Unveiling the third dimension: vertical structure as a probe of planet formation conditions

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English summary

In the north of Chile, due to its natural conditions and isolation, the Atacama desert is a unique window to observe the universe. For many centuries the local native indigenous groups, called in their language *Lickan Antay* and in current spanish *Atacameños*, looked up at the universe and focused not only on the bright stars, but on the dark areas that contrasted against the glow. We now know that these regions are dark because small dust grains absorb the starlight at optical frequencies and that these dark clouds are associated with star-forming regions. While our eyes are not able to see past the dust, instruments such as the Atacama Large Millimeter/submillimeter Array can reveal their secrets. ALMA is built on the Chajnantor plateau, a sacred place for the *Lickan Antay* in the Atacama desert, that means "place of departure" in their language. Located at an altitude of 5000 meters, one of the main science goals of ALMA is to look into these dark and cold regions to understand the processes that lead to star and planet formation.

The analysis and results presented in this thesis have been possible due to the capabilities of ALMA, that since the start of its operations in 2013 has revolutionized the view of planet formation. Through observations and theoretical understanding of the universe as traced at (sub-)millimeter wavelengths we have the unique opportunity to look back towards our origins. How did the earth form? May other planetary systems have similar conditions? What are the key processes that govern the initial epochs?

Star and planet formation

The process of planet formation is intrinsically linked to stellar formation. First, stars form from the collapsing material of molecular clouds that contracts into a pre-stellar core. From core to planetary system, young stellar objects (YSOs) are classified into Classes (0, I, II or III). In the earliest Class 0/I stage, a protostar will be actively accreting material from its surrounding protostellar envelope, then, due to conservation of angular momentum, the infalling material will spread out to form a rotating disk-like structure around the protostellar system. These disks are named protoplanetary or planet-forming disks, as they are the birthplaces and host the material reservoir of planetary systems.

The Class II protoplanetary disk stage lasts ~1-10 million years and ends when most of the disk material has either accreted onto the star, formed planets or dispersed, after which a Class III planetary system is revealed. This thesis focuses on the protoplanetary disk phase, where the primordial planet-forming material can be observed at high resolution (sub-)millimeter wavelengths.

Protoplanetary disks

Like their parent clouds, protoplanetary disks are gas-rich structures with solid particles (dust) that account for only a few percent of their mass. The bulk of the gaseous disk material is molecular hydrogen (H_2), however its emission is extremely faint and inaccesible with current telescopes. Carbon monoxide (CO) is the second most abundant molecule after H_2 and frequently detected, making it the preferred probe of the material reservoir. Other gas tracers commonly observed in protoplanetary disks are; CN, HCN, H_2CO, CS, HCO^+, N_2H^+, H_2O and C_2H.

Figure 6 presents the radial and vertical material distribution within a disk, together with the main features and ongoing processes. Radially, the disk is divided between a hot inner disk (<20 au) and a cold outer disk. ALMA observations can access the outer disk at a spatial resolution of a few astronomical units. Understanding the morphology, properties and dynamics of any radial, azimuthal or vertical substructures is a key goal of planet-formation studies in order to directly probe ongoing processes.

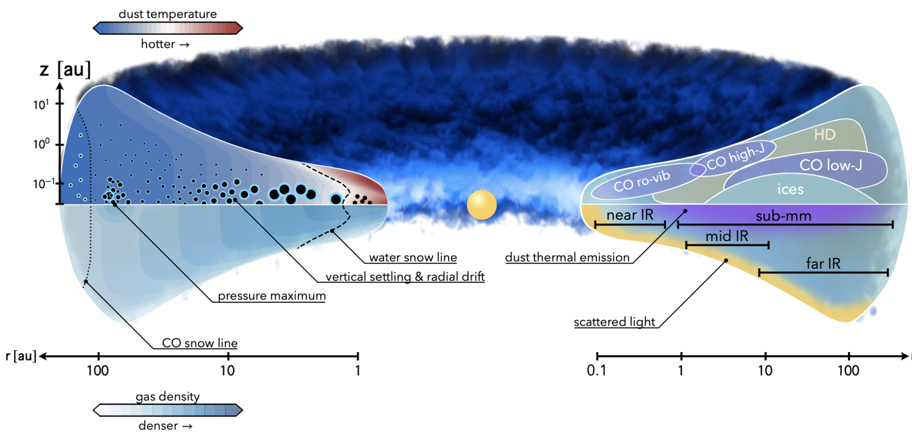

Figure 3: Illustration from Miotello et al. (2023) indicating the emission regions, relevant scales, dust temperature and gas density structure in protoplanetary disks. Left side shows the distribution of dust particles in black circles with different sizes represented as symbol size. Right side presents a simplified view of the molecular layering for the main gas-phase molecules. In the bottom the dust thermal and scattered light emission regions are highlighted in purple and yellow.

In their vertical dimensions, disks have an extent that is set by hydrostatic equilibrium. This means that the balance between the gravitational potential of the star and thermal support of the material will shape their vertical distribution.

Therefore, the vertical distribution of protoplanetary disks contains information on key physical properties such as the thermal and density structure. Vertical structure may also be used as a probe for the ionisation field and the presence of hydrodynamical instabilities and winds. However, observationally probing the vertical dimension in large disk samples has only been possible over the past few years and, in particular, through the results of this thesis.

Studying the disk vertical structure

Accessing the vertical dimension of protoplanetary disks with ALMA will depend on the inclination angle at which the disk is viewed from earth. There are two extreme cases; 1) edge-on disks with high inclinations ($\gtrsim 75°$) and 2) face-on disks at low inclinations ($\lesssim 35°$). In both cases only two dimensions can be accessed, for edge-on disks the vertical and radial, for face-on disks the radial and azimuthal. The remainder of the protoplanetary disk sample, with observed inclinations between $\sim$35-70° are classified as mid-inclination disks. Our work focuses on these sources, as they allow for an accurate representation of the ongoing processes throughout their whole three-dimensional structure, including the vertical axis. Figure 4 shows each of the inclination scenarios.

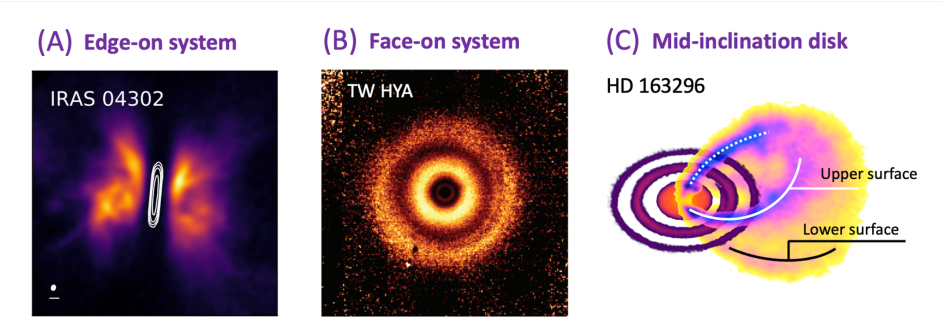

Figure 4: Three protoplanetary disks systems with different viewing inclinations. For IRAS 04302 colors trace the small dust grain distribution, which is well coupled to the gas, and white contours show the mm-continuum disk (van't Hoff et al. 2020). TW Hya is observed in ALMA mm-continuum (Andrews 2020). HD 163296 shows the rings from ALMA mm-continuum tracing the disk midplane and a single CO gas channel where the upper and lower emission surfaces extend vertically.

In mid-inclination disks observed by ALMA, the vertical dimension can be directly probed through the emission channel maps by tracing the emission maxima, as shown in the right panel of Figure 4. This methodology is sensitive to any substructure or asymmetry that may be present and has been implemented in public algorithms such as ALFAHOR (see Chapter 3 of this Thesis).

The immediate applications of measuring the vertical molecular layers in protoplanetary disks are many, depending on the selected tracers, the resolution and the available information from any radial or azimuthal structures. The temperature structure can be traced through the peak brightness temperature of CO isotopologues, providing strong constraints to benchmark thermochemical models and precise temperature measurements, which are critical in turbulence studies (see Chapter 4 of this thesis for an application). If spatially resolved kinematic information is available, recent methods allow to separate the radial, azimuthal and vertical components of the material motion, combining this with the location of the vertical emission surfaces it is possible to directly trace and test the presence of meridonial flows or disk winds which are crucial for understanding disk dynamics. Most recently, by tracing the vertical location of atomic carbon, early studies are being conducted to understand the location of the hot irradiated disk surface and the properties of this region.

This thesis

Recognizing the importance of characterizing the vertical protoplanetary disk structure to further understand the conditions and governing processes of planet formation, this thesis presents an in-depth observational and theoretical analysis of the vertical dimension. Here is an outline of the upcoming chapters and conclusions of this work,

Chapter 2: **Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk.** We analyse CN $N = 3 - 2$ in two different transitions and compare it to CO isotopologue emission. Our results show that the vertical location of CN and CO in Elias 2-27 is layered and consistent with predictions from thermochemical models. The inferred CN column densities, low optical depth ($\tau \leq 1$), and location near the disk surface agree with thermochemical disk models where CN formation is initiated by the reaction of N with UV-pumped H_2. This study highlights the importance of tracing the vertical location of various molecules to constrain the physical disk conditions.

Chapter 3: **Directly tracing the vertical stratification of molecules in protoplanetary disks.** The ALFAHOR code is presented, this is an implementation of the Pinte et al. (2018a) method and obtains accurate vertical profiles even for low signal-to-noise molecules using interactive masking of emission channel maps. Using ALFAHOR we study the molecular emission surfaces of Elias 2-27, WaOph 6, and the five sources from the MAPS ALMA Large Program. Thermal structure, gas pressure scale heights, substructure and modulations in the vertical profiles and relations to the chemical origin of each observed molecule are discussed. Overall, we show that it is possible to trace the vertical locations of multiple molecular species and relate this information to a wide variety of physical and chemical disk properties.

Chapter 4: **High turbulence in the IM Lup protoplanetary disk. Direct observational constraints from CN and C_2H emission.** Constraining turbulence in disks is key to understanding their evolution, however its measurement relies on knowledge of the thermal conditions for the molecular emission. Combining the information on the physically resolved temperature structure that can be obtained from the vertical structure analysis, we present a new way of directly measuring turbulence. This method is benchmarked using CN and C_2H molecular emission from the protoplanetary disk of IM Lup. Our analysis retrieves high turbulence of Mach 0.4-0.6 at $z/r \sim 0.25$. This study presents the first empirical evidence for a vertical gradient in the disk turbulence, which is a key prediction of magneto rotational instabilities.

Chapter 5: **Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion.** Using thermochemical models we study the protoplanetary disk and stellar host properties that most affect the vertical location of CO $J = 2 - 1$ emission surfaces. The modelling predictions are benchmarked against data of CO emission from nineteen disks. We find that the CO emission surface is most affected by the total disk mass (M_d) and volatile carbon abundance, which leads to a z/r-M_d relationship. In order to reconcile total disk mass estimates from the characteristic z/r and the values obtained based on dust continuum analysis, a volatile carbon depletion of 10-100 (with respect to the ISM) is needed for the majority of sources.

Future outlook

Studies of vertical disk structure in large samples are in early stages, to date only ~ 20 disks have vertical CO surfaces characterized and $\sim$8 (Paneque-Carreño et al. 2023; Law et al. 2024) have measured vertical profiles of more than three different molecules. The overall work from this thesis has shown that it is possible to use ALMA observations to study the vertical molecular layering and relate it to a number of physical processes.

Future work must focus on expanding the sample of disks with characterized molecular surfaces and combine the chemical information with knowledge on the dust grain distribution to accurately characterize disk processes. This requires high spatial and spectral resolution observations of molecules beyond CO, which is typically time consuming due to the low signal-to-noise of less abundant tracers. The upcoming ALMA Wideband Sensitivity Upgrade in the next decade will allow us to do these studies in less time and for larger samples.

Overall, the possibility of studying the protoplanetary disk material distribution across all three dimensions offers unique insight into the process of forming planets. Observational constraints are now catching up to theoretical models, which must be revised in order to explain the totality of observed features. In the same way that for the past years studies have focused on explaining the existence of radial and azimuthal substructure, we must now look at the third dimension and understand the information that comes from it. The techniques and results from this thesis have laid the foundations for many future studies that will for sure answer the questions we now leave open.