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A sub-grid model for molecular gas in a cosmological galaxy formation simulation

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A thesis submitted for the degree of
MSc Physics - Theoretical Astrophysics and Cosmology

September 20, 2018

Acknowledgements

First and foremost, I would like to express my thanks to my supervisor, Prof. (Dr.) Romain Teyssier, for his patient guidance, encouragement and useful critiques of this research work. He has been a great support and has followed my work with lots of dedication and time throughout the course of my research. He has also helped me broaden my mind and obtain a deeper understanding of astrophysics. To a large extent I owe it to him that I have enjoyed my research at all stages of the project.

I would also like to thank Mr. Michael Kretschmer and Ms. Tine Colman, for their valuable and constructive suggestions during the planning and development of this project and their assistance in keeping my progress on schedule. Their willingness to give their time so generously has been very much appreciated.

I would also like to extend my thanks to the Institute of Computational Science for their help in offering me the resources needed for this project.

Finally, I wish to thank my parents and sister for their support and encouragement throughout my study.

Amandeep Singh *September 20, 2018*

Abstract

The spectral energy distribution, line luminosity, and molecular fraction of CO in galaxies are studied. For this aim, a model is constructed which uses Jeans length and Virial theorem to establish a relation between the radius and density of the turbulent molecular cloud. Then, a simplified model for radiative transfer is introduced which accounts for the clumpy nature of the molecular clouds. The results from this sub-grid model are used to post-process and resolve a cosmological simulation of a main-sequence ($M_* \approx 10^9 \mathrm{M}_\odot, \mathrm{SFR} \approx 100 \mathrm{M}_\odot \mathrm{yr}^{-1}$) galaxy. The luminosity for the $[\mathrm{C}_{II}]158\mu$m emission computed after post-processing the simulation is $L_{\mathrm{CO}(1-0)} = 10^4 \mathrm{L}_\odot$, which is comparable to observations of galaxies having similar characteristics.

Key words: Jeans length, Lyman-Werner photons, photo-dissociation, molecular fraction, optical depth, emissivity, escape probability, luminosity.

Chapter 1

Introduction

To understand the process of star formation in galaxies, we need to study and constrain the microscopic properties.

Molecular hydrogen (H_2) is the most abundant molecule in the universe and is the main ingredient in star formation. But H_2 is not a polar molecule, so it's first quadrupole line excitation temperature ($T_{exc} \approx 500K$) is much higher than the temperature of surrounding molecular cloud ($T \approx 10 - 20K$)(ref_e). This makes H_2 a difficult tracer of the properties of the giant molecular cloud. Carbon monoxide (CO) is the second most abundant molecule in the Universe. The first CO rotational transition occurs at $T_{exc} \approx 5K$ (ref_e), which means that it is easily excited inside the molecular clouds. This is the reason why the rotational transitions of CO are used as tracers for detection of molecular gas in galaxies.

The different emission line of CO have different requirements for excitation. These requirements can be used to constrain different gas properties (e.g. density, temperature, etc.) and the gas heating mechanisms (e.g. FUV photon flux, shocks, etc) in the molecular cloud. One way to do it is by analysing the CO Spectral Line Energy Distribution (CO-SLED) flux in each emission line. (ref_e)

The goal here is to develop a model that works at: (1) small scales ($\approx 0.1 - 1pc$) by taking into account the physical and chemical reactions taking place in the photo-dissociation layer in the molecular parts of the molecular clouds, and (2) large scales ($\approx 30pc$) by referencing the properties of the interstellar medium (ISM) (density, turbulence, metallicities, background radiation field, etc.) from the hydrodynamical simulation.

This kind of approach of constructing sub-grid models to predict the luminosity of CO emission lines tracing the diffused gas and dense photo-dissociation regions in galaxies has proven to be an optimal strtegy to study molecular clouds. (ref_e)

This report is structured as follows. The outline of the sub-grid model and then the implementation of a simplified radiative transfer model is explained in Chapter 2. In Chapter 3, the results of the model are compared with local observations. Chapter 4 details the application of this model to post-process a sample cosmological galaxy simulation and computation of the CO emission. Conclusions are drawn in Chapter 5.

Chapter 2

Model Outline

The outline of the model structure is represented in Figure-1 (fig_s). The first part (Section 2.1) details the analytical description the internal density structure of the molecular cloud and its time evolution. The second part (Section 2.2) deals with the simplified radiative transfer model to compute the CO line emission once the density profile is established.

