Dusty perspectives on the cradles of planets

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Introduction

Studying the origins of life on planet Earth has always been one of the most prominent pursuits in human history. With the increasing advances in astronomy, we began observing other stellar systems closely and discovered that they host a variety of planets with different compositions and sizes. This led to the study of planet formation, aiming to understand how planetary systems like our own and those around other stars originate. By doing so, we hope to uncover not only how Earth and the Solar System formed but also whether life exists elsewhere in the universe or not. Today it is known to be a fact that the process of planet formation begins in the early stages of what are known as protoplanetary disks.

1.1 The beginning and evolution of protoplanetary disks

Classification of young stellar objects

Before discussing the current challenges in studying protoplanetary disks and planet formation, it is important to first consider how far our understanding of their origins has come. The formation of stars and, eventually, planets begins in what is known as a molecular cloud (e.g., Ballesteros-Paredes et al. 2007). These molecular clouds originate from the atomic gas found in the interstellar medium (ISM), the gas and dust that fill the space between stars in galaxies such as our own Milky Way.

As regions within this gas become denser, they reach the physical conditions necessary for molecule formation (Glover & Mac Low 2007; Valdivia et al. 2016; Ballesteros-Paredes et al. 2020), where these dense, molecule-rich regions are the birthplaces of stars and what we call molecular clouds. Initially, the material in these clouds is concentrated in a localized region called a core, but as the system evolves, it begins to evolve away from simple spherical symmetry. Through a process known as accretion, the material (gas and dust) is channeled inward via a rotating disk structure, feeding the growing central protostar (Zhao et al. 2020b), forming the disk that we refer to as a protoplanetary disk. One of the earliest, and still used, observational classifications for Young Stellar Objects (YSOs) was introduced by Lada (1987), dividing them into three categories: Class I, Class II, and Class III sources. This classification was based on spectral energy distribution (SED) observations of these protostars at infrared wavelengths (between 2 and 25 μm, see Fig 1.1). As observational techniques improved and became more sensitive, the classification was extended to include Class 0 objects (Andre et al. 1993). While these classifications have some limitations, they remain widely used today to categorize the evolutionary stages of protoplanetary disks and their host stars.

The evolutionary transition from the initial collapse and disk formation phase (Class 0/I) to the Class II stage occurs very quickly, within approximately 0.5 Myr (Evans et al. 2009). Class II objects, however, persist for a longer period, with median lifetimes between 2–3 Myr, though they can last up to 10 Myr (Fedele et al. 2010; Michel et al. 2021). Although each phase of star evolution presents its own details and challenges, throughout these evolutionary stages, one crucial component shapes the evolution of protoplanetary disks in ways beyond planet formation alone. This component will be studied in detail in this thesis: the interstellar dust grains.

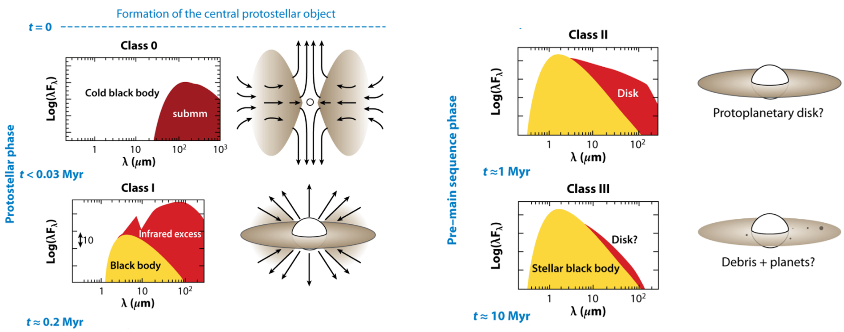

Figure 1.1: Star and disk formation stages classified based on the spectral energy distribution (SED) at micrometer wavelengths, adapted from Dauphas & Chaussidon (2011).

1.1.1 Interstellar dust and its influence in protoplanetary disks

Dust grains significantly influence the composition of the ISM, the appearance of galaxies, and the process of star formation. The term dust grains or interstellar dust is commonly understood, following Draine (2003), as solid particles consisting of tens or more atoms. Although this includes large molecular structures, dust grains are typically larger in size and possess more complex compositions, often involving silicates, carbonaceous materials, and ices. The origin of this dust is believed to be primarily from stellar outflows of red giants, giant stars, and planetary nebulae (stardust). However, it is important to note that the majority of interstellar dust is not pristine stardust; rather, its composition and properties are largely shaped and altered by various physical and chemical processes that occur within the ISM (Draine 2003). The exact composition of these small dust grains remains somewhat controversial, as it can only be inferred indirectly through e.g. spectral emission features, scattered light or optical extinction. These three processes can be explained as follows: Extinction refers to the dimming of optical and near-infrared starlight as it passes through dust. Scattering is the process where light is redirected in multiple directions as it encounters the surface of a dust grain, and emission occurs when dust grains absorb energy from different sources and then re-emit this energy at longer wavelengths, predominantly in the infrared. From observations of these spectral features, the main probable components of interstellar dust have been narrowed down to the following:

