The puzzle of protoplanetary disk masses

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SUMMARY

The cosmos is within us.
We are made of star-stuff.
We are a way for the universe to know itself.
Carl Sagan

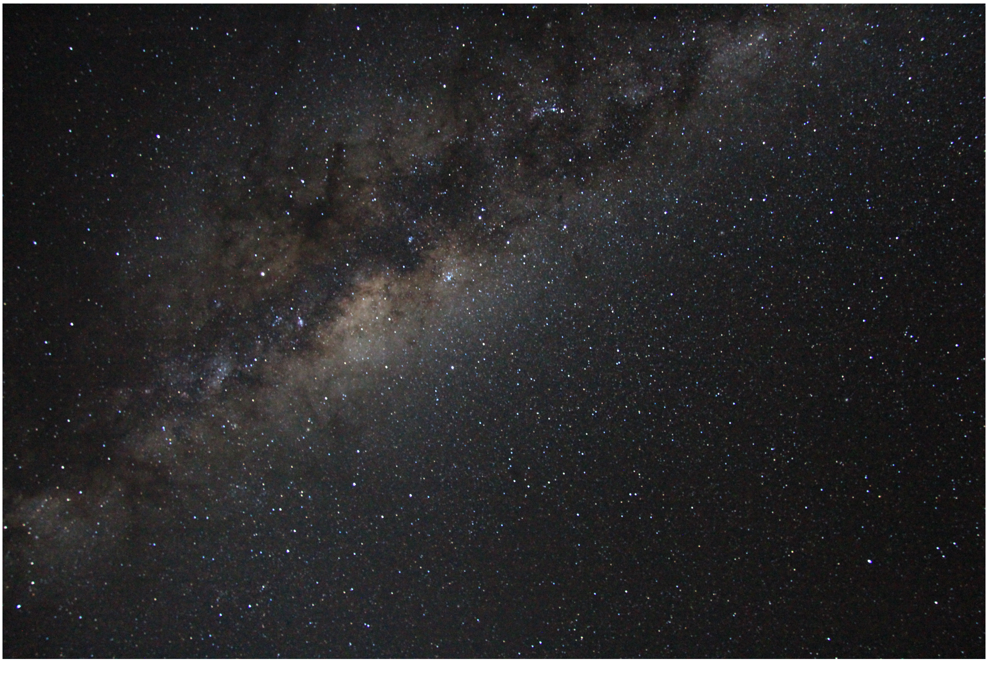

Figure 8.1: The galactic center and dusty Milky Way as seen on March 26, 2017 on a new moon night from Cerro Paranal (photo taken by the author with Reflex camera, exposure 30s).

Since the beginning of human history, men have raised their eyes to the night sky and wondered about the meaning of such a majestic show (Fig. 8.1). Ancient civilizations from different parts of the world, from Egypt to China, from Oceania to southern America, have given life to myths and legends about the constellations and nebulosities that they could spot in the sky. Even throughout our European history many poets, painters and artists have taken inspiration from celestial events. The astonishment in front of the sky has always been accompanied by the need to understand the link between mankind and the universe. Now that science and technology have advanced and we are able to explain the physical and chemical structure of astronomical objects, this question has not been abandoned. Science has revealed to us that the connection of the cosmos with our existence is much deeper than any pre-scientific vision had dared to imagine. For example our knowledge on our hosting galaxy tells us that all phenomena happening in the Milky Way, from the presence of a black hole to that of supernova explosions up to the actual location of our Solar System, have cooperated to allow life to evolve up to the current status. Also, the growing zoo of discovered exoplanets allows us to compare their characteristics with those of our planetary system. Despite the large statistics, it seems that the configuration of our own Solar System is very “special”. Based on exoplanet observational surveys, the Sun-Jupiter system is as common as one in a thousand. On the other hand theoretical modeling favors Jupiter as the fundamental player in the Solar System’s evolution.

Star formation and protoplanetary disks

The question about our origins centers around star and planet formation. How do stars and planets orbiting around them form? What are the initial conditions needed to generate a planetary system similar to our own? Which roles do the physical architecture and chemical composition of these forming systems play?