2.1 Structure of the Cloud

Fragmentation of gas clouds has been intensively studied in the past, and both numerical and analytical models (ref_e) have shown that the density field of an isothermal, non-gravitating, turbulent gas of mean number density $\bar{n}_H$ is well described by a lognormal probability distribution function (PDF). The volume-weighted PDF ($P_V(s)$) can be written as:

$$P_V(s) = \frac{1}{(2\pi\sigma_s^2)^{1/2}} \exp\left[-\frac{1}{2}\left(\frac{s-\bar{s}}{\sigma_s}\right)^2\right], \tag{2.1}$$

where:

$$s = \ln\left(n_H/\bar{n}_H\right), \tag{2.2}$$

$$\bar{s} = -\sigma_s^2/2, \tag{2.3}$$

where $\bar{n}_H$ is the mean number density of the cloud, $\bar{s}$ is related to the volume-averaged value of the logarithm of the density (ref_e). σ_s depends on the sonic Mach number ($\mathcal{M}$) as:

$$\sigma_s^2 = \ln\left(1 + b^2\mathcal{M}^2\right), \tag{2.4}$$

where b parametrises the kinetic energy injection mechanism driving the turbulence. In this model $b = 0.3$ everywhere.

When self-gravity becomes important, the probability of finding dense regions increases and a power-law tail develops on the high-density side of the PDF. The occurrence of the power-law tail is confirmed both theoretically (ref_e), and observationally via molecular line detections (ref_e). Treating properly the high-density tail of the density PDF is pivotal when computing the emission of CO emission lines as they trace the densest regions of the clouds (ref_e).

In this model, the time evolution of the density PDF of self-gravitating molecular clouds is described via the formalism developed by Girichidis et al. (2014)(ref_e). Assuming a pressure-free collapse, these authors provide a set of analytical equations to calculate the functional form of the PDF at any given time, $P_V(s,t)$, given the initial $P_V(s,0)$. According to their model, the high-density tail of the PDF quickly asymptotes to a power law consistently with observations.

In this model, as the initial PDF, $P_V(s,0) \equiv P_V(s)$ where $P_V(s)$ is given by equation (2.1).

(Formulae and description of pdf evolution)

The size of the molecular cloud is given by the Jeans length λ_J of the cloud, which depends on the density n_H of the cloud,

$$\lambda_{\rm J} = \frac{c_s}{\left(\sqrt{4\pi G \cdot n_H \cdot m_p}\right)}, \tag{2.5}$$

where c_s is the isothermal sound speed given by:

$$c_s = \sqrt{\left(K_b \cdot \overline{T}/m_p\right)}, \tag{2.6}$$

where K_b is the Boltzmann constant, $\overline{T}$ is the mean cloud temperature taken in this model such that, $\overline{T} = 10K$, and m_p is proton mass.

Now, to describe the chemistry of the cloud, the chemical reaction rate equation has to be solved. The construction rate (CR) of H_2 molecules per unit time on the surface of dust particles and destruction rate (DR) of H_2 molecules per unit time due to photo-dissociation is given as:

$$CR = k \cdot n_H \cdot Z \cdot n_{H1}, \tag{2.7}$$

$$DR = \sigma_{dust} \cdot c \cdot n_{H2} \cdot n_{LW}, \tag{2.8}$$

where k is the construction coefficient, such that $k = 2.5 * 10^{-17} cm^3 s^{-1}$, Z is the metallicity of the cloud, σ_{dust} is the mean cross-section of the dust particles, n_{H1} is the number density of H atoms, n_{H2} is the number density of H_2 molecules, and n_{LW} is the number of Lyman-Werner photons responsible for photo-dissociation of the H_2 molecules. n_{H1} and n_{H2} are related to n_H as:

$$n_H = n_{H1} + 2 \cdot n_{H1}, \tag{2.9}$$

In equilibrium, construction and destruction rates are equal. Equating equations (2.7) and (2.8), and using equation (2.9):

$$n_H = \left[\frac{\sigma_{dust} \cdot c \cdot n_{H2} \cdot n_{LW}}{k \cdot Z \cdot n_H} + 2\right] * n_{H2}, \tag{2.10}$$