- Silicates: Infrared extinction curves show a strong absorption feature peaking at approximately 9.7 μm, associated with silicate minerals. It is well established that a large fraction of the ISM dust mass is in silicates, with at least 95% of it being amorphous (Li & Draine 2002).

- Carbonaceous materials: A broad spectral feature in the dust extinction curve centered near 0.21 μm is typically attributed to carbon-rich materials, such as graphite or diamond-like carbon.

- Silicon Carbide (SiC): SiC is commonly detected in meteorites and as an emission feature in the spectra of many carbon stars (Treffers & Cohen 1974; Blanco et al. 1998). Although SiC is a confirmed part of interstellar dust grains, its abundance is estimated to be less than 5% that of silicates (Whittet et al. 1990).

- Carbonates: Some carbonates have been detected around dusty disks (Kemper et al. 2002), but these exist only in very small quantities and are not considered a major component of interstellar dust.

Regarding grain sizes, Mathis et al. (1977) showed that the observed extinction curve in the ISM can be reproduced by assuming a grain size distribution following a power law, $\mathrm{dn}/\mathrm{da} \propto \mathrm{a}^{-3.5}$, with grain sizes ranging from 5 nm to 0.25 μm, consisting mainly of graphite and silicate grains. Since then, various modifications have been made to the assumed composition, opacities, and size distributions of dust grains present in protostellar objects. Despite these refinements, the detailed size distribution in these systems remains uncertain and although larger dust grains are expected in protoplanetary disks (from 5 nm to 1 mm and even cm, Testi et al. (2014)), many assumptions about dust in disks are still based on the properties derived for the ISM.

While it constituting only about 1% of the total YSO mass, dust plays an indispensable role in numerous pathways and aspects of disk and planet formation (e.g., Birnstiel 2024). For example, the continuum dust opacity plays a critical role in regulating disk heating and photodissociation, shaping the disk's structure (Jonkheid et al. 2004; Aikawa & Nomura 2006). Additionally, dust traces the hydrostatic structure of disks, as small dust particles absorb and emit stellar radiation, heating the disk and influencing the thermal balance (Gorti & Hollenbach 2009; Woitke et al. 2009). Dust grains also provide the surface area for the formation of volatile and complex organic molecules (COMs) (e.g., Garrod & Herbst 2006), which are considered precursors to prebiotic chemistry and their formation in early star-forming regions may determined the potential habitability of new forming planets. Moreover, depending on the disk's dynamics and the locations where molecules freeze-out or form, dust contributes to the redistribution and structural variation of chemical abundances (e.g., Cyr et al. 1998; Ciesla & Cuzzi 2006; Krijt et al. 2016; Stammler et al. 2017) which may set a diversity in the atmospheric conditions of exoplanets.

Observationally, dust can be traced in both scattered light and thermal dust emission. Scattered light originates from small dust particles in the upper layers, whereas thermal dust emission ranges from optically thick continuum emission in the infrared to optically thin continuum emission at millimeter wavelengths. Modern telescopes such as the Atacama Large Millimeter Array (ALMA) can detect this millimeter emission, offering valuable insights of the disk structure, but more importantly of the disk's mid-plane where it is believed that dust grows, collides, accumulates, migrates, and eventually leads to the formation of planets (Brauer et al. 2008). This underscores the crucial role of dust in shaping not only

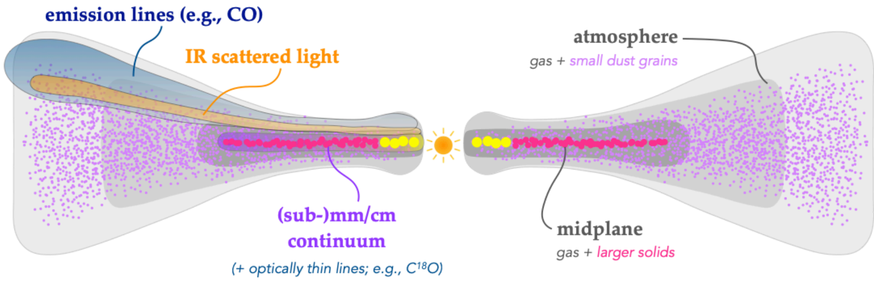

Figure 1.2: Protoplanetary disk structures as traced by emission lines, infrared scattered light (small dust grains), and sub-mm/cm continuum emission (large dust grains), adapted from Andrews (2020).