On large scales, star formation begins with the formation of filamentary structures inside giant molecular clouds. Observations have shown that filaments are elongated structures, within which typically several dozens of smaller fibers are created and eventually fragment into dense cores. These are defined as *prestellar cores*, as they will likely collapse to form one or more stars. As the collapse proceeds, due to conservation of angular momentum a rotating disk-like structure is formed, through which matter accretes onto the forming protostar (Fig. 8.2). This is called *protoplanetary disk* as it is also the place where planets, like our own Earth and the other Solar System planets, are formed.

Disks evolve from an initial phase where they are still embedded in their extended envelope (Class 0 and Class I objects), to a more typical stage in which they are gas-rich and the envelope has been dissipated (Class II objects), to a more evolved

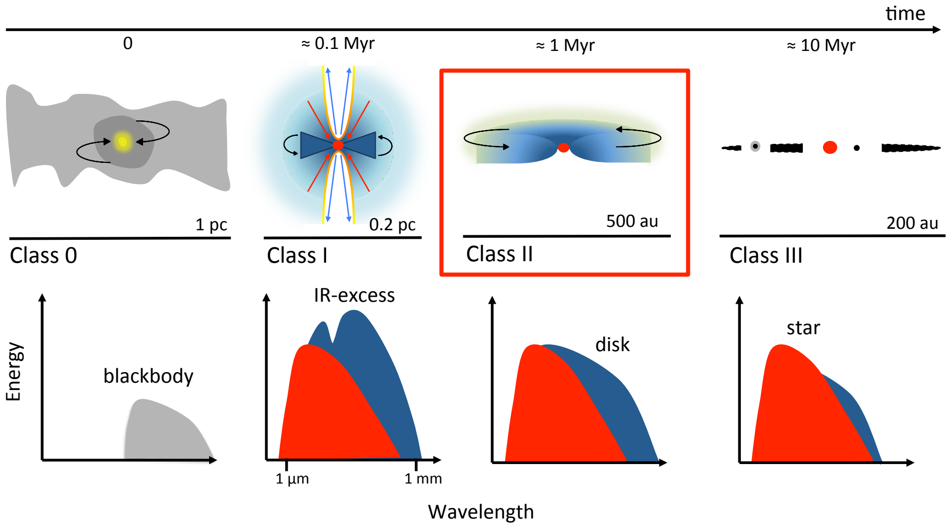

Figure 8.2: Sketch of the star and planet formation process in isolation. In the upper panel different evolutionary classes are sketched, while in the lower panel the respective observational features are shown through schematic SEDs. This thesis focuses on the stage of a pre-main sequence star with a disk, called the Class II stage.

phase where they are gas-poor and larger bodies, such as planets and asteroids, must be already formed (Class III objects). As shown by the sketch in Fig. 8.2, the different evolutionary stages have different slopes in their Spectral Energy Distributions (SED). The focus of this thesis is on protoplanetary disks in their gas rich Class II phase through the modeling of their bulk gas component and comparing with brand-new observations of images of gas and dust in disks from the Atacama Large Millimeter/submillimeter Array (ALMA, see Fig. 8.3).

Open questions in the study of protoplanetary disks

One of the fundamental properties of disks is the total *mass*, as it determines their physics, evolution and the characteristics of the planetary outcomes. Nevertheless disk masses are not yet observationally determined with high confidence. Disks are composed of gas, accounting for 99% of the mass, and dust, which in turn dominates the emission. The bulk of the dust mass is in mm-sized grains, which are not necessarily well mixed with the gas. Accordingly the mass determination of the gaseous and dusty components should in principle be carried out independently. Most of

