6TH SEMESTER PROJECT REPORT

RADIATIVE TRANSFER MODELING OF PRESTELLAR CORE

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I am thankful to my project group members for their helping me out with doubts.

Finally, I would like to thank my peers and seniors for their constant support during these rough times.

Abstract

In this project, various radiative transfer models where studied under multiple conditions and parameters. The models are basically python codes built to run simulations and get the desired result. The codes are computationally expensive as they include various complexities to be as realistic as possible. Equations of radiative transfer have application in many fields including optics, astrophysics, atmospheric science, and remote sensing.

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1

Introduction

1.1 Radiative transfer

Radiative transfer is the phenomenon of transfer of thermal energy in the form of electromagnetic radiation[1]. The propagation of radiation through a medium is affected by absorption, emission, and scattering processes by the intermediate medium. The equation of radiative transfer describes these interactions mathematically.
Flux(F_ν) is defined as energy passing through a unit area per unit time per frequency.

$$F_\nu = \frac{dE}{d\nu.d\sigma.dt}$$

dE is the energy from the source, F_ν is frequency, $d\sigma$ is the area element and dt is time
We define a term, "Specific intensity" which is also referred as spectral radiance, is a fundamental quantity in radiative transfer, denoted by I_ν and defined as:-

$$I_\nu = \frac{dE}{dt.d\nu.d\sigma.d\omega} \tag{1}$$

where, $d\omega$ is the solid angle.

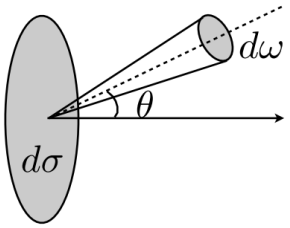

Figure 1

[1]https://en.wikipedia.org/wiki/Radiative_transfer

θ equals to angle between dA and the ray for which we measure I_ν, which implies,

$$F_\nu = \iint I_\nu cos\theta \, d\omega$$

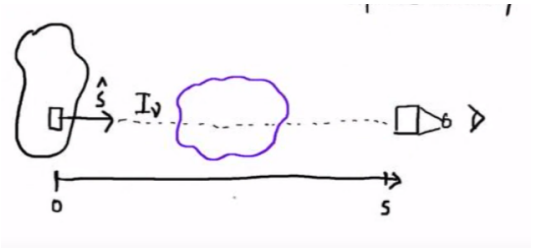

Figure 2

The physics involved in I_ν in the figure 2 is determined by the radiative transfer equation,

$$\frac{dI_\nu}{ds} = j_\nu - a_\nu . I_\nu \tag{2}$$

where,
s is the distance.
j_ν is the emission coefficient, which is function of s).
$a_\nu . I_\nu$ is the absorption scattering term, which is function of I_ν at that point.
In the absence of sources and sinks (perfect vacuum), intensity along a ray s is a conserved quantity. Therefore,

$$\frac{dI_\nu}{ds} = 0$$

In any medium, there will be emission and absorption (and possibly scattering) along any ray s. The emission coefficient j_ν is energy emitted over unit time per frequency in a specific direction from a unit volume.

$$j_\nu = \frac{dE}{dt.d\nu.dV.d\omega}$$

Absorption coefficient a_ν is the energy absorbed per unit time, which depends on the density of the medium as well as its ability to absorb, known as opacity.

$$a_\nu = \rho . \kappa_\nu$$

The source function is defined as the ratio of the emission coefficient to the absorption coef-

ficient.

$$S_\nu = \frac{j_\nu}{\alpha_\nu} \tag{3}$$

In a case where there is no emission,

$$dI_\nu = -\alpha_\nu I_\nu . ds \tag{4}$$

The equation (4) has the following solution,

$$I_\nu(s) = I_{\nu 0} . e^{-\alpha_\nu . s} \tag{5}$$

We define a term- optical depth τ_ν which is,

$$\tau_\nu = \int \alpha_\nu(s) . ds \tag{6}$$

From (2) and (3) we get,

$$\frac{dI_\nu}{d\tau} = S_\nu + I_\nu \tag{7}$$

which has the solution-

$$I_\nu(\tau_\nu) = I_{\nu_0} e^{-\tau_\nu} + \int_0^{\tau_{\nu 0}} S_\nu(\tau'_\nu) . e^{-(\tau_\nu - \tau'_\nu)} \, d\tau'_\nu \tag{8}$$

The first term is the background intensity attenuated by the medium (exponential term) and the integral term is due to the medium emission attenuated by exponential term due to self absorption. This equation is not trivial to solve because the source function is a function of the optical depth. An analytic solution exists only for the case where emission and absorption is not function of τ_ν, then the integration simplifies,

$$I_\nu(\tau_\nu) = I_{\nu_0} e^{-\tau_\nu} + S_\nu(1 - e^{\tau_\nu})$$

$\tau \gg 1$ optically thick medium : leads to $I_\nu \approx S_\nu$
$\tau \ll 1$ optically thin medium : leads to $I_\nu \approx I_{\nu 0} + I_\nu . S_\nu$

1.1.1 Black Body radiation

The medium in thermodynamic equilibrium will emit radiation with a spectrum which is a function of temperature and frequency only. This thermal radiation is known as blackbody radiation.

$$S_\nu(\text{at LTE}) = B_\nu$$

An object which is non-reflective and opaque (not transparent) is a blackbody and emits blackbody radiation.
By Planck's law,

$$B_\nu(T) = \frac{2h\nu^3}{c^2}[\exp(h\nu/K_bT) - 1]^{-1} \tag{9}$$

1.2 Line processes

Let us consider a two level system,

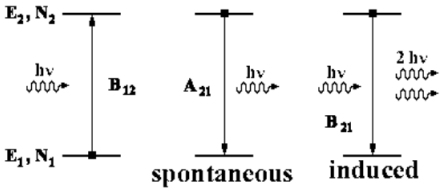

Figure 3

Let ni and nj are the populations of the energy levels i and j and Rij and Rji are transition rates between levels i and j. At statistical equilibrium,

$$n_i \sum_j R_{ij} = \sum_j n_j R_{ji} \tag{10}$$

The transition rates contain contributions from: There are three basic processes spontaneous emission, absorption, and stimulated emission. These processes are described statistically by the Einstein coefficients, Aij, Bji, and Bij respectively. The Einstein coefficients give how often the transition happens for a single state. It also has contributions from collisional excitation and dexcitation ($n_{col}.C_{ij}$). Rij in equation(10),

$$R_{ij} = n_i B_{ij} \int_0^\infty J_\nu \varphi_{ij}(\nu).d\nu$$

where $\varphi_\nu(\nu)$ is the line profile function (explained later), and J_ν is defined as the integral of the

specific intensity I_ν over the source of emission:

$$J_\nu = \frac{1}{4\pi} \int I_\nu d\omega$$

Now, (10) becomes,

$$n_i \left[\sum_j (n_{col} C_{ij} + B_{ij} \int_0^\infty J_\nu \varphi_{ij}(\nu).d\nu) + \sum_{j<i} A_{ij} \right] = \sum_j n_j (n_{col} C_{ij} + B_{ji} \int_0^\infty J_\nu \varphi_{ji}(\nu).d\nu) + \sum_{j>i} n_j A_{ji} \tag{11}$$

With i as lower energy level l and j as upper level u, which implies $\sum_{j<i} A_{ij} = 0$. Therefore,

$$n_i (n_{col} C_{lu} + B_{lu} \int_0^\infty J_\nu \varphi_{lu}(\nu).d\nu) = n_u (n_{col} C_{ul} + B_{ul} \int_0^\infty J_\nu \varphi_{ul}(\nu).d\nu) + A_{ul} \tag{12}$$

At this point, we can derive the Einstein relations Aul, Bul and Blu. Considering only radiative excitation (Clu = Cul = 0) and complete redistribution over the line profile $[\varphi_{lu} = \varphi_{ul}]$. Physically, this means that emitted and absorbed photons are completely independent. Hence :

$$n_l B_{lu} J_\nu \varphi_{lu} = n_u B_{ul} J_\nu \varphi_{lu} + n_u A_{ul} \tag{13}$$

In case of thermal equilibrium the relative populations follow the relation:

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} exp\left(-\frac{h\nu}{KT}\right)$$

Using this relation and equation (9) in (13), we get:

$$\left(\frac{c^2}{2h\nu^3} A_{ul} - \frac{g_l}{g_u} B_{lu}\right) \left[exp\left(\frac{h\nu}{KT}\right) - 1\right] = \frac{g_l}{g_u} B_{lu} + B_{ul} \tag{14}$$

From the above equation we get our Einstein relations,

$$g_l B_{lu} = g_u B_{ul} \tag{15}$$

$$A_{ul} = \frac{2h\nu^3}{c^2} B_{ul} \tag{16}$$

The absorption and emission coefficients in terms of Einstein coefficients,

$$\alpha_\nu = \frac{h\nu}{4\pi}(n_l B_{lu} - n_u B_{ul})\varphi_\nu$$

$$j_\nu = \frac{h\nu}{4\pi} A_{ul} n_u$$

1.2.1 Local thermal equilibrium

The medium is in thermodynamic equilibrium if the populations ni are described by a Boltzmann distribution. The excitation is determined by the kinetic temperature Tkin. The excitation can still be described by a Boltzmann distribution, even when not in thermodynamic equilibrium. However, in that case, the temperature is called excitation temperature. Therefore in general,

$$\frac{n_i}{n_j} = \frac{g_i}{g_j} exp(\frac{h\nu}{K_B T_{kin}})$$

In LTE, $T_{kin} = T_{ex}$.
In non-LTE, $T_{kin} \neq T_{ex}$.
For an infinitely large medium, the radiation field would be defined as blackbody: $I_\nu = B_\nu$.
Assuming excitation temperature, Tex, which is defined as-

$$T_{ex} = \frac{h\nu/k}{ln(\frac{n_l g_u}{n_u g_l})}$$

where n is the number density. At local thermal equilibrium, we know $S_\nu = B_\nu$, hence from (8)-

$$I_\nu(\tau_\nu) = I_{\nu_0} e^{-\tau_\nu} + \int_0^{\tau_{\nu 0}} B_\nu . e^{-(\tau_\nu - \tau'_\nu)} \, d\tau'_\nu \tag{17}$$

Assuming excitation temperature is constant,

$$I_\nu = I_{\nu_0} e^{-\tau_\nu} + B_\nu . [1 - e^{-\tau_\nu}] \tag{18}$$

Molecular spectral line measurements requires difference in the measured intensity toward a reference position that contains only background intensity from that measured toward a molecular line source position:

$$\begin{aligned}\Delta I_\nu &= I_\nu - I_{\nu 0} \\ &= I_{\nu 0} e^{-\tau_\nu} + B_\nu [1 - e^{-\tau_\nu}] - I_{\nu 0} \\ &= [B_\nu - B_{\nu 0}][1 - e^{-\tau_\nu}]\end{aligned}$$

where $B_{\nu 0}$ is Planck's function at background temperature T_{bg}. Using Rayleigh–Jeans approximation:

$$\frac{T_R}{d\tau_\nu} = -T_{bg} + T_{ex}$$

where T_R is radiation temperature. Therfore,

$$T_R = T_{ex}(1 - e^{-\tau_\nu}) + T_{bg} e^{-\tau_\nu}$$

The number population is set by Boltzmann function and the source function is equal to Planck function at T_{kin} in case of thermal equilibrium.

1.3 Radiative problem solution

1.3.1 Collisional Rates

In radiative transfer problems we have to consider the discuss collision rates. The rates Cij are the collision rates per second per molecule. They depend on the density of the collision partner,

$$C_{ij} = K_{ij} n_{col}$$

where n_{col} the density of the collision partner (usually H2) and Kij is the collisional rate coefficient which are velocity-integrated collision cross sections, and depend on temperature.
For a two-level system in thermodynamic equilibrium,

$$n_l C_{lu} = n_u C_{ul}$$

Pluging the relation into the relative population density equation we get,

$$\frac{C_{lu}}{C_{ul}} = \frac{g_u}{g_l} exp\left(\frac{hv}{KT}\right) \tag{19}$$

Thereby,

$$\frac{dn_l}{dt} = -n_l(B_{lu}\bar{J} + C_{lu}) + n_u(A_{ul} + B_{ul}\bar{J} + C_{ul}) \tag{20}$$

$$\frac{dn_u}{dt} = n_l(B_{lu}\bar{J} + C_{lu}) - n_u(A_{ul} + B_{ul}\bar{J} + C_{ul}) \tag{21}$$

where $\bar{J}$ is J_v over line profile function $\varphi(v)$.

1.3.2 Escape probability method

This method involves figuring out factor that determines the probability that a photon in the medium can escape the system. Now we will estimate $\bar{J}$ to find the level populations(20 and 21). The amount of radiation coming from the the source is equal to the profile averaged source function S, for a completely opaque source . Hence it can be formulated as,

$$\bar{J} = S(1\beta)$$

where β is the probability that a photon can escape from the system.
This makes the equilibrium equations (20 and 21) easier to evaluate. Now we have yet to know the value of β. In one-dimensional case, it can be estimated as,

$$\beta = < e^{\tau} > = \frac{1}{\tau}\int_0^{\tau} e^{-\tau'} d\tau' = \frac{1 - e^{-\tau}}{\tau}$$

For a uniform sphere,

$$\beta = \frac{1.5}{\tau}[1 - \frac{2}{\tau^2} + (\frac{2}{\tau} + \frac{2}{\tau^2})e^{-\tau}]$$

1.4 Non LTE excitation

1.4.1 Collisions

We can recall the discussion on the collisional excitation and de-excitation, and how they are dependent on the density of collision partner. The most common collisional partners are H2, electrons.

Collision rates apart from density also depend on the cross-section σ_v and velocity distribution at temperature T.

$$C_v = \int_{v_0}^{\infty} \rho v \sigma_v dv \tag{22}$$

Now for condition of Non LTE condition.

1.4.2 Critical Density

In LTE, we assume level populations relation (section 1.2.1) and also is independent of the radiation field. In reality most of the interstellar medium donot follow this conditions as the density is too low to be thermalised. Hence we define critical density $n_{crit}(=\frac{A_{21}}{K_{21}})$for reference.

- $n >> n_{crit}$: collisional de-excitation will be more, and the level population will fulfill LTE condition.
- $n < n_{crit}$: radiative de-excitation will be more, and the excitation is not in equilibrium (non-LTE condition).
- $n \approx n_{crit}$: de-excitations via collisions and radiative interactions are equally likely.

1.5 Exact solutions

- Monte Carlo :Sampling the radiation field randomly , and using a given set of rays, the radiative transfer problem is solved iteratively (convergence).
- ALI : Convergence is done faster by splitting the coupling operation into a local and a non-local part.

2

Model based on LTE

This code reads molecular data from an SPCAT catalog file, and simulate a spectrum of the molecule. It uses a number of parameters and provides stick spectra or Gaussian simulations using the input .cat file for large number of lines. It can plot over a given observational spectrum.

2.1 Catalog File

The main input follows the SPCAT[2] format:

$$1, 2, 3, 4, 5, 6, 7, 8, 9$$

$$FREQ, ERR, LGINT, DR, ELO, GUP, TAG, QNFMT, QN$$

1. FREQ : Frequency of the line
2. ERR : Estimated / experimental error
3. LGINT : Logarithm of integrated intensity in base 10 (units - nm^2 MHz)
4. DR : Degrees of freedom in the rotational partition function
   - = 0 - atoms
   - = 2 - linear molecules
   - = 3 - nonlinear molecules
5. ELO : Lower state energy (units in cm^{-1})
6. GUP : Upper state degeneracy

[2]http://www.ifpan.edu.pl/ kisiel/asym/pickett/crib.htmspcat

7. TAG : Molecular identifier or unique tag.
   Its generally positive. In case of negative value tag implies that the line frequency has been measured in the laboratory or observation is recorded. The absolute value is considered as the species tag.
8. QNFMT : Identifies the format of the quantum numbers given in the field QN.
9. QN (qn1, qn2, qn3, qn4, qn5, qn6, qn7, qn8, qn9, qn10, qn11, qn12) :
   Quantum numbers coded according to QNFMT. Upper state quanta start in character 1. Lower state quanta start in character 14. For quanta shown as:
   - larger than 99 or smaller than –9 are shown with alphabetic characters or **. These are unused quanta.
   - between –10 and –19 are shown as a0 through a9.
   - from –20 to –259, which are shown as b0 upto z9.
   - between 100 and 109 are shown as A0 through A9.
   - from 110 to 359, which are shown as B0 upto Z9

2.2 Parameters used

2.2.1 Defaults:

- Temperature : 300 K
- LSR(Local standard of rest) Velocity : 0.0 km/s
- Column Density: 1E13 cm-2
- Lower Limit Cut-off for Simulation: none
- Upper Limit Cut-off for Simulation: none
- Linewidth: 5.0 km/s
- Temperature Catalog was Simulated At: 300 K
- Simulate Gaussian Profiles: True
- Thermal Continuum: 2.7
- RMS: none
- Simulation Resolution: 10 kHz

2.2.2 Start:

- quietflag = False
  Turn on to suppress warnings about how long the simulation will take.
- rms = float('-inf')
  Rms noise.
- thermal = float('inf')
  initial default cutoff for optically-thick lines
- T = 300
  temperature for simulations. Default is 300 K.
- catalog_file = None
  catalog file to load in. Call load_mol()
- C = 1e13
  column density. Units are cm-2.
- vlsr = 0.0
  velocity of lsr offset applied to simulation.
- ll = float('-inf')
  lower limit for the simulation range.
- ul = float('inf')
  upper limit for the simulation range.
- spec = None
  file of a laboratory or observational spectrum to load in for comparison. Default is none.
- dV = 5.0
  linewidth of the simulation in km/s.
- CT = 300.0
  temperature the catalog is simulated at in K.
- gauss = True
  toggle for simulating Gaussians or a stick spectrum.

- dish_size = 100
  for use if beam corrections are desired; given in meters
- source_size = 1E20
  for use if beam corrections are desired
- eta = 1.0
  beam efficiency of the telescope.
- res = 0.01
  resolution used in Gaussian simulation.
- cavity_ftmw = False
  if set to True, simulates doubler doublets from the cavity FTMW.
- cavity_dV = 0.13
  sets the default cavity linewidth to 0.13 km/s
- cavity_split = 0.826
  sets the default doppler splitting in the cavity to 0.826 km/s in each direction.
- planck = False
  flag to use planck scale. If planck = True is enabled, a synthesized beam size must also be provided using synth_beam = [bmaj,bmin] below.
- synth_beam = ['bmaj','bmin']
  to be used with planck = True conversions.
- vibs = None
  *This is a list of vibrational *frequencies* in units of* cm^{-1}

2.3 Data

2.3.1 H-atom

res = 1e-2

line = 1

Q(T = 300K) = 4 (*Partition function*)

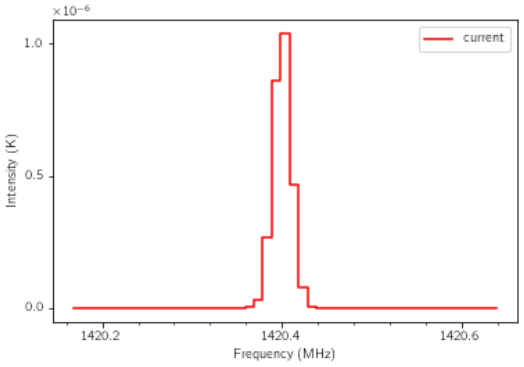

Figure 4

2.3.2 N-atom

res = 1e-8

line = 1

Q(T = 300K) = 12.001 (*Partition function*)

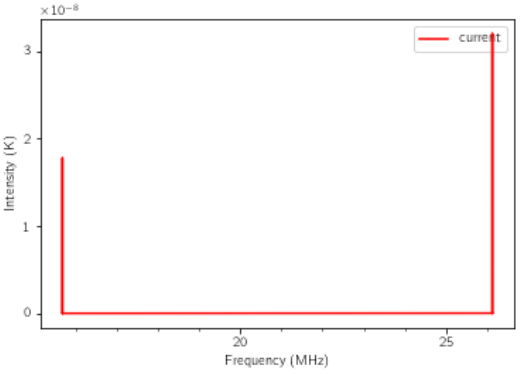

Figure 5

2.3.3 D-atom

res = 1e-2

line = 1

Q(T = 300K) = 6 (*Partition function*)

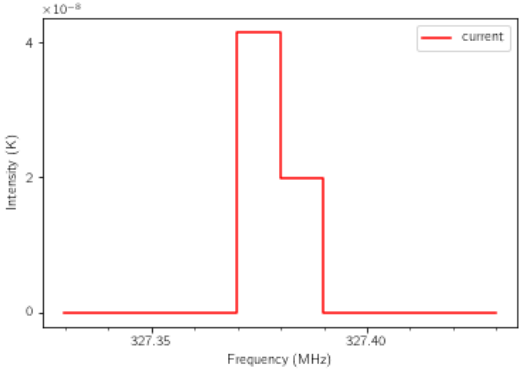

Figure 6

2.3.4 O-atom

res = 1e-2

line = 2

Q(T = 300K) = 6.741 (*Partition function*)

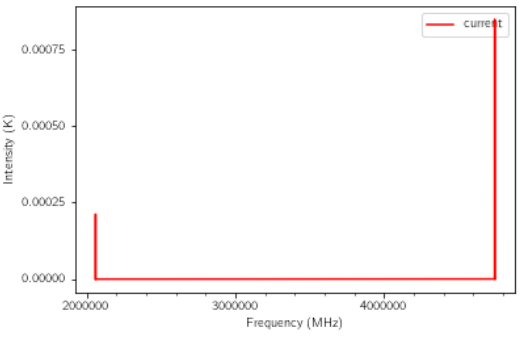

Figure 7

2.3.5 CH

res = 1e-2

line = 508

Q(T = 300K) = 120.841 (*Partition function*)

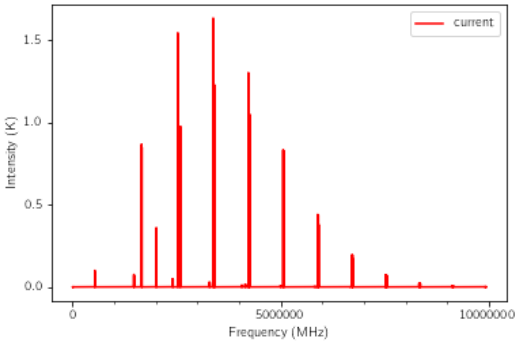

Figure 8

2.3.6 CH_3D

res = 1e-2

line = 203

Q(T = 300K) = 896.191 (*Partition function*)

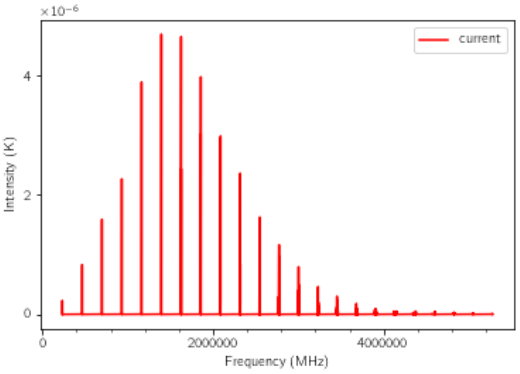

Figure 9

2.3.7 H_2D+

res = 1e-2

line = 32

Q(T = 300K) = 76.452 (*Partition function*)

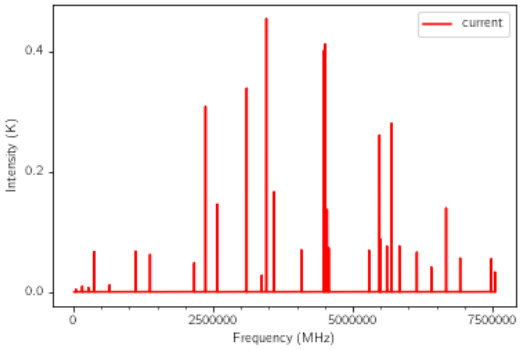

Figure 10

2.3.8 NH

res = 1e-2

line = 1416

Q(T = 300K) = 236.347 (*Partition function*)

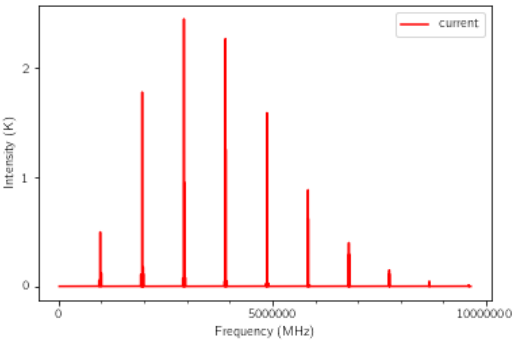

Figure 11

3

Model based on Non LTE (1D)

3.1 Based on RATRAN

Molecule - HCO+ (*From the LAMBDA database*[3])

3.1.1 Parameters

1. Dust parameters = "jena , thin , e5"
2. Goal signal to noise ratio = 20
3. Number of photons for simulation = 1000
4. Background temperature = 2.735
5. Minimum population = 1e-4
6. Transitions to trace = [0,1,2]
7. Channel resolution = 0.1 km/s
8. Line blending = False
9. Seed - 1971

[3]https://home.strw.leidenuniv.nl/ moldata/

3.1.2 Plots

Intensity (calculated for line transitions)

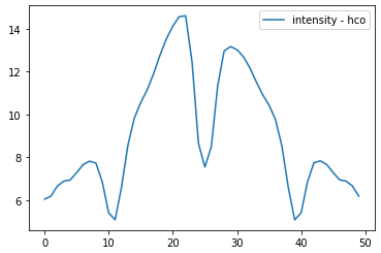

Figure 12

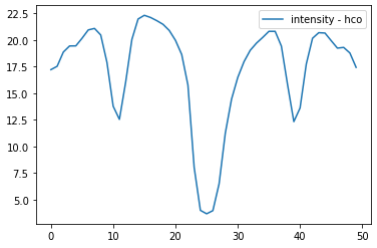

Figure 13

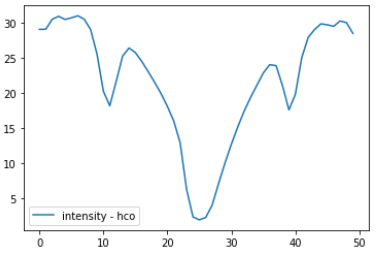

Figure 14

Optical Depth

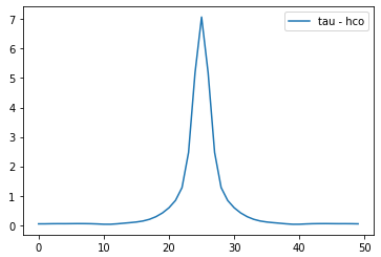

Figure 15

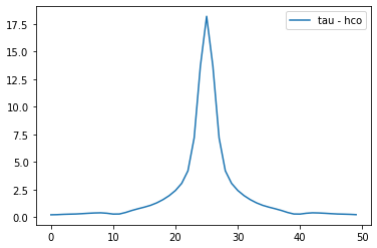

Figure 16

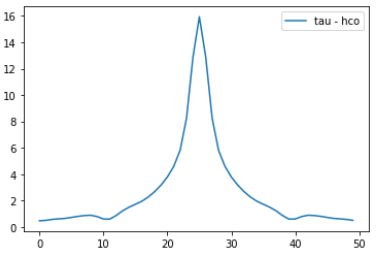

Figure 17

3.2 NDRADEX

It uses grid parameters for non-LTE molecular transfer and gives multidimensional arrays as output.

3.2.1 Parameters

Molecule - CO

I - Example

1. LAMBDA datafile : CO+.dat
2. Transition : 1 - 0
3. T_{kin} : 100 K
4. CO column density : 1e15 cm^{-2}

5. H2 (collisional partner) density : 1e3 cm^{-3}

I- Output:

Table 1

Variable	Description	Value
QN_{ul}	Transition	1-0
T_{kin}	Kinetic Temperature	100 K
N_{mol}	Column density	1e15
T_{bg}	Background temperature	2.73
dV	Linewidth	1.0
geom	Geometry of escape velocity	'uni'(*uniform*)
description		LAMBDA-CO
E_u	Upper state	5.5
freq	Frequency	115.3
wavel	Wavelength	2.601e+3
T_{ex}	Excitation temperature	132.5
tau	Optical depth	0.009966
T_r	Radiation temperature	1.278
pop_u	Population at U	0.4934
pop_l	Population at L	0.1715
I	Intensity	1.36
F		2.864e-08
n_{H2}	625.6	2576

II - Grid parameter input

1. LAMBDA datafile : CO+.dat
2. Transition : '1 - 0' , '2 - 1'
3. T_{kin} : [10,15,20,25,30] K
4. CO column density : 1e15 cm^{-2}
5. H2 (collisional partner) density : [1e3, 5e3, 1e4, 5e4, 1e5, 5e5] cm^{-3}

II- Output:

Dimensions: QN_{ul} - 2, T_{kin} - 5, n_{H2} − 6

No of variables = 60 for each $(QN_{ul}, T_{kin}, n_{H2})$

Table 2

Variable	Description	Value
QN_{ul}	Transition	1-0 , 2-1
T_{kin}	Kinetic Temperature	10,15,20,25,30 K
N_{mol}	Column density	1e3, 5e3, 1e4, 5e4, 1e5, 5e5
T_{bg}	Background temperature	2.73
dV	linewidth	1.0
geom	Geometry of escape velocity	'uni'(*uniform*)
description		LAMBDA-CO
E_u	Upper state	5.5,5.5,5.5....16.6,16.6
freq	Frequency	115.3,115.3,115.3....230.5,230.5
wavel	Wavelength	2.601e+3,2.601e+3,2.601e+3.....,1.3e+3,1.3e+3
T_{ex}	Excitation temperature	5.336,8.937,9.811,....,29.24,29.87
tau	Optical depth	0.4152,0.2083,...,0.07337,0.06692
T_r	Radiation temperature	0.7475,1.056,1.049,....,1.688,1.585
pop_u	Population at U	0.4817,0.5131.....,0.2809,0.2628
pop_l	Population at L	0.4527, 0.3176, ...0.2461,0.2284
I	Intensity	0.7957,1.124,1.117,....,1.797,1.687
F		1.569e-08,2.217e-8,...,2.662e-07

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Conclusion

Various models where studied and got plots for the inputs as shown.
For the LTE model, we go with the radiative and collision rates, along with the escape probability assumptions. The codes uses extrapolation technique to get the collision rates due to limited data range. Model utilises the assumption that lines used in the simulation are thermalised or $T_{ex} = T_{kin}$. And we get spectral line in the given range. The codes are given more computational capability like storing data, comparing laboratory data, storing a simulation, redefining parameters and so on.
Non-LTE is added with complications, the lines being not thermalised. The model follows the Monte Carlo method to converge upon the next new level populations. We also found line center optical depths using the relation

$$\varphi(\nu) = \frac{1}{\Delta\nu}$$

and with taking the change in optical depth with the line profile into consideration.
For future, the goal would be to use the models in depth understanding the physical processes ongoing in the interstellar medium.

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