planet formation, but also the overall structure, evolution, and chemical composition of protoplanetary disks, by both tracing and influencing different regions within them. Figure 1.2 illustrates the current understanding of disk structure. Infrared scattered light traces small dust grains in the upper, flared surface layers of the disk. Sub-millimeter continuum emission, probes larger, millimeter-sized grains that have settled closer to the mid-plane. Meanwhile, molecular line emission, such as CO and its isotopologues, traces the gas component across different vertical layers. Together, these tracers provide a more complete view of the physical and chemical environment within protoplanetary disks that will be studied in this thesis.

1.1.2 Dust evolution: Radial Drift

To understand how dust evolves in protoplanetary disks, it is essential to comprehend the drag forces that enable various interactions between these dust particles, including collisions, sticking, fragmentation, and growth. These interactions are the building blocks of dust dynamics in protoplanetary disks (Brauer et al. 2008; Birnstiel et al. 2010; Zsom et al. 2010; Windmark et al. 2012). In particular, drag forces occur due to the interaction between dust particles and the surrounding gas, which depends on the relative motion between them and the particle size (e.g., Testi et al. 2014).

The most important consequence of drag forces is the dust radial drift (Whipple 1972; Adachi et al. 1976; Weidenschilling 1977). In a disk with gas, where centrifugal forces, gravitational forces, and pressure gradients are in balance, the gas orbits at a slightly sub-Keplerian speed, caused by an outward pressure gradient. Dust particles, however, depending on their degree of coupling to the gas, are primarily influenced by gravitational and centrifugal forces and, as a result, they tend to move at Keplerian velocities. This slight difference in orbital velocities between the gas and dust leads to the dust experiencing a headwind, which results in dust particles eventually slowing down and spiraling inward towards the star. The rate of radial drift then depends on how strongly the dust is coupled to the gas, which is quantified by the dimensionless Stokes number, $\mathrm{St} = t_{\mathrm{stop}}\Omega_{\mathrm{K}}$ (Cuzzi et al. 2001). This number relates the stopping time to the orbital timescale, and depends on particle size and composition, meaning that particles of different sizes drift at varying speeds in different regions of the disk (Testi et al. 2014).

One of the main unresolved issues that will be mentioned throughout this thesis is that, unless the disk is exceptionally massive (which is unlikely), large dust particles on the order of mm to cm in size will spiral into the star very quickly, within a short fraction of the disk's lifetime. This rapid inward motion makes it difficult for dust to interact, grow, and finally, form planetesimals or planets. Numerous studies were conducted to understand and solve the problem of radial drift (e.g., Whipple 1972; Weidenschilling 1977; Youdin & Shu 2002; Brauer et al. 2007). Even then, a proposed solution to this problem was an inversion of the pressure gradient in the disk to help halt radial drift (Nakagawa et al. 1986; Pinilla et al. 2012b), though observational capabilities were limited at the time, and results were primarily theoretical.

1.1.3 Dust evolution: Settling and turbulent mixing

In addition to radial drift, there is another important type of drag force that exist in protoplanetary disks and shapes the pathway of planet formation: Turbulent mixing and settling. Under the influence of gravitational force, dust particles were initially thought to follow inclined orbits, oscillating vertically and constantly through the mid-plane. However, due to strong gas drag-forces, these particles tend to gradually settle toward the mid-plane over timescales of a few hundred thousand years (Goldreich & Ward 1973; Weidenschilling 1980; Nakagawa et al. 1986; Dullemond & Dominik 2004). Understanding vertical settling is vital, as it directly shapes and regulates the concentration of dust in the disk mid-plane, that allows dust to gather and grow. This process, however, does not occur unimpeded. Turbulent mixing, which is often attributed to instabilities such as the Magneto-Rotational Instability (MRI) or other hydrodynamic instabilities, counteracts settling by stirring particles upward, preventing excessive dust accumulation at the mid-plane. This process typically acts within a specific vertical region of the disk: above a certain height, vertical settling can proceed efficiently, causing small grains to settle rapidly and disappear from the upper layers; below that, turbulence maintains the balance within a more uniform dust distribution for grains of certain sizes and establishing a balance that defines the vertical distribution of solids (Dullemond & Dominik 2004). In this context, Dubrulle et al. (1995) was able to calculate the vertical structure of the dust layer by solving the equilibrium between the effects of settling and turbulent mixing, which defines the dust scale height.

Settling has profound implications for the observational appearance of disks. It can lead to the formation of a thin mid-plane layer of large grains (e.g., pebbles). Additionally, settling alters the disk's optical depth and temperature structure, affecting the emission and scattering properties observable in infrared and millimeter wavelengths (Chiang et al. 2001; D'Alessio et al. 2001; Dullemond & Dominik 2004). High-resolution observations of edge-on protoplanetary disks at both millimeter and infrared wavelengths have confirmed a certain degree of settling by measuring the vertical extent of the dust continuum emission at different wavelengths (e.g., Villenave et al. 2019, 2020, 2022).

Both drag forces (radial drift and vertical settling), shape the appearance of protoplanetary disks and influence their observational signatures (Fig. 1.2). In this thesis, understanding these processes is key to interpreting the emission observed from such disks with one of the most advanced astronomical instruments of our era.

1.2 Protoplanetary disks in the modern era with ALMA

The Atacama Large Millimeter/submillimeter Array (ALMA) is a state-of-the-art telescope located on the Chajnantor Plateau in the Chilean Andes. It was built by the collaboration between the European Southern Observatory (ESO), the National Radio Astronomy Observatory (NRAO) and the National Astronomical Observatory of Japan (NAOJ) to study the universe in unprecedented detail. One of ALMA's primary goals is to observe the coldest objects in the universe, such as molecular gas and dust, which emit radiation at millimeter and submillimeter wavelengths.

ALMA consists of 66 individual antennas, each operating at wavelengths ranging from 0.32 to 3.6 millimeters at high sensitivity. It functions as an interferometer, meaning the signals from multiple antennas are combined to simulate a much larger telescope, with the resolution of such an array being comparable to that of a single dish with a diameter equal to the maximum separation between antennas. The main array includes fifty 12-meter antennas, complemented by an additional four 12-meter and twelve 7-meter antennas in the Atacama Compact Array (ACA). The distance between antennas can be adjusted from 150 meters up to 16 kilometers, allowing ALMA to achieve some of the highest angular resolutions ever achieved to study the universe.

Over the last decade, the capabilities of ALMA have significantly advanced our understanding of protoplanetary disks, not only in terms of dust evolution and continuum emission at sub-millimeter wavelengths, but also concerning molecular line emission and the gas structure within these disks.

1.2.1 Gas and ice content of protoplanetary disks

The chemical composition of protoplanetary disks depends on two main factors: the chemical processes occurring within the disk itself and the chemical inheritance passed down from the interstellar cloud (e.g., Visser et al. 2009). While the first molecules form in the interstellar cloud, most remain frozen in icy mantles on the dust grains. During the protostellar phase, however, more complex molecules form in the ice through processes such as hydrogenation and irradiation. These molecules, along with pre-existing volatiles, then sublimate before being incorporated into the disk (e.g., Öberg et al. 2023).

The gas and chemical structure in the disk also experiences redistribution, similar to dust, and is influenced by processes such as advection, turbulent diffusion, and disk winds. One of the most important factors affecting the gas distribution in disks is the location of condensation fronts, or snowlines (e.g., Öberg et al. 2023), which impact the chemistry in both radial and vertical direction. Snowlines mark the regions where molecules freeze out in the disk, depending on the vertical and radial temperature gradients. It is believed that these snowlines play a critical role in planet formation (e.g., Hayashi 1981) for three main reasons:

- The surface density of dust particles is thought to be enhanced beyond the snowlines, meaning that outward past a snowline, gas-phase molecules freeze onto grains, increasing their mass and surface density (Zhang 2024).

- Depending on the local temperature, snowlines could facilitate the formation of planetesimals since the fragmentation thresholds (maximum velocity at which dust particles can collide without breaking apart) and sticking properties of the dust change given their icy composition or lack thereof after crossing a snowline. (Gundlach & Blum 2015; Gundlach et al. 2018)

- Snowlines create distinct regions within the disk that have different elemental ratios, as various molecules freeze out at different distances from the central star depending on the temperature. The classical picture suggests that measuring elemental ratios in planetary atmospheres can reveal their formation locations within the disk (Öberg et al. 2011). However, more recent studies have shown that in reality, the elemental ratios are more complicated due to effects of dust transport (e.g., Krijt et al. 2023).

