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

Paneque Carreño, T.

Chapter 1

Introduction

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. What western cultures decided to name the Milky Way was known as the River of Life, River of Stars or River Above to the *Lickan Antay.* Within this River of Stars, which we now know is the projection of our galaxy seen in the sky, the *Lickan Antay* observed the dark regions to mark their constellations. In these obscure zones they drew a number of creatures seen in the Andes such as a llama and her baby, a fox, a snake and a toad. This interpretation of the sky was related to their cosmovision, where they proposed that all the beings and experiences they had on earth should have a representation in the stars.

Thousands of years later, many astronomers remain interested in those dark regions and, from the same Atacama desert, point the largest telescopes in the world to observe them. It is now known that they are dark because small dust grains absorb the starlight at optical frequencies, leading to high visual extinctions (Bergin & Tafalla 2007). Most importantly, these dark clouds are associated with star-forming regions (Bok 1948) and, while our eyes are not able to see past the dust, instruments such as the Atacama Large Millimeter/submillimeter Array (ALMA[1]) can reveal their secrets. ALMA is built on the Chajnantor plateau, a sacred place for the *Lickan Antay* that means "place of departure" in the Kunza 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.

[1]ALMA is a partnership of ESO (representing its member states), NSF (USA) and NINS (Japan), together with NRC (Canada), NSTC and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO and NAOJ

Such fundamental questions regarding the origin of our planet must be answered through global participation and, indeed, ALMA is a testimony to scientific and international collaboration. The observatory is composed of 66 antennas that work simultaneously while they are spread over nearly 16 kilometers in the Chajnantor plateau. Groups of antennas and their technology are provided by consortiums from more than 20 countries across North America, Europe and East Asia, including Chile as host country and collaborator.

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 (see for example the iconic first high-resolution image of a protoplanetary disk around HL Tau, ALMA Partnership et al. 2015). Through observations and theoretical understanding of the cold 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? As the *Lickan Antay* did centuries ago - and are still doing to this day - we observe the conditions in our surroundings and look for them in the skies, only going a bit further. In practice, we measure abundances and take data from the Solar System, predict possible scenarios for earth's formation and search the dark clouds for clues as to whether we may or may not be correct.

1.1 Star and planet formation

The process of planet formation is intrinsically linked to stellar formation. Stars form from the collapsing material of dark and cold molecular clouds with characteristic densities $>10^2 n_{\mathrm{H}}\mathrm{cm}^{-3}$ (hydrogen nuclei per cubic centimeter, Öberg & Bergin 2021a). The initial cloud composition is expected to be mostly gas, with one percent of sub-micron dust particles formed of silicates and carbonaceous material (Bohlin et al. 1978; Henning 2010). Through their high densities, molecular clouds shield themselves against external radiation and achieve low temperatures (10-20 K) in their centers, where denser structures, known as pre-stellar cores, can assemble (Bergin & Tafalla 2007). Pre-stellar cores slowly rotate while they reach densities of $\sim 10^6$, temperatures of $\sim$10 K and sizes of order $\sim$0.1 pc (Terebey et al. 1984; Myers & Benson 1983; Bergin & Tafalla 2007). Cores that are dense enough to overcome turbulence, thermal and magnetic pressure, gravitationally collapse inwards conserving angular momentum to form one or multiple protostars (Shu 1977; Galli & Shu 1993).

Going from a pre-stellar core to a planetary system, young stellar objects (YSOs) are classified into Classes (0, I, II or III) through the analysis of the slope of their spectral energy distribution (SED) between 2-25μm (Lada 1987, see also Figure 1.1). In the earliest Class 0/I stage, a protostar will be actively accreting material from its surrounding cloud core or protostellar envelope while angular momentum conservation acts by spreading out the accreting material to form a rotating disk-like structure (Cassen & Moosman 1981). This deeply embedded Class 0/I phase is hard to observe at millimeter wavelengths, as the envelope material blocks the emission from the protostar and disk (Williams & Cieza 2011; Tobin et al. 2015; Ohashi et al. 2023).

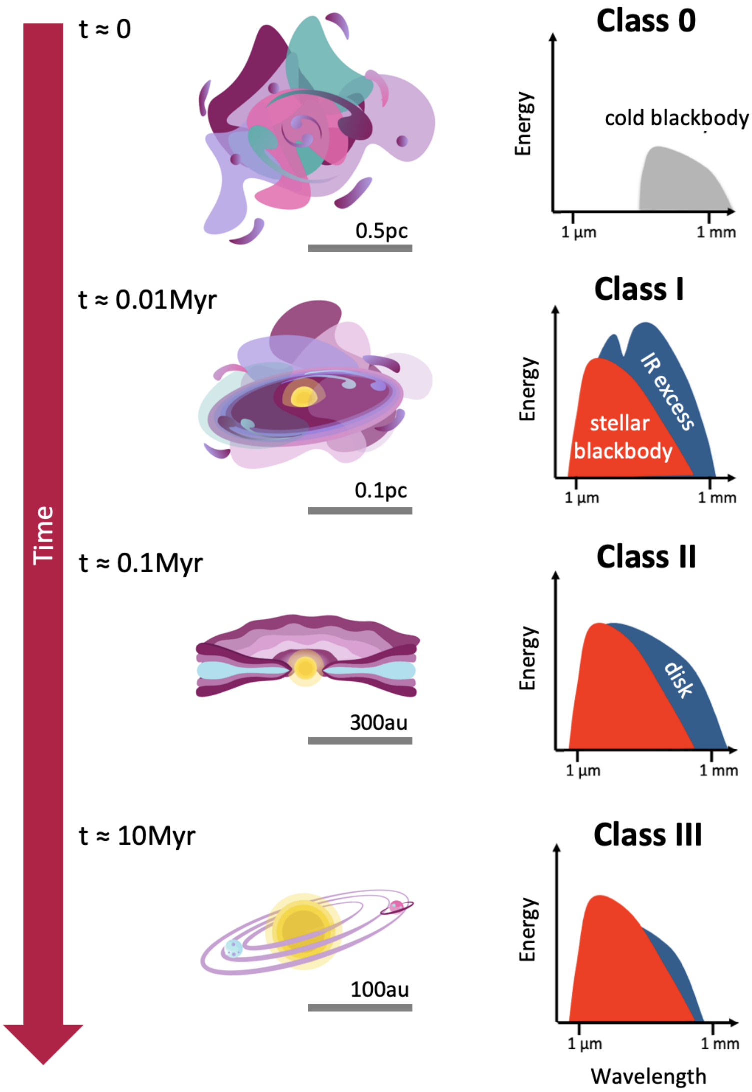

Figure 1.1: Schematic of star and planet formation timeline. Left: evolutionary stages from pre-stellar core to planetary system. Right: typical SEDs and respective classification, corresponding to each stage. SEDs adapted from A. Miotello's PhD thesis.

As time passes, in ∼0.5-1 Myr, the protostellar envelope is dispersed via molecular outflows and accretion, revealing a pre-main sequence star and a Keplerian disk (Williams & Cieza 2011; Öberg & Bergin 2021a). These circumstellar accretion 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 may last ∼1-10 Myr (Mamajek 2009) and ends when most of the disk material has either accreted onto the star, formed planets, or has been dispersed through photoevaporative winds and other processes (Alexander et al. 2006a,b; Pascucci et al. 2023). Finally, a planetary system is produced, which may continue evolving through collisions or interactions between its components (e.g., Wyatt 2018).

This thesis focuses on the protoplanetary disk phase, where the primordial planet-forming material can be readily observed and characterized at (sub-)millimeter wavelengths at high spatial and spectral resolution (e.g., Andrews et al. 2018; Öberg et al. 2021b). By tracing the material composition and distribution at mm wavelengths, it is possible to probe the ongoing processes and understand the planet-forming environment.

1.2 Protoplanetary disks

1.2.1 Composition and mass

1.2.1.1 Dust

Like their parent clouds, protoplanetary disks are gas-rich structures with solid particles accounting for only a few percent of their mass. Studying the dust component of disks is crucial for understanding planetesimal core and rocky-planet formation (Testi et al. 2014). The amount of solid particles will inform on how much material remains to form planetary cores, to obtain this number one must have an estimate of the total dust surface density or total dust mass. It is also relevant to estimate the size of these particles, as it can be used to predict their aerodynamic behavior when interacting with the gas reservoir (Whipple 1972; Weidenschilling 1977).

Assuming optically thin dust continuum emission, the total flux of the disk (F_ν) can be related to the total dust mass ($M_{\rm dust}$) following,

$$F_\nu = \frac{B_\nu(T_d)\kappa}{d^2} M_{\rm dust} \tag{1.1}$$

where d is the distance to the source, B_ν the Planck spectrum at the assumed dust temperature T_d and κ the dust opacity. This relationship was first proposed by Hildebrand (1983). In most studies, T_d and κ are disk-averaged values calculated from the stellar properties and an assumed grain porosity. From the estimated dust mass, typically an ISM-like gas-to-dust ratio of 100 is considered to calculate the total disk (e.g., Andrews et al. 2013; Ansdell et al. 2016; Barenfeld et al. 2016; Pascucci et al. 2016; Ansdell et al. 2017; Cazzoletti et al. 2019; Stapper et al. 2022). Overall, estimates of the disk mass extracted from the continuum flux can be uncertain, given the number of assumptions used to estimate the physical parameters (temperature, porosity, gas-to-dust ratio), however this approach to extract dust masses has been largely used in the literature and may give a first-order approach to measuring the disk material (for further discussion see Miotello et al. 2023).

The initial dust reservoir consists of μm-sized grains, however as these solids grow, the presence of large dust grains will alter the dust opacity of the emission, which in the (sub-)millimeter regime is related to the frequency of the observations such that $\kappa \propto \nu^{\beta}$. For grains of millimeter or larger sizes, β becomes smaller. In the Rayleigh-Jeans regime ($h\nu << kT$), the intensity of optically thin emission relates to the frequency as $I_{\nu} \propto \nu^{\alpha}$, where $\alpha = \beta + 2$ (Draine 2006; Testi et al. 2014). Studies of the opacity spectral index β confirm dust growth in protoplanetary disks, as they find dust aggregates larger than millimeter sizes (e.g., Tazzari et al. 2021a,b). Including more realistic processes affecting dust emission, such as scattering (e.g., Sierra et al. 2021; Carrasco-González et al. 2019) or polarization effects (e.g., Kataoka et al. 2016) can vary these values. The presence and distribution of large and small dust grains will have a direct effect on the protoplanetary disk heating processes, as μm-sized dust will couple to the gas and effectively shield disk regions from energetic radiation, while larger particles will settle towards the midplane and affect the chemical reservoir by sequestering volatiles in their ice mantles or creating dust over-densities (D'Alessio et al. 2005; Henning 2010; Andrews 2020).

1.2.1.2 Gas

The bulk of the gaseous disk material is molecular hydrogen (H_2), however due to the lack of permanent dipole moment, its emission is extremely faint at the typical temperatures (20-30 K) and conditions of the outer (>20 au) disk (Field et al. 1966). A less abundant isotopologue, hydrogen deuteride (HD), can be detected at protoplanetary disk conditions in its fundamental rotational transition ($J = 1 - 0$), however, there are some caveats to interpreting HD emission (e.g., Trapman et al. 2017; Calahan et al. 2021) and there are no current facilities that may observe it at 112 μm (Kamp et al. 2021). Realistically, the best alternative for probing the gas reservoir is carbon monoxide (CO). CO is the second most abundant molecule after H_2 and its chemistry has been deeply studied in many astrochemical contexts, as it is the most abundant gas-phase carrier of interstellar carbon (van Dishoeck & Black 1988; Miotello et al. 2023).

CO is readily detected at (sub-)millimeter wavelengths in protoplanetary disks, particularly in its main isotopologue $^{12}C^{16}O$ (Dutrey et al. 1997; Ansdell et al. 2016; Pascucci et al. 2016; Eisner et al. 2016; Cieza et al. 2019; Long et al. 2018; Ansdell et al. 2017; Cazzoletti et al. 2019). The survival of CO in gas phase is regulated by its photodissociation due to UV photons and CO freeze-out onto dust grains at low ($\leq$20 K) temperatures. CO manages to achieve column densities sufficient to self-shield from UV photons and survive at high abundance throughout the disk (Aikawa et al. 2002; van Dishoeck & Black 1988). Its characteristics have made it the most used molecular probe of disk conditions and it is used to trace the disk extent (Ansdell et al. 2016; Law et al. 2022), hunt for kinematical signatures (Teague et al. 2018a; Pinte et al. 2018b; Izquierdo et al. 2022, 2023), as a temperature probe (Law et al. 2021b) and disk mass tracer (Miotello et al. 2014, 2016; Stapper et al. 2024).

Beyond CO and its isotopologues, molecules that have been frequently detected in protoplanetary disks environments include; CN, HCN, H_2CO, CS, HCO^+, N_2H^+, H_2O, C_2H, among others (e.g., Dutrey et al. 1997; Thi et al. 2004; Dutrey et al. 2007; Hogerheijde et al. 2011; Öberg et al. 2021a,b; Booth et al. 2023). Precursors of complex organic molecules such as methanol (Walsh et al. 2016; Booth et al. 2021) and dimethyl ether (Brunken et al. 2022) are less frequently observed, but exemplify the rich chemistry that may be occurring in these epochs (see also Booth et al. 2024). It is still an open question whether the chemical composition of the disk gas is directly inherited from the interstellar medium and molecular cloud or if significant reprocessing occurs during/before this phase. Indeed, for the most studied case of CO, multiple studies support that CO abundance considerably reduces (between one or two orders of magnitude) throughout the early stages of planet and stellar formation passing from an abundance of $\sim 10^{-4}$ (with respect to H_2) to $10^{-5} - 10^{-6}$ (e.g., Zhang et al. 2019, 2020; Schwarz et al. 2016; Bergin et al. 2014; Bosman et al. 2018).

1.2.2 Disk evolution

Above all, protoplanetary disks are accretion disks and their main physical process is to funnel material onto the central stellar object (Hartmann et al. 2016; Manara et al. 2023). Accretion is a fundamental problem in astrophysics, as it requires a mechanism through which particles lose angular momentum in order to move closer and accrete onto the central object (for dedicated reviews see Hartmann et al. 2016; Lesur et al. 2023). In protoplanetary disks there are two main scenarios proposed to enable this process; (1) viscosity inside the disk that transports angular momentum to the outer disk (Shakura & Sunyaev 1973) or (2) magnetically-driven disk winds that disperse mass from the upper layers, thus taking angular momentum away (Blandford & Payne 1982).

Viscous evolution has traditionally been the preferred theory for driving protoplanetary disk evolution due to its simplicity (i.e., it can be expressed analytically), but the the exact physical origin of the viscosity is still not clear. Considering the disk as a viscous fluid, the first cause of viscosity would be the random collisions between gas particles, creating a molecular viscosity. However, protoplanetary disks are not viscous like honey or other thick fluids, in fact, the viscosity of a gas can be estimated as $\nu \sim v_{th}\lambda$ where v_{th} is the thermal speed of the molecules and λ the mean-free path. We can estimate these parameters based on reasonable assumptions of disk conditions and calculate $\lambda \sim 1/n\sigma$, where n is the molecular number density and σ the collision cross-section. Overall, estimates of molecular viscosity yield $\nu \sim 10^5\ \mathrm{cm^2\,s^{-1}}$ (Armitage 2015). For a disk with characteristic size r, the viscously-driven evolution timescale (t_ν) follows,

$$t_\nu = \frac{r^2}{\nu} \tag{1.2}$$

Therefore, on its own, the estimated molecular viscosity would drive disk evolution within a timescale of $\sim 10^{13}$ yr, much larger than the protoplanetary disk lifetime, which survives roughly for a few Myr (Williams & Cieza 2011; Mamajek 2009). This large viscous timescale proves that molecular viscosity alone cannot be responsible for disk evolution. Shakura & Sunyaev (1973) solved the viscous problem by proposing that random velocity fluctuations, known as turbulence, might act as an effective viscosity, removing angular momentum and driving disk evolution in reasonable timescales. In this case viscosity is parametrized as,

$$v = \alpha c_s H \tag{1.3}$$

where c_s is the sound speed and H the hydrodynamical pressure scale height (described in section 1.2.3.2). Typically an α of $\sim 10^{-2}$ is required to match observational constraints of timescales and accretion rates (Armitage 2015). While this prescription is a sensible solution, it still poses the question regarding the origin and strength of turbulent motions. Various hydrodynamical instabilities have been proposed to cause turbulence, with distinct vertical patterns and launching mechanisms (Lesur et al. 2023). Magneto-rotational instability (MRI, Balbus & Hawley 1991) and vertical shear instability (VSI, Urpin & Brandenburg 1998) will produce high values of turbulence in the upper disk and smaller fluctuations near the midplane (Shi & Chiang 2014; Simon et al. 2015). Comparatively, gravitational instability (GI, Lynden-Bell & Pringle 1974) is expected to launch turbulent motions that will be constant throughout the disk vertical structure (Forgan et al. 2012). We will discuss turbulence in depth and the relevance of resolving its value across the vertical structure in chapter 4.

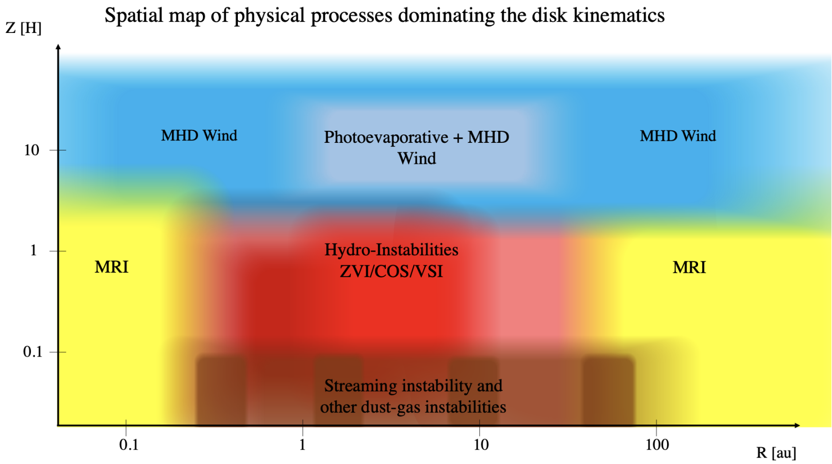

Figure 1.2: Figure from Lesur et al. (2023) indicating the spatial map of dominant physical processes (hydrodynamical instabilities and winds) relevant for the evolution of protoplanetary disks. Distribution of specific instabilities can be model dependent, but in general their effects may be characterized through their local vertical and radial perturbations.

Evolution may also be driven or aided by external torques, specifically, the presence of magneto-hydrodynamical (MHD) winds could cause a magnetic torque on the disk surface and drive mass loss (Blandford & Payne 1982; Wardle & Koenigl 1993). MHD processes require the disk material to be ionized, as the gas must support electrical currents in order to interact with the magnetic field and launch the wind (Lesur et al. 2023). It has been shown that even for weakly ionized disks, magnetised outflows may be launched resulting in a mass loss rate within the order of measured accretion rates (Bai & Stone 2013; Simon et al. 2013; Bai 2017; Lesur et al. 2014; Gressel et al. 2015). Unfortunately, while many theoretical models predict the effectiveness of MHD winds, observational confirmation has been scarce. Winds have been identified in a number of systems, but determining their nature (MHD or thermal) is still a complication within the field (see discussion in Pascucci et al. 2023). Upcoming facilities such as the Next Generation Very Large Array (ngVLA), could make advances in this matter (Ricci et al. 2021). Figure 1.2 maps the regions where winds may be relevant ($z/r \gtrsim 10$) compared to the previously discussed hydrodynamical instabilities which may drive turbulent motions in disk layers between the midplane and $z/r \sim 8$.

1.2.3 Disk structure

In simple terms a protoplanetary disk consists of material orbiting around the star following (mostly) Keplerian motion. As discussed in previous sections, dust aggregates have their dynamics determined by gravitational and centrifugal forces, together with the drag they feel from the gas (Whipple 1972; Weidenschilling 1977). Gas particles are also subject to gravitational and centrifugal forces, but in addition feel radial and vertical pressure support which will directly depend on the gas temperature (Pinte et al. 2023). Overall, pressure support will create a force pointing outwards from the inner disk, causing the gas to have a slightly sub-Keplerian motion. This velocity difference with respect to the dust particles (that are not pressure supported) will decelerate the dust, causing solids to loose angular momentum and drift towards the inner disk (Whipple 1972; Weidenschilling 1977). To avoid this *radial drift* and fast accretion of the solid reservoir, radial pressure gradients must exist, to accumulate and allow dust growth to happen at locations of pressure maxima (Pinilla et al. 2012a,b). This is particularly relevant for large (mm-cm) solids, as the smaller μm dust will be well coupled to and follow the molecular gas dynamics and structure. Figure 1.3 represents the radial and vertical material distribution and main processes discussed in the following sections.

1.2.3.1 Radial distribution

Radially, the disk can be divided between a hot inner disk (<20 au) and a cold outer disk. Infrared telescopes such as the James Webb Space Telescope (JWST) study the emission at several 100 K of the inner disk and many ongoing studies are trying to understand the structure and processes in the terrestrial-planet forming zone, close to the star. These topics, however, are outside the scope of this thesis and we will not refer to them beyond acknowledging their importance towards characterizing the innermost planet-forming zone.

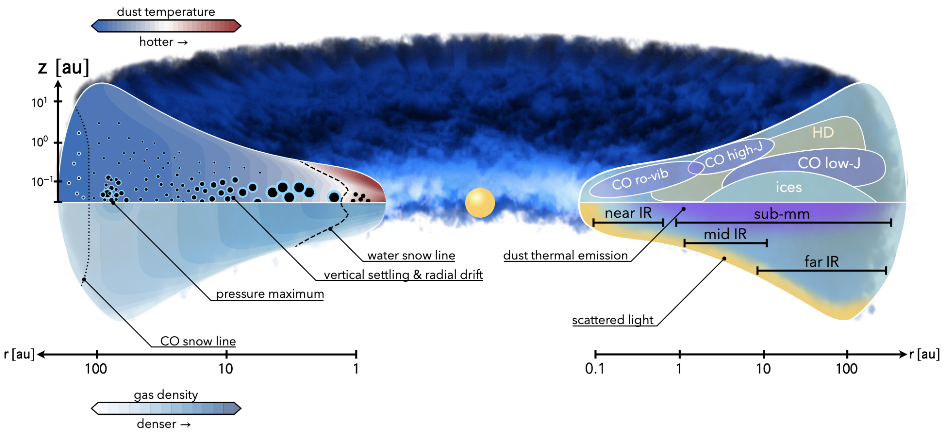

Figure 1.3: Illustration from Miotello et al. (2023) indicating the emission regions, relevant scales, dust temperature and gas density structure in protoplanetary disks. Left side shows the distribution of dust particles in black circles with different sizes represented as symbol size. Right side presents a simplified view of the molecular layering for the main observed gas-phase molecules. In the bottom the main dust thermal and scattered light emission regions are highlighted in purple and yellow.

On the other hand, ALMA observations can access the outer disk at a spatial resolution of a few au (depending on the observing frequency, ALMA Partnership et al. 2015) when observing systems at ∼150 pc distance (the typical distance of nearby Star-Forming Regions, Gaia Collaboration et al. 2023), obtaining high spatial resolution data of the material beyond ∼20 au (e.g., Andrews et al. 2018; Öberg et al. 2021b). Several systems have now been observed at the highest resolution possible with ALMA, revealing a plethora of continuum and gas substructures, from axisymmetric rings, cavities and gaps (ALMA Partnership et al. 2015; Huang et al. 2018b) to azimuthally concentrated vortices (Pérez et al. 2018a), spirals (Pérez et al. 2016; Huang et al. 2018c) and extreme asymmetries (van der Marel et al. 2013). Radial substructure is ubiquitous and expected, as it is the physical representation of accumulation of dust grains in pressure maxima, overcoming the radial drift problem (Pinilla et al. 2012b; Testi et al. 2014). By analyzing the morphology, properties and dynamics of these substructures, studies aim to determine their physical or chemical origin (Andrews 2020).

Assuming that substructures are only a lower-order modulation of the radial disk structure, most works assume that the radial distribution of material (surface density, $\Sigma(R)$ profile) follows a radial power-law dependence, typically with an exponential taper at large radii. The precise prescription for the surface density will depend on the governing evolution mechanism and different prescriptions have been proposed in individual disk studies. The most used form is the self-similar solution for a viscously evolving disk (Lynden-Bell & Pringle 1974; Andrews et al. 2011), such that the surface density follows,

$$\Sigma(R) = \Sigma_c \left(\frac{R}{R_c}\right)^{-\gamma} \exp\left[-\frac{R}{R_c}\right]^{2-\gamma} \tag{1.4}$$

where R_c is the characteristic radius and γ the surface density exponent. It is important to note that dust and gas will likely have different radial distributions; indeed the MAPS ALMA large program (Öberg et al. 2021b) showed that molecular emission substructure is rarely coincident with the continuum substructure (Law et al. 2021a). Multiple studies have also shown that gas outer radii are generally many times larger than the dusty mm-disk edge, indicating a more extended distribution for the gas (see discussion in Miotello et al. 2023).

1.2.3.2 Vertical structure

From a theoretical standpoint, disks are well described in their vertical dimension. Hydrostatic equilibrium between the gravitational potential of the star and thermal support will shape the vertical distribution of the gaseous material and of the small dust grains coupled to it (Armitage 2015). In cylindrical coordinates, the hydrostatic equilibrium equation for the vertical direction follows,

$$\frac{1}{\rho}\frac{dP}{dz} = -\frac{d\phi}{dz} \tag{1.5}$$

where ρ is the gas density, P the gas pressure and ϕ the gravitational potential. Strictly speaking, both the central star and the disk material contribute to the gravitational potential, however, in most cases the disk self-gravity is negligible and therefore we consider only the stellar gravitational potential,

$$\phi = -\frac{GM_*}{(r^2 + z^2)^{1/2}} \tag{1.6}$$

For an ideal gas, pressure and density can be related such that $P/\rho = c_s^2 = kT/(\mu m_p)$, where c_s is the sound speed. The differential equation to solve for P is,

$$\frac{1}{P}\frac{dP}{dz} = -\frac{z\,GM_*}{c_s^2(r^2 + z^2)^{3/2}} \tag{1.7}$$

which in the most general form can be solved through,

$$P(z) = c_s(z)^2\rho(z) = C\exp\left(-\int \frac{z\,GM_*}{c_s^2(r^2 + z^2)^{3/2}}dz\right) \tag{1.8}$$

where C is an integration constant. The latter equation describes the gas density throughout the vertical extent at each radial position, which will depend on the thermal structure through c_s. Indeed, disks are not isothermal, but it is not possible to analytically determine their thermal gradient, as it will depend on the stellar radiation parameters, dust distribution (which affect in cooling and shielding) and material density. Numerical models that aim to solve this equation must do so self-consistently, assuming a previously computed thermal structure to iterate from (e.g., D'Alessio et al. 1998, see also Chapter 5 of this thesis). A common approximation to the vertical density distribution is to assume a thin disk such that $z << r$ where the disk is vertically isothermal. This simplifies our general equation as c_s will no longer have a vertical dependence, therefore the solution follows,

$$\rho(z) = \rho_c(r)\exp\left[-\frac{z^2}{(2H^2)}\right] \tag{1.9}$$

Here $\rho_c(r)$ is the gas density at the midplane ($z = 0$) and H is known as the gas pressure scale height such that,

$$H = \sqrt{k\,T\,r^3/(\mu m_p\,GM_*)} = c_s/\Omega \tag{1.10}$$

where T is the midplane temperature, constant across the vertical extent in this approximation and Ω the disk angular velocity. Upcoming sections and chapters in this thesis will discuss observational proof that this is not an adequate solution to the vertical structure, however it is a first-order approximation used in many state-of-the-art hydrodynamical and thermochemical models to set the vertical material distribution.

1.3 Studying the disk vertical structure

As discussed in the previous sections, the vertical structure of disks contains information on key physical disk properties such as the thermal, ionisation and density structure, characteristic hydrodynamical instabilities and winds. However, probing this dimension observationally in large disk samples has only been possible over the past few years. Many of the data-driven advances presented in this section are also addressed in throughout the thesis and will be discussed in depth along the upcoming chapters. To avoid reiterating results, only conclusions from other groups are presented in this section.

1.3.1 Framework from theoretical models

A number of thermochemical models that account for the physics and chemistry of protoplanetary disks have been developed in the past years (e.g., D'Alessio et al. 1998; Bruderer 2013; Woitke et al. 2016), allowing for predictions and analysis focused on the thermal, chemical and density disk structure (for an overview see Dutrey et al. 2014). These models have confirmed that protoplanetary disks should be characterized by vertical and radial temperature and density gradients, affected by varying UV radiation and X-ray intensities, depending on the stellar parameters and dust properties. Indeed, it is important to consider that the dust distribution will strongly affect the gas temperature (Jonkheid et al. 2004, 2007; D'Alessio et al. 2005, 2006) which, while not a main topic of this thesis, should be a focus of future work obtaining observational constraints of the vertical distribution of both molecular gas and dust reservoirs simultaneously. Overall, in the disk vertical extent, three regions can be characterized as shown in Figure 1.4; (1) the cold, dense and dusty midplane, (2) a warm molecular layer and (3) a hot, ionized and heavily irradiated upper disk (Aikawa & Herbst 1999; Dutrey et al. 2014).

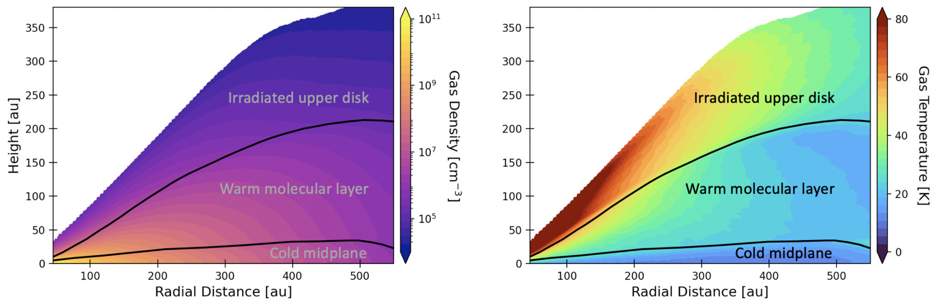

Figure 1.4: Output from thermochemical DALI (Bruderer 2013) models of the disk material surrounding a 1 solar mass star. Left panel shows the gas density distribution and the right panel displays the gas temperature, accounting for stellar, dust and molecular cooling and heating processes. Overlayed are rough estimations of the key vertical regions, the midplane, molecular layer and irradiated upper disk. Details on the model are presented in Chapter 5 of the thesis.

The dense midplane is also considered the "planet-forming zone" as larger (mm-sized) solids will settle towards it (Testi et al. 2014) and form or accrete onto planetesimals through various processes (for a review see Drążkowska et al. 2023). This region is shielded from high-energy stellar radiation through the layers of material above it, which makes it "darker" and colder than the more vertically extended material. Nevertheless, the inner ($\lesssim$10 au) disk will be extremely hot and the high densities will allow optically thick continuum emission to be used as a probe for the dust and gas temperature in that area (which will be in equilibrium due to collisional coupling, Dutrey et al. 2014), if the spatial resolution is sufficient to avoid beam-dilution effects (Andrews et al. 2018). The outer disk midplane will be extremely cold, therefore dust grains will be covered in icy mantles, that may host a reservoir of volatile rich and organic molecules (Henning & Semenov 2013; Sturm et al. 2023).

Above the midplane, a warmer ($\gtrsim$20 K) and less dense molecular zone is located. This molecular layer has boundaries loosely defined between the CO freeze-out and photodissociation layer (Aikawa et al. 2002). Conditions in this region have hydrogen densities of $n_H \sim 10^5$-10^8 cm^{-3}, allowing for multiple gas-phase and gas-grain reactions and leading to the synthesis of molecular species commonly observed in disks such as CO, CN, C_2H, H_2CO, HCN and CS, among others (Aikawa et al. 2002). Finally, a diluted, heavily irradiated and ionized layer is located at the disk surface, resembling the photodissociation regions (PDRs) at the edge of dense clouds (van Dishoeck 2006). Here ions, photostable radicles and polycyclic aromatic hydrocarbons (PAHs) may survive as molecules are photodissociated by the intense UV radiation from the central star. Atomic carbon (CI) or molecules such as C_2H and CN have been proposed to be tracers of the lower boundary for this zone, given their UV-chemistry origin (Bergin et al. 2016; Cazzoletti et al. 2018; Law et al. 2023a), however there is a lack of observational agreement or understanding about the location and properties of this region (see discussion in Urbina et al. 2024).

1.3.2 Extreme inclination disks

1.3.2.1 Edge-on

Vertical structure can be immediately accessed in edge-on disks, where high inclinations ($\gtrsim 75°$) allow observations to directly probe the 2D radial and vertical material distribution. Protoplanetary disks from evolved systems (Class II, Guilloteau et al. 2016a; Dutrey et al. 2017; Louvet et al. 2018; Ruíz-Rodríguez et al. 2021; Villenave et al. 2020, 2022) and younger stars (Class I/0, Podio et al. 2020; van't Hoff et al. 2020; Villenave et al. 2023) at high inclinations have been studied at millimeter wavelengths thorough dust continuum and molecular line emission. Figure 1.5 shows an example from dust and gas emission in an edge-on system.

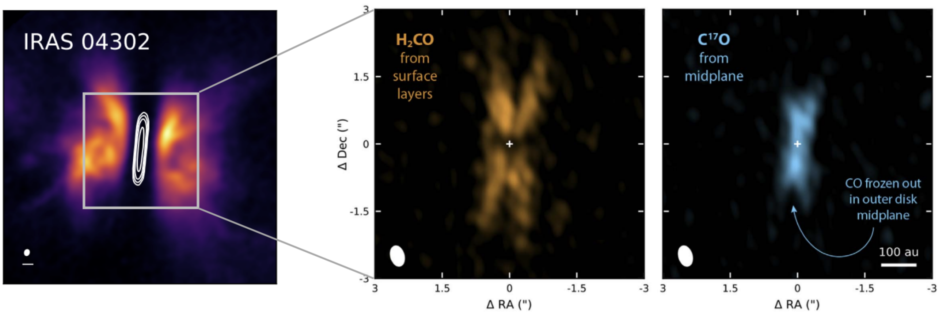

Figure 1.5: Data from edge-on source IRAS 04302. Data on left panel shows the dust continuum traced at mm wavelengths by ALMA (white contours) and the μm grains observed through scattered light (colors) shown in Villenave et al. (2020). The right two panels present molecular emission from H_2CO and $C^{17}O$ studied in van't Hoff et al. (2020).

Continuum emission data show that the millimeter-sized grains in Class II disks are significantly settled vertically, while earlier epochs show a measurable vertical extent or cannot be characterized due to their large optical thickness (Villenave et al. 2023, 2022). This offers observational evidence for dust settling processes affecting larger grains, while the small μm sized particles are coupled to the gas and trace a much more vertically and radially extended region. Observations of scattered light taken both from ground and space observatories show with exquisite detail the separation between the vertical zones traced by each grain size in edge-on systems (e.g., Padgett et al. 1999; Stapelfeldt et al. 2014).

Constraints from the distribution of molecular gas in edge-on disks have given crucial insight into processes such as CO freeze out (see rightmost panel in Figure 1.5) and allowed for a direct comparison to thermochemical models in order to better understand processes affecting temperature and density throughout the disk extent (Dutrey et al. 2017; Ruíz-Rodríguez et al. 2021; van't Hoff et al. 2020). Unfortunately, the sample of edge-on disks is a small fraction of all detected protoplanetary disks and their high inclinations make it extremely complex to compare the observed features to any azimuthal or radial structure. Attempts to deproject the emission and obtain the 3D material distribution at high inclination have been scarce due to their complexity and the need for high spatial resolution and sensitivity (e.g., Dent et al. 2014; Teague et al. 2020).

1.3.2.2 Face-on

On the other side of the inclination spectrum lie face-on disks. These low-inclination objects ($\lesssim$35° inclination) show the 2D radial and azimuthal material distribution, but lack the orientation to easily access the vertical structure. There are many examples of such disks, more than for edge-on systems given the broader inclination range, but for this section we focus on TW Hya as a representative of face-on systems hosting a protoplanetary disk with an inclination of ∼6°.

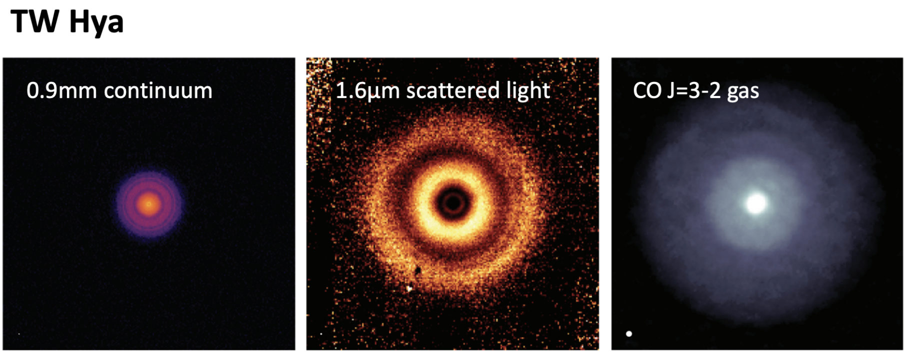

Figure 1.6: Panels with data from continuum (mm ALMA and μm scattered light) and CO gas emission observed in TW Hya. Adapted from Andrews (2020).

TW Hya is one of the most studied systems due to its closeness to earth (∼60 pc Gaia Collaboration et al. 2023) and bright protoplanetary disk studied in dust (e.g., Kim et al. 2019; Ilee et al. 2022; Macías et al. 2021; Nomura et al. 2016; Wilner et al. 2000; Andrews et al. 2012; Tsukagoshi et al. 2022; Hogerheijde et al. 2016; Jayawardhana et al. 1999) and gas (e.g., Huang et al. 2018a; Walsh et al. 2018; Nomura et al. 2021; Teague et al. 2017; Kastner et al. 2015; Salinas et al. 2016; Yoshida et al. 2022; Rosenfeld et al. 2012; Vlemmings et al. 2019; Bergin et al. 2013; Schwarz et al. 2016; Teague et al. 2016). Adequately constraining its thermal vertical structure has been at the core of many TW Hya studies, as interpretation of the total disk mass (e.g., Calahan et al. 2021), turbulent motions (Teague et al. 2016, 2018b), dynamics (e.g., Rosenfeld et al. 2012) and dust properties (e.g., Macías et al. 2021) all require assumptions on the vertical material distribution and properties. Uncertainties in this dimension may be a reason as to why, for example, the disk mass estimates using different tracers and approaches yields differences of up to two orders of magnitude between methods (see discussion in Miotello et al. 2023). Indeed, Calahan et al. (2021) discusses the importance of accurately defining the vertical thermal disk structure to obtain reliable results, something they achieve through a detailed fit of various molecular emission profiles. This is the challenge of face-on disk studies, while they display a unique view of radial and azimuthal substructures, interpretation of their physical properties can be hindered due to the unknown vertical properties.

A way of overcoming the challenges of accessing the vertical dimension in face-on disks is to study the kinematics, which, if the disk is not at an inclination of 0°, may offer insight into the vertical structure through its effect on the velocities (Rosenfeld et al. 2013a; Teague 2019a). However, the effect of the disk back surface will be unconstrained and could become, particularly for optically thin tracers, an important source of contamination in the data. Like in the edge-on case, it is not trivial to access all three dimensions when only two (radial and azimuthal here) are displayed clearly.

1.3.3 Mid-inclination disks

The remainder of the protoplanetary disk sample, with observed inclinations between ∼35-70° are classified as mid-inclination disks. These are objects where all three dimensions may be probed. As indicated in panel (A) of Figure 1.7, the azimuthal and radial material distribution can be observed from continuum (e.g., ALMA Partnership et al. 2015; Andrews et al. 2018) or intensity-integrated moment 0 molecular emission maps (e.g., Law et al. 2021a). At millimeter wavelengths, the vertical dimension can be directly probed through the emission channel maps, following the methodology presented by Pinte et al. (2018a) which is detailed below and in the sketch of Figure 1.7. If azimuthally symmetric structures are present, scattered light images of mid-inclination disks may also be used to trace the vertical location where μm-sized grains reside (e.g., Avenhaus et al. 2018).

The method of Pinte et al. (2018a) recovers the vertical structure from a given molecule using spatially and spectrally resolved data such that the emission within multiple channel maps is resolved, this allows us to trace the maxima of emission in each channel emission. The recovered maxima is identified in cartesian coordinates such that the x-axis and y-axis fall along the semi-major and semi-minor axis respectively, as defined by the disk position angle (PA). It is assumed that for a same x position, the maxima obtained at y_n ("near" side) and y_f ("far" side) will come from the same vertical height with respect to the disk midplane. For each x position where y_n and y_f values are extracted, the coordinates of the centre of the projected circular orbit passing through the two points are (x_c, y_c). These projected orbit coordinates relate to the stellar position (x_*, y_*) and maxima coordinates following $x_c = x_*$ and $y_c = (y_f + y_n)/2$. Considering this, for each duo of identified emission maxima at x position, a single radial (r) and height (h) point are computed accounting for the system inclination angle (i) following,

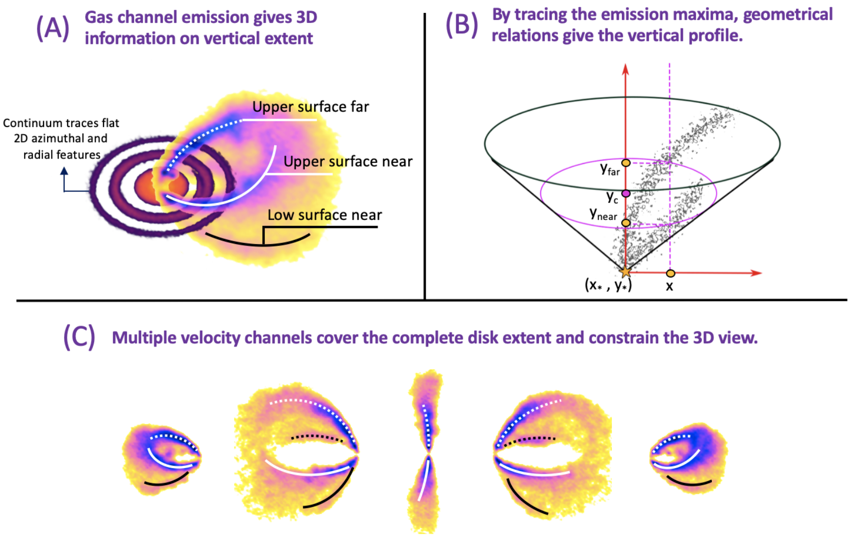

Figure 1.7: Sketch of key coordinates and steps for extracting the vertical disk profiles from emission channel maps of protoplanetary disks following the method of Pinte et al. (2018a). Panel (A) shows the position-angle corrected continuum and CO emission data, where the continuum characterizes the disk midplane and the upper and lower gas surface emission can be identified, tracing the vertical disk extent. Panel (B) presents the geometrical coordinates and assumptions used in the method, as explained in the main text. Panel (C) displays channel map emission at various velocities, where the emission maxima are traced in the upper and lower surfaces, as an example of how mutliple channels are used to trace the vertical extent accross the disk. Data are taken from the ^{12}CO $2-1$ emission and 1.3mm continuum of HD 163296 (Öberg et al. 2021b).

$$r = \sqrt{(x - x_c)^2 + \left(\frac{y_f - y_c}{\cos(i)}\right)^2} \tag{1.11}$$

$$h = \frac{y_c - y_*}{\sin(i)}. \tag{1.12}$$

An overview of the methodology and coordinates is presented in Figure 1.7. This methodology has been implemented in public algorithms DISKSURF (Teague et al. 2021b) and ALFAHOR (Paneque-Carreño et al. 2023, see Chapter 3) and used in multiple studies to extract the molecular surfaces of upper and lower sides in a growing sample of disks (Pinte et al. 2018a; Rich et al. 2021; Paneque-Carreño et al. 2021, 2023, 2024; Law et al. 2021b, 2022, 2023a,b, 2024; Urbina et al. 2024; Hernández-Vera et al. 2024). Alternatively, as with the face-on disks, parametric models can be fit in the image plane to account for the vertical distribution together with other molecular emission properties such as linewidth and intensity (Rosenfeld et al. 2013a; Izquierdo et al. 2021). While parametric models can give good estimates of the overall emission vertical location, they are generally not sensitive to any substructure or asymmetry that may be present in the surfaces.

1.3.4 Applications of vertical structure analysis in mid-inclination disks

The immediate applications of directly measuring the molecular layering in protoplanetary disks are many, depending on the selected tracers, the resolution and the available information from any radial or azimuthal structures. In this section we mention some examples of interest, many will be discussed in upcoming chapters.

By using optically thick CO isotopologues; ^{12}CO, C^{13}O and, if the disk is massive enough, C^{18}O, the temperature structure can be traced through their peak brightness temperature. The brightness temperature (T_b) relates to the effective disk temperature (T_{eff}) as $T_b \sim T_{eff}(1 - e^{-\tau})$, where τ is the optical depth of the tracer. Recent works have exploited the spatially resolved vertical and radial CO isotopologue profiles to empirically trace the 2D thermal structure (e.g., Pinte et al. 2018a; Law et al. 2021b). This provides strong constraints to benchmark thermochemical models and provides precise temperature measurements, which, for example, are critical in turbulence studies (e.g., Guilloteau et al. 2012; Flaherty et al. 2015, 2017, 2020, see Chapter 4 of this thesis for an application). For observations at lower spatial resolution or emission from less abundant complex molecules where the vertical structure may not be directly extracted, empirical thermal maps may be used to spatially locate these tracers, while their temperature is estimated using alternative methods such as rotational diagrams or hyperfine structure ratios (e.g., Ilee et al. 2021; Bergner et al. 2021).

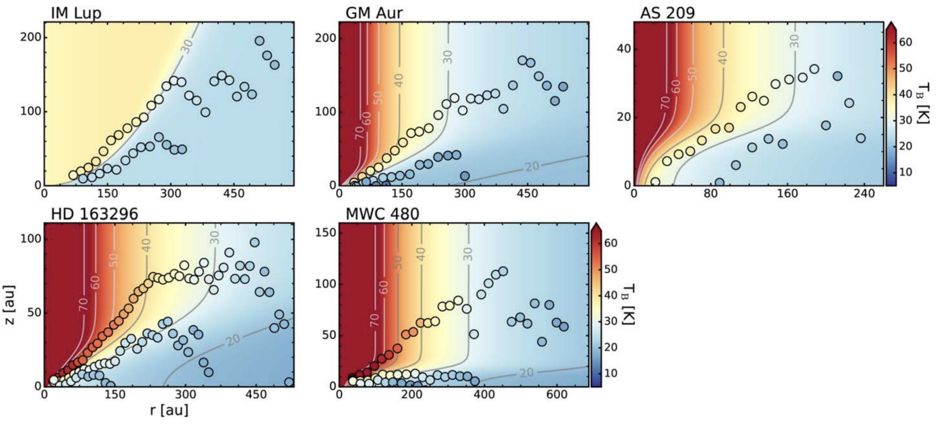

Figure 1.8: Results from empirical temperature maps extracted for the MAPS sample (Öberg et al. 2021b) by Law et al. (2021b). In each panel the circle symbols trace the optically thick CO emission surfaces and the circle colors are the peak brightness temperature extracted from the data. The colored background indicate the parametric fit to the data used to extrapolate the temperature values to other disk regions.

If spatially resolved kinematic information is available, at high spectral resolution, recent methods allow to separate the radial, azimuthal and vertical components of the material motion (e.g., Teague et al. 2018a; Pinte et al. 2023; Izquierdo et al. 2023). By 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 (Teague et al. 2019; Galloway-Sprietsma et al. 2023), crucial for understanding ongoing processes and disk dynamics.

Most recently, by tracing the vertical location of atomic carbon, early studies are being conducted to understand the disk layering and location of the hot irradiated surface (Law et al. 2023a; Urbina et al. 2024). In principle, any parameter may be traced in the vertical dimension, for example the ionization structure through observations and characterization of the HCO^+, DCO^+ and N_2H^+ emission surfaces. Observations of UV-sensitive molecules, such as CN and C_2H will give an overview of the energetic radiation field, which studies have found may be deeper penetrating than previously expected (Ruíz-Rodríguez et al. 2021, see also Chapter 2 of this thesis).

1.4 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 this third dimension. An initial question from the beginning of the PhD was if it was possible to extract vertical surfaces for molecules beyond the routinely studied CO, focusing particularly on expected tracers of the upper disk region; CN and C_2H. The existence of vertical substructure, never before characterized in detail, was also studied through the creation of a sensitive algorithm capable of accurately tracing the vertical profiles even in low signal-to-noise data. Finally, comparisons of large observational samples with thermochemical models and parametric prescriptions are done, in order to link our theoretical understanding of disk vertical structure to the observational constraints. Here is an outline of the upcoming chapters and main conclusions of this work,

Chapter 2: **Vertically extended and asymmetric CN emission in the Elias 2-27 protoplanetary disk.** Based on its chemistry, cyanide (CN) emission is predicted to originate in the upper layers of protoplanetary disks, tracing UV-irradiated regions. This hypothesis, however, has been observationally tested only in a handful of disks. Elias 2-27 is a young star that hosts an extended, bright, and inclined disk of dust and gas. The inclination and extreme flaring of the disk make Elias 2-27 an ideal target to study the vertical distribution of molecules. We analyse CN $N = 3 - 2$ emission in two different transitions $J = 7/2 - 5/2$ and $J = 5/2 - 3/2$ and compare it to CO isotopologue emission. Our results show that the vertical location of CN and CO isotopologues in Elias 2-27 is layered and consistent with predictions from thermochemical models. We characterize the optical depth and column densities for CN, ^{13}CO and $C^{18}O$. Overall, the inferred CN column densities, low optical depth ($\tau \leq 1$), and location near the disk surface are consistent with thermochemical disk models in which 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 disk physical conditions.

Chapter 3: **Directly tracing the vertical stratification of molecules in protoplanetary disks.** This work focuses on showing the power of the method from Pinte et al. (2018a) to extract vertical surfaces of multiple molecular lines in a sample of protoplanetary disks. The ALFAHOR code is presented in this work, which is an implementation of the method that obtains accurate vertical profiles even for low signal-to-noise molecules implementing an interactive masking procedure. Our sample of disks consists of Elias 2-27, WaOph 6, and the five sources targeted by the MAPS ALMA Large Program (Öberg et al. 2021b). The set of molecules studied includes CO isotopologues in various transitions, HCN, CN, H_2CO, HCO^+, C_2H, and c-C_3H_2. We are able to extract vertical profiles for ten different molecules and transitions in HD 163296. In the rest of the sample it is possible to vertically locate between four and seven lines. 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. The vertical layering of molecules is in agreement with theoretical predictions in some systems, but not in all. Therefore, dedicated physical-chemical models are needed to further study and understand the diversity of the emission surfaces.

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 via the transport of angular momentum. Measurements of turbulence through its line-broadening effect rely 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 without the need of complex radiative transfer or thermochemical models. 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 $z/r \sim 0.25$. Considering previous estimates of low turbulence near the midplane, this may indicate for the first time evidence of a vertical gradient in the disk turbulence, which is a key prediction of magneto rotational instabilities that may be occurring in the IM Lup disk.

Chapter 5: **Vertical CO surfaces as a probe for protoplanetary disk mass and carbon depletion.** The growing sample of mid-inclination disks with measured CO emission surfaces grows and a fundamental but unanswered question is how these vertical profiles connect to their host properties. In this chapter we address this question by using thermochemical models to study the protoplanetary disk parameters that most affect the recovered 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. A z/r-M_d relationship is derived, which varies depending on the carbon abundance. 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 our sources.

The main results and conclusions of this thesis are the following;

1. Vertical emission surfaces of molecules in protoplanetary disks can be directly extracted from ALMA observations of gas emission in mid-inclination disks. This is possible even for optically thin and low signal-to-noise molecular tracers. *(Chapters 2, 3, 4)*

2. The disk thermal structure follows a radial and vertical gradient. This can be empirically probed using optically thick tracers such as ^{12}CO and ^{13}CO. The physical conditions of the gas (e.g., turbulence and density) may be inferred by combining the thermal structure with information on the spatial location from various molecules. *(Chapters 2, 3, 4)*

3. CO isotopologues show a clear vertical layering, with ^{12}CO being the most vertically extended tracer and both ^{13}CO and $C^{18}O$ $J = 2-1$ tracing similar regions. *(Chapters 2, 3)*

4. CN $3-2$ and C_2H $4-3$ emit from a vertically constrained and mostly optically thin slab high up in the disk. This is in agreement with theoretical predictions and makes them ideal tracers of the conditions and location of the upper disk layers. *(Chapters 2, 4)*

5. Vertical emission surfaces of various molecular tracers display modulations and peaks (vertical sub-structure). In the case of CO isotopologues these are correlated with the radial location of millimetre continuum gaps and kinematic perturbations. *(Chapter 3)*

6. Turbulence may have higher values in the upper disk layers than the midplane. The empirically-derived thermal structure can be combined with spatially resolved emission from optically thin molecules to directly measure turbulence across the disk extent using a simple parametric model. *(Chapter 4)*

7. Total disk mass and volatile carbon depletion can be probed through the vertical location of the CO emission surface using a $z/r - M_d$ relationship. *(Chapter 5)*

8. Most protoplanetary disks show indications of volatile carbon depletion, between 1-2 orders of magnitude with respect to the ISM. T Tauri disks are more carbon depleted than Herbig systems. *(Chapter 5)*

1.4.1 Future prospects

Studies of vertical disk structure in large samples have only just begun, to date only ~ 20 disks have vertical CO surfaces characterized and ∼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 observationally 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. Looking forwards to the ALMA Wideband Sensitivity Upgrade, in the upcoming years it will be possible to do these studies in less times and larger samples. Small μm-sized dust, as traced by scattered light images, plays a key role in regulating the thermal and radiation fields towards the disk. Combining information from the solid and molecular material distributions will allow us to obtain a much better overview of the disk conditions.

Characterizing turbulence in disks or localizing features related to winds through tracers of the upper disk atmosphere will also be an interesting avenue of research in the coming years. Both of these processes have been suggested to drive disk evolution, but the complexity of detecting them has made them difficult to study. Through the analysis of vertical structure in mid-inclination disks a new avenue of observational constraints for these theories opens. In particular, high spatial and spectral resolution observations of CN $3-2$ and C_2H $4-3$ in ALMA Band 7, together with atomic Carbon at higher frequencies, should be key targets for this goal.

This thesis has shown that CO surfaces, combined with other methods, may be good probes of disk mass and volatile carbon depletion, other molecules must also be studied to see how their location may be exploited to learn about their host's properties. It is expected that UV tracers might be strongly affected by stellar parameters, or maybe less abundant CO isotopologues could be more sensitive to other parameters beyond the mass. Dedicated thermochemical models that test these hypothesis will be useful as the number of disks with molecular surfaces grows.

Overall, the possibility of studying the planet-forming material distribution across all three dimensions offers unique insight into the process of forming planets. Observational constraints are now catching up to the questions posed by theoretical models, which must be revised in order to explain the observed features. In the same way that for the past decade studies have focused on explaining the existence of radial and azimuthal substructure, we must now look at the third dimension and digest 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 have left open.