This gives the molecular fraction X_{H2} of H_2:

$$X_{H2} = \frac{n_{H2}}{n_H}, \tag{2.11}$$

$$= \frac{1}{2 + \left(\frac{\sigma_{dust} \cdot c \cdot n_{H2} \cdot n_{LW}}{k \cdot Z \cdot n_H}\right)}, \tag{2.12}$$

Here, the number of photo-dissociating photons (n_{LW}) is given as:

$$n_{LW} = (BGRF) \cdot \exp(-\tau), \quad (2.13)$$
$$\tau = 1000 * m_p \cdot Z \cdot n_H \cdot \lambda_J, \quad (2.14)$$

where τ is the optical depth and BGRF is the Background Radiation Flux of the photo-dissociating photons responsible for the destruction of H_2 molecules. In this model, BGRF is taken as the far-ultraviolet(FUV) flux, denoted by G_0 (in Solar units).Young, massive stars are the main source of the FUV photons which permeate the ISM and readily photo-dissociate interstellar molecules, such as H_2 and CO. This model does include an H2-dissociating FUV photo-background, though assumed it to be constant in both space and time. ($G_0 = 1(Solar)$)

(Formulae and description of self shielding)
Self-shielding of molecular hydrogen has been studied extensively since the pioneering work of Stecher Williams (1967). A commonly used formula that conveniently parametrises the self-shielding effects for H2 with (local) one-dimensional velocity dispersion was given by Draine Bertoldi (1996),

$$S_{\mathrm{H_2}} = \frac{0.965}{(1+x/b_5)^2} + \frac{0.035}{\sqrt{1+x}} \exp\left(-\frac{\sqrt{1+x}}{1180}\right) \quad (2.15)$$

where $x \equiv N_{\mathrm{H_2}}/5 \times 10^{14}\mathrm{cm}^{-2}$, and $b_5 \equiv b/\mathrm{km/s}$, with $b \equiv \sqrt{2}\sigma_v$. Here $N_{\mathrm{H_2}}$ is the column density of $\mathrm{H_2}$.
The accuracy of this shielding function has been confirmed by recent work Sternberg et al. 2014 who also explicitly accounted for line overlap in the Lyman-Werner bands. Using this formula, the new number of dissociating photons, the new molecular fraction of H_2, and the new number density of H_2 can be calculated:

$$n_{LW,ss} = (BGRF) \cdot S_{H_2} \cdot \exp(-\tau), \quad (2.16)$$
$$X_{H2,ss} = \frac{1}{2 + (\frac{\sigma_{dust} \cdot c \cdot n_{H2} \cdot n_{LW,ss}}{k \cdot Z \cdot n_H})}, \quad (2.17)$$
$$n_{H2,ss} = n_H \cdot X_{H2,ss}, \quad (2.18)$$

Significant CO fractions only form in the densest gas where a combination of dust, H_2, and self-shielding attenuates the far-ultraviolet (FUV) background. Using n_{H2} and X_{H2}, the molecular fraction (X_{CO}) and the number density (n_{CO}) of CO can be calculated:

$$X_{CO} = , \quad (2.19)$$
$$n_{CO} = 10^4 * Z \cdot n_H \cdot X_{CO}, \quad (2.20)$$

The results for CO given by this model are accurate enough to not consider self-shielding of CO.

2.2 Radiative Transfer

A simplified version of radiative transfer is adopted in this model, which assumes Local Thermodynamical Equilibrium (LTE) to calculate the occupation number (n_i) of the molecules in each excited state. The energies (E_i), emitted frequencies(ν_{ij}), statistical weights(g_i), and the Einstein coefficients (A_{ij}, B_{ij}, B_{ji}) are read from the Leiden Atomic and Molecular Database (LAMDA) file.

Since the PDF ($P_V(s)$), number density of CO molecules (n_{CO}), and Jeans length (λ_J) are provided by the model, the emissivity for CO(1-0) transition (j_{10}) can be computed as:

$$j_{10} = \frac{h \cdot \nu_{10}}{4\pi} n_{CO} \cdot n_1 \cdot A_{10}, \tag{2.21}$$

where ν_{10} is the frequency of the emitted photon, and A_{10} is the Einstein coefficient from the CO(1-0) transition, and n_1 is the occupation level of CO molecules in the 1st excited state.

Finally, using emissivity (j_{10}), the luminosity of the CO(1-0) emission line can be calculated:

$$l_{10} = \overline{j_{10}} \cdot (dx^3), \tag{2.22}$$