Although chemical characterization of disks has been conducted observationally across a wide range of frequencies and energy scales, from UV to millimeter wavelengths observations, our focus on this thesis will be on submillimeter and millimeter observations, which probe the cold gas, the bulk of the disk's gas reservoir (e.g., Öberg et al. 2023). Depending on dust optical depth and the specific spectral lines observed, it is possible to trace gas from the disk's upper layers down to the mid-plane regions of protoplanetary disks. More specifically, with ALMA's long baselines and sensitivity, rarer molecules can be detected, enabling high spatial resolution studies of disk chemistry on scales smaller than 10 au (Öberg et al. 2015; Huang et al. 2018a). To date, 31 molecules have been detected in Class II protoplanetary disks (McGuire 2022; Booth et al. 2021; Canta et al. 2021; Phuong et al. 2021; Brunken et al. 2022), yet more complex molecules are still being observed and discover within the earlier stages of disk formation.

1.2.2 Complex organic molecules in YSOs

The study of molecular emission in YSOs has progressed significantly in recent years, particularly with the discovery of several complex molecular species from within the interstellar medium (ISM) to the core of protoplanetary disks. According to Herbst & van Dishoeck (2009), a complex organic molecule (COM) is defined as a carbon-bearing molecule containing at least six atoms, the term COM (or COMs) has become widely adopted in the literature. Although other nomenclature exists, for the purposes of this thesis, we will consistently use the term COM. Understanding the abundances and distributions of COMs in YSOs and how they eventually make their way into protoplanetary disks is crucial, as these COMs in the Solar Nebula were potential building blocks for life (Zhang 2024).

Advancements made possible by ALMA and other facilities have greatly expanded our understanding of COMs. Initially, they were only identified in the ISM or in high-mass star-forming regions. However, more recent observations have shown that most of the same COMs are also present in low-mass star-forming regions, with no clear difference in abundances ratios and therefore chemical complexity between high- and low-mass environments (Jørgensen et al. 2020).

As the number of observational samples has increased, the number of open questions has increased as well. For instance, Bisschop et al. (2007) studied COM emission in seven high-mass YSOs and found that the molecules fell into two distinct groups: one tracing hot gas ($T > 100$ K) and the other associated with cold gas ($T < 100$ K). While several subsequent studies attempted to establish some chemical patterns between these sources, their efforts were often limited by insufficient spatial resolution, the number of detectable COMs, and different spectral coverage (e.g., Calcutt et al. 2014; Suzuki et al. 2018; Taniguchi et al. 2018).

Despite these limitations, these early studies were fundamental and critically important, as they allowed researchers to begin distinguishing between different physical regions and processes in young stellar objects.

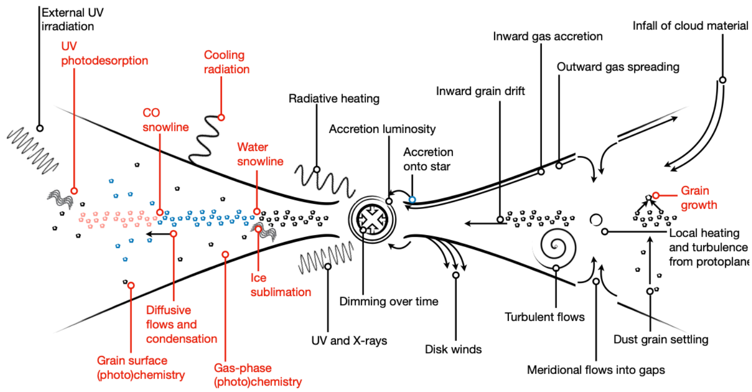

Figure 1.3: An overview of all the chemical processes occurring in protoplanetary disks taken from Öberg et al. (2023). In this schematic, processes shown in black are stellar and dynamical ones, while those in red correspond to chemical processes that directly depend on the disk's chemical composition.

For example, in the case of the young high-mass YSO G328.2551–0.5321, ALMA observations at small spatial scales (a few hundred AU) revealed clear chemical differentiation (Csengeri et al. 2018, 2019). This was interpreted as evidence of accretion shocks combined with a rotational pattern. From a theoretical perspective, the formation of a circumstellar disk is thought to be closely tied to the presence of such accretion shocks, where infalling material transitions into the disk structure (e.g., Cassen & Moosman 1981; Neufeld & Hollenbach 1994). These findings underscore the importance of high-resolution chemical studies in unraveling the physical mechanisms that govern disk formation and early stellar evolution. However, this is only a brief overview, and it is important to acknowledge the wide range of processes involved in the chemistry of protoplanetary disks and the distribution of complex organic molecules (COMs), as illustrated in Fig. 1.3.

1.2.3 Early disk formation and spatial distribution of dust and COMs

Observations with ALMA and other sub-millimeter facilities have gradually revealed the presence of Keplerian disks in embedded objects or Class I protostars, confirming their existence (e.g., Harsono et al. 2014; Yen et al. 2015a; Artur de la Villarmois et al. 2019b), including in some Class 0 sources (Tobin et al. 2012; Murillo et al. 2013; Yen et al. 2017). However, there are also notable cases where no clear signs of Keplerian rotation are detected, even down to 10 au scales (e.g., Yen et al. 2015b; Jacobsen et al. 2019).

Despite the non-detections, these youngest circumstellar disks provide a crucial link between the complex organic molecules (COMs) observed in warm gas regions and the initial conditions for subsequent dust evolution and planet formation. As noted by Harsono et al. (2018), many embedded disks may already harbor millimeter-sized dust grains, which can lead to optically thick dust that obscures the underlying gas emission. Consequently, careful interpretation is required when analyzing the spatial differentiation between molecular species and dust emission at these scales. Even in the absence of large grains, high continuum optical depths can significantly affect the observed gas emission.

The exact distribution and origin of complex organic molecules (COMs) around Class 0/I protostellar sources remains an open question. Observations from the ALMA Ophiuchus survey suggest that CH_3OH is very limited in spatial extent toward certain protostars (Artur de la Villarmois et al. 2019a). Additionally, Lee et al. (2017) conducted an in-depth study of the HH 212 protostellar system in the L1630 cloud of Orion, leading to the suggestion that some COM species may reside in the “atmosphere” of the disk. These molecules may either originate from cold regions on larger scales, sublimating upon heating in the disk atmosphere, or form in situ through rapid gas-phase reactions under high-temperature conditions.

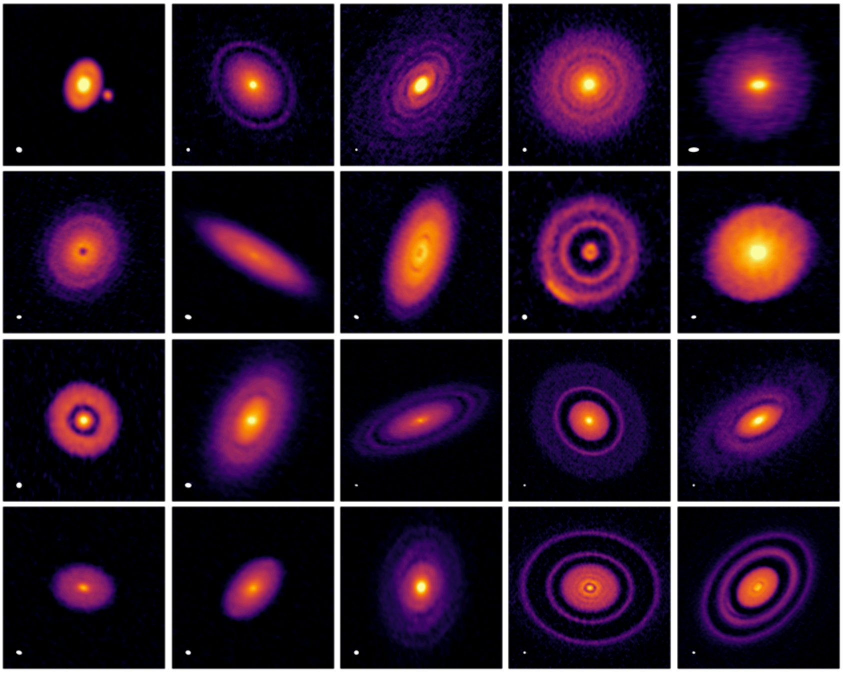

Figure 1.4: ALMA observations at 240 GHz from the DSHARP survey (Andrews et al. 2018a) revealing a variety of substructures in the dust continuum emission, indicating a more complex dust surface density distribution.

Nevertheless, this investigation is ongoing, and to properly constrain the spatially resolved abundance profiles of COMs in protostellar envelopes, high-sensitivity ALMA observations are essential. Such studies should be extended to larger, statistically significant samples of young stellar objects. This is the only way to robustly test the predictions of astrochemical models, derive accurate molecular abundances, and identify systematic patterns in the chemical structure and distribution of COMs during the earliest stages of star and planet formation (Jørgensen et al. 2020).

1.2.4 Substructures in protoplanetary disks

Regarding more evolved disks, early high-resolution, high-sensitivity ALMA observations (e.g., ALMA Partnership et al. 2015; Andrews et al. 2016; Isella et al. 2016) revealed that Class II disk density distributions are not as smooth as once thought, but instead exhibit distinct radial structures and variations. These findings supported the idea that pressure gradients, originally proposed as a solution to the efficiency of radial drift as mentioned before, may indeed be present and play a role in dust trapping, bringing us closer to understanding planet formation.

Subsequent studies showed that the most common substructures in these disks appear as bright rings and deep gaps, while less frequently observed features include spiral arms and asymmetries. (e.g., Pérez et al. 2016; Dong et al. 2018; Andrews et al. 2018a), as shown in Figure 1.4. Despite these observations, how and when these substructures originate remains an open question. Among some of the proposed mechanisms, the most widely accepted explanation involves planet-disk interactions (e.g., Zhu et al. 2014; Bae et al. 2017; Zhang et al. 2018). However, while planets can create the substructures needed to halt radial drift, such structures may also be necessary to grow dust and form planets themselves creating a chicken and egg problem.

Moreover, the increasing number of substructures detected in protoplanetary disks without any clear planetary signatures has motivated alternative theories. These include zonal flows and MHD-induced pressure bumps, gravitational instabilities, condensation fronts such as snow lines, and other dust evolution processes like sintering (Zhang et al. 2015b; Flock et al. 2015; Okuzumi et al. 2016; Dong et al. 2018).

Given this paradigm, determining when exactly these substructures emerge, particularly during the early, embedded Class 0/I phases, is critical for interpreting the substructures observed in more evolved, Class II disks.

1.3 The current problems in planet formation

While significant advances in planet and disk formation since the early ALMA years have been made, several key challenges remain. In this section, we highlight two of these unresolved issues that are particularly relevant to this thesis. These problems will be introduced here and discussed in greater detail in the following chapters.

1.3.1 Early substructure formation and unsettled Disks in YSOs

Ohashi et al. (2023) conducted high-resolution ALMA observations of several Class 0/I disks, revealing a strong connection between the physical structure, chemical composition, and evolution of young stars and their surrounding disks. Despite the remarkable resolution of these observations, most of the YSO disks showed little to no substructure in the dust continuum at 1.3 mm, at least at the wavelength at which the data was taken (see Fig. 1.5). This raised several questions about the true origin and timing of substructure formation in disks. The authors suggested that the apparent absence of substructures may be either due to high optical depths obscuring them or that the substructures that we commonly observed in Class II disks form very quickly during the transition from Class I to Class II, which would support scenarios involving early and thus rapid planet formation.

For optical depth to effectively obscure substructures, the disk must exhibit significant vertical structure. This requires a degree of stratification, where smaller grains trace upper layers of the disk, while larger grains, and substructures, reside closer to the mid-plane. In fact, studies of edge-on Class I protoplanetary disks by Villenave et al. (2020, 2023) show that disk layers probed by infrared scattered light have a much larger vertical extent than those traced by ALMA at millimeter wavelengths. Also in more evolved Class II disks, several observations show that the scale height increases with decreasing wavelength (Villenave et al. 2020). While

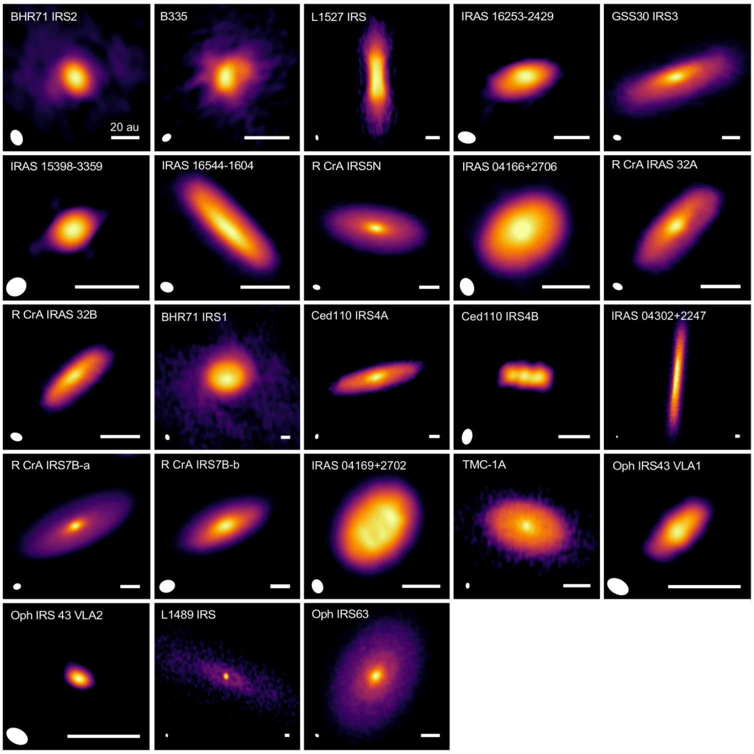

Figure 1.5: ALMA observations of protoplanetary disks around Class 0/I sources by Ohashi et al. (2023), revealing that most of these disks exhibit little to no substructure.

this stratification depends on the optical depth at the observe wavelengths and the structure of the disk itself, not all dust grains appear to be fully settled, particularly those traced at the shortest sub-millimeter wavelengths with ALMA, where the emission is expected to be optically thick.

These optically thick observations often provide very limited insight into disk substructures and, therefore, into potential signs of planet formation. Such observations, however, may contain information about the vertical structure of disks and the degree of dust settling. Understanding the settling and the vertical distribution of solids in disks is just as important as understanding radial drift. Settling governs how much dust

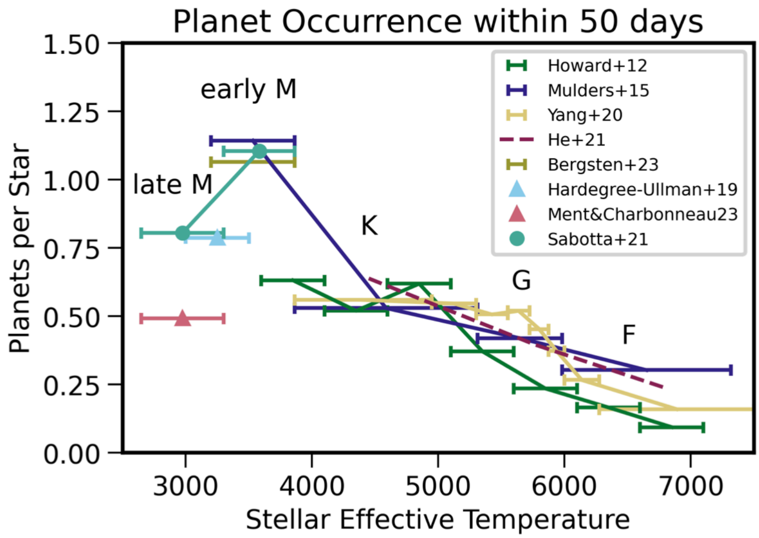

Figure 1.6: The occurrence rate of sub-Neptunes with orbital periods of less than 50 days as a function of stellar spectral type, source from Mulders (2018).

accumulates in the mid-plane, where grain growth and planet formation take place. Ignoring the vertical structure (scale height) of dust in protoplanetary disks risks overlooking a critical mechanism that could replenish the mid-plane with material that allows for planet formation to happen.

1.3.2 Exoplanet demographics vs protoplanetary disks surveys

Another challenge in planet formation studies has been the reconciling of the growing exoplanet catalog with the structures observed in Class II protoplanetary disks. Since the discovery of the first exoplanet, thousands of planets have been identified, with many exciting findings, such as the relation between the occurrence rate of giant planets and stellar mass (e.g., Johnson et al. 2010). However, the majority of giant exoplanets are detected at orbital radii between 1 and 10 au (Fernandes et al. 2019;

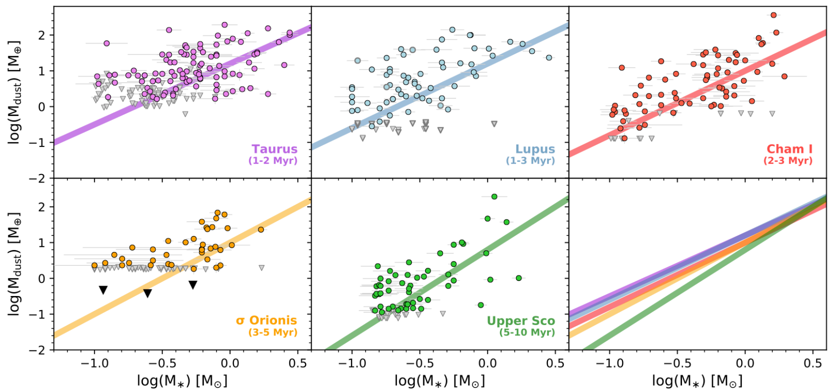

Figