to find the logical errors, loopholes, and cul-de-sacs of your hasty programming. Save yourself the frustration, disappointment, and anger!
1. General Program Planning: It is a good idea to lay out the program as general as possible. This makes it easier to include other effects, or to try out other situations. E.g. keep the number of levels as a parameter which is assigned a value in the main program, rather than being specified everywhere in the loop limits. Checking the program for other numbers of levels can thus be done easily at any time. Or one can try out how many levels are really necessary for a paricular model and accuracy.
2. Modular Construction: It is also a good idea to break up the program into mathematically or physically sensible units. This allows a better testing of these individual modules — and most of the time is spent in tracing an error — a more flexible use of them for other purposes, and their exchange against improved or alternative methods, improved data, other physical processes, etc. For example, if the solution of the system of linear equations is contained in an independent unit, one simply exchanges this against a more sophisticated method, if need arises, but without the trouble of having to change the program at a dozen places. For testing, a simple main program has to be written which supplies the neccessary input data to this unit.
3. Check Everything by Hand: Often, we understimate our ingenuity to make small logical mistakes or simple typing errors, which may cause faulty results. The worst kind of mistakes are those which produce results that look as one would

expect them to be. Take the trouble of check everything the program does, until you are sure it does only what you want it to do. In programs about physical things, basic physics must be obeyed: conservation of particles, energy, etc. Also, all the simple and limiting cases which we do understand, must be reproduced accurately.

4. Be Highly Skeptic of anything the program produces.
5. Be Careful with the indices: (I,J) is easily confused with (J,I), so is I and 1. If one tries to find the origin of some error in the results, one may **never** notice in the program's listing that the two letters were interchanged. Thus, just merely writing (J,K) is preferable to (I,J).
6. When you are making tests, and later running the program for various situations and parameters, try to keep a careful written record of what you do, noting input parameters and results. This will make it easier for you later to compare results with earlier ones, in case you have to hunt for an error that has crept in yesterday when you "just changed a few things, almost nothing — but the program doesn't work any more".

4.2 Iterations

Fortunately this program has only one iteration. But nonetheless it is a good idea to take measures to prevent the iteration to hang up into an eternal loop: Therefore one should not just check the accuracy, but also specify a maximum number of iterations, after which there will be a control output for the next (say) 10 iterations, after which the program is halted. In this way one gets important information about the iteration's behaviour if ever something makes the program to take more than the usual number of steps. This control output should give all relevant information. Sometimes it is better to have printed out more than really necessary. This pertains not only to the testing phase of the program, when one still has to hunt for the errors one has programmed in, but also for the production phase, especially if one wants to try out a different molecule, and uses the program in situations it has not yet tested with.

4.3 Excitation Temperature

To judge the behaviour of any transition ($i \to k$, $i > k$), it is useful to define the excitation temperature $T_{ex}(i,k)$ of the line:

$$\frac{n_i}{n_k} = \frac{g_i}{g_k} \exp(-\frac{E_i - E_k}{kT_{ex}}) \tag{14}$$

Note that the excitation temperature may be larger than the kinetic temperature T_{kin}. In this case one speaks of suprathermal excitation. If population of the upper level is even stronger, the excitation temperature increases, and may even become negative. Then one has an population inversion. Note that the absorption coefficient is negative, so is the optical depth. This leads to an **amplification** of the external radiation field rather than an attenuation: the cloud has become a maser amplifier.

4.4 Limiting Cases

Here are some limiting situations which are useful for testing whether the whole program converges to the correct solutions:

(a) Optically thin cloud (small R) and little collisional excitation (small N): Then the excitation temperatures of all transitions should be equal to the temperature of the external radiation field, since it completely dominates the rates of all transitions and is thus responsible for the population of the energy levels. $T_{ex}(i,k) = T_{BG}$ for all i, k.

(b) Optically thick cloud (large R): When the cloud is opaque in all transitions, the radiation field at the centre is only due to what the local molecules radiate themselves. The net radiative rates are all zero, and only the collisions are responsible for the populations of the levels. As can be ascertained from (7), then the excitation temperatures of all transitions are equal to the (local) kinetic temperature. $T_{ex}(i,k) = T_{kin}$ for all i, k.

(c) Collisionally dominated case (large N): When the density is increased, the collisional rates will eventually surpass all radiative rates. So collisions will set up the level populations, and the excitation temperatures of all transitions will equal the kinetic temperature. $T_{ex}(i,k) = T_{kin}$ for all i, k.

4.5 Computing a Series of Models

Since the population numbers n_i for the limiting cases can be easily calculated, and actually the iteration usually converges there quickly, it is advisable to compute always a series of models, starting at one of the limiting cases, then changing the model parameters in small steps, while using the solution of the previous model as the starting guess for the n_i in the next model.

5. Tasks

(1) For which values of the parameters (R, N, T_{kin}) one gets in the $J = 1 \rightarrow 0$ line a population inversion, i.e. a maser?

(2) Are these masers "strong", i.e. how large is the negative optical depth, and is the amplification factor $e^{-\tau}$ much greater than one?

(3) The reason for the population inversion is the fact that whereas collisions can cause a change between any two energy levels of the CO molecule, radiative processes affect only transitions between neighbouring levels. Since the spontaneous rates A increase for higher energy levels, molecules will tend to get stuck at higher levels, like in a traffic jam.

(4) If this explanation is true, changing the dependence of the Einstein A-values with angular quantum number J should could produce bigger or smaller traffic jams,

thus bigger or smaller population inversions. Can you make a maser with an amplification factor of say 2 or 10? Try it! Everything is allowed for changes in the molecular constants, energy levels, and collisional rates.

```
      SUBROUTINE SOLVE(N, IERR)
C=============================================================
C    PROGRAM TO SOLVE THE SYSTEM OF LINEAR EQUATIONS:
C
C         SUM( A(I,J) X(J) ) = B(I)
C
C          BY GAUSSIAN ELEMINATION
C-------------------------------------------------------------
C    INPUT:   A( , ), B( ), N
C    OUTPUT:  B( ), IERR
C
C    ERROR CODE:   IERR = 0   EVERYTHING O.K.
C                       = 1   MATRIX HAS ZERO DETERMINANT
C
C    NOTE: MATRIX A AND VECTOR B ARE MODIFIED BY THE PROGRAM
C-------------------------------------------------------------
      DOUBLE PRECISION A,B,BIGA,SAVE
      COMMON /S1/ A(10,10), B(10)
      DATA  TOL  / 1.0D-30 /
C
      N1   = N-1
      N2   = N*N
      IERR = 0
C
C        GOING THROUGH ALL COLUMNS...
C
      DO 50 J = 1, N
C
C        FIND THE EQUATION WITH THE BIGGEST MATRIX ELEMENT
C
      BIGA = 0.0D0
      DO 10 I = J, N
      IF(DABS(BIGA) .LT. DABS(A(I, J))) THEN
        BIGA = A(I, J)
        IMAX = I
      ENDIF
10    CONTINUE
C
C         THE MATRIX IS NOT REGULAR!
C
      IF(DABS(BIGA) .LE. TOL) THEN
        IERR = 1
        RETURN
      ENDIF
```

```
C
C        EXCHANGE THE PRESENT EQUATION WITH THE ONE WITH THE
C        BIGGEST ELEMENT, AND DIVIDE ALL COEFFICIENTS BY BIGA
C
      DO 20 K = J, N
      SAVE       = A(IMAX, K)
      A(IMAX, K) = A(J, K)
20    A(J, K)    = SAVE/BIGA
C        ...AND THE VECTOR AS WELL
      SAVE       = B(IMAX)
      B(IMAX)    = B(J)
      B(J)       = SAVE/BIGA
C
C        NOW REDUCE ALL EQUATIONS 'BELOW' THE PRESENT ONE
C
      IF(J .LT. N)   THEN
        J1 = J+1
        DO 40 I = J1, N
        DO 30 L = J1, N
30      A(I, L) = A(I, L) - (A(J, L)*A(I, J))
40      B(I)    = B(I)    - (B(J)   *A(I, J))
      ENDIF
50    CONTINUE
C
C        FILL B-VECTOR WITH THE SOLUTION
C
      DO 60 I = 2, N
      J  = N+1-I
      J1 = J+1
      DO 60 K = J1, N
60    B(J) = B(J) - A(J, K)*B(K)
      RETURN
      END
```