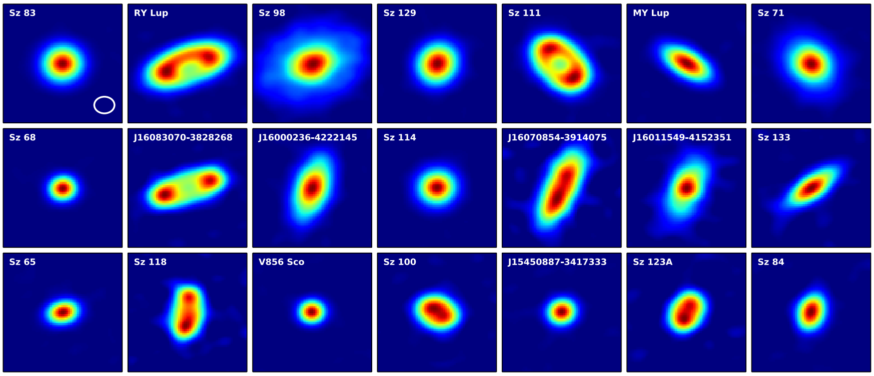

Figure 8.3: Image showing the zoo of protoplanetary disks observed with ALMA in the Lupus Star Forming region. These images show the dust thermal emission at 890 μm caused by mm-sized grains present in the disks (Credit: M. Ansdell).

the disk mass is expected to be in the form of molecular gas, essentially molecular hydrogen (H_2). However, H_2 is not easily excited and observable at the cold temperatures in the bulk of the disk. Hence, traditionally, the presence of gas in disks has been constrained through carbon monoxide (CO) emission lines, easily excited in disks. However the emission is generally very optically thick, so using CO to measure accurately the gas mass is very difficult and model dependent. The main questions that are tackled in this PhD thesis are the following.

- Which is the best gas mass tracer in protoplanetary disks? Could the less abundant isotopologues[1] of CO serve this purpose? Would hydrogen deuteride (HD) be a good alternative and what are its limitations?

- How can current and future ALMA observation be used to determine the masses of a statistically significant sample of disks?

- What is the actual gas-to-dust mass ratio in disks and how is its determination affected by the fact that a fraction of the carbon and oxygen may be locked up in refractory material?

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[1] Isotopologues are molecules that differ only in their isotopic composition. Simply, the isotopologue of a chemical species has at least one atom with a different number of neutrons than the parent.

This thesis and future outlook

Determining disk gas masses has been the leading question of this PhD thesis since its origin. CO isotopologues have been promising gas mass tracer candidates for many years and with the advent of ALMA their detection in disks has become routine. The still open question is if chemical isotope-selective effects play a major role in setting the mutual abundance ratios of CO isotopologues and in the determination of disk masses. The rarer isotopologue $C^{18}O$ is indeed destroyed by UV radiation faster than the main form of carbon monoxide, $^{12}C^{16}O$. Therefore this thesis starts from the modeling perspective. Subsequently a larger sample of CO isotopologues observations in disks has been provided by the *Lupus Disk Survey* with ALMA . The grid of models presented in Chapter 3 has therefore been compared with observations and some more observation-motivated projects have been carried out.

- In Chapter 2 isotope-selective photodissociation, the main process controlling the relative abundances of CO isotopologues in the CO-emissive layer, was properly treated for the first time in a physical-chemical disk model called DALI. The chemistry, thermal balance, line, and continuum radiative transfer were all considered together with a chemical network that treats ^{13}CO, $C^{18}O$ and $C^{17}O$, isotopologues as independent species. The main result is that isotope selective processes lead to regions in the disk where the isotopologues abundance ratios are considerably different from the elemental ratios. Accordingly, considering CO isotopologue ratios as constants may lead to underestimating disk masses by up to an order of magnitude or more.

- In Chapter 3 the small grid of models used in Chapter 2 to investigate the effects of CO isotope-selective photodissociation has been expanded. More than 800 disk models have been run for a range of disk and stellar parameters. Total fluxes have been ray-traced for different CO isotopologues and for various low $J-$ transitions for different inclinations. This chapter shows that a combination of ^{13}CO and $C^{18}O$ total intensities allows inference of the total disk mass, although with larger uncertainties, compared with the earlier studies. These uncertainties can be reduced if one knows the disk's radial extent, inclination and flaring from other observations. Finally, total line intensities for different CO isotopologue and for various low-J transitions are provided as functions of disk mass and fitted to simple formulae. The effects of a lower gas-phase carbon abundance and different gas-to-dust ratios are investigated as well.

- In Chapter 4 the grid of physical-chemical models presented in Chapter 3 has been employed to analyze continuum and CO isotopologues (^{13}CO $J = 3-2$ and $C^{18}O$ $J = 3-2$) observations of Lupus disks. Disk gas masses have been calculated for a total of 34 sources, expanding the sample of 10 disks studied previously. This chapter shows that overall CO-based gas masses are very low for disks orbiting a solar mass-like star, often smaller than $1 M_{\rm J}$ (mass of Jupiter), if volatile carbon is not depleted. Accordingly, global gas-to-dust ratios are much lower than the expected ISM-value of 100, being predominantly between 1 and 10. Low CO-based gas masses and gas-to-dust ratios may indicate rapid loss of gas, or alternatively chemical evolution, e.g. via sequestering of carbon from CO to more complex molecules, or carbon locked up in larger bodies. The first hypothesis would imply that giant planet formation must be quick or rare, while for the latter the implication on planet formation timescales is less obvious.

- In Chapter 5 another important disk property has been investigated with DALI models, i.e. the gas surface density distribution $\Sigma_{\rm gas}$. Reliable observational measurements of $\Sigma_{\rm gas}$ are key to understand disk evolution and the relative importance of different processes, as well as how planet formation occurs. This chapter investigates whether ^{13}CO line radial profiles, such as those recently acquired by ALMA, can be employed as a probe of the gas surface density profile. By comparing with DALI simulations we find that ^{13}CO radial profiles follow the density profile in the middle-outer disk. The emission drops in the very inner disk due to optical depth, and in the very outer disk due to a combination of freeze-out and inefficient self-shielding.
- In Chapter 6 simple deuterium chemistry has been added to the chemical network in DALI to simulate HD lines in disks. The aim is to examine the robustness of HD as a tracer of the disk gas mass, specifically the effect of gas mass on the HD far infrared emission and its sensitivity to the disk vertical structure. The uncertainty on HD-mass determination due to disk structure is found to be moderate and HD observations should be considered as an important science goal for future far-infrared missions, such as SPICA.

The main conclusions of this thesis are the following:

1. CO isotope-selective photodissociation needs to be properly considered when modeling rare CO isotopologues emission. Otherwise, C^{18}O lines emission could be overestimated and the derived gas masses could be underestimated by up to an order of magnitude or more.
2. Disk gas masses can be inferred by a combination of ^{13}CO and C^{18}O total intensities, although with non-negligible uncertainties, up to two orders of magnitude for very massive disks.
3. CO-based disk gas masses derived in Lupus are extremely low, often smaller than 1 $M_{\rm J}$ and the global gas-to-dust ratios are predominantly between 1 and

10. This may be interpreted as either rapid loss of gas, or fast chemical evolution.

4. The shape of the disk surface density distribution can be constrained by spatially resolved ^{13}CO observations, if optical depth, freeze-out and self shielding are properly considered in the modeling.
5. HD far-infrared emission can be used to determine disk gas masses with moderate uncertainty which depends mainly on the disk vertical structure. Such observations should be considered as an important science goal for future far-infrared missions.

The question on disk gas masses remains open. CO isotopologues are still promising mass tracers candidates, as their detection is routine for ALMA, but they need to be calibrated. This thesis shows that the process of isotope-selective photodissociation is important for a good interpretation of CO isotopologues as gas mass tracers. However photodissociation, at least for the case of TW Hya and possibly for other disks, is not the main process responsible for the observed faint CO isotopologues lines. In turn, volatile carbon depletion is a process that needs to be further investigated and understood. Where does the carbon go? The detection of slightly more complex molecules, such as the hydrocarbons C_2H and c-C_3H_2 could be a way to calibrate CO-based gas masses. Another option is to enlarge the sample of [CI] line detections, which allow inference of the volatile carbon abundance in the upper regions of the disk. Finally, if the HD fundamental lines can be covered at high enough spectral resolution with SPICA, their detection will provide an unique independent tracer of the disk mass.

Determining the total mass of protoplanetary disks is challenging but crucial, as this is the main disk property that one needs in order to understand how planets such as our own Earth or the diverse observed exo-planets[2] form.

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[2] Exo-planets are planets orbiting a star that is not the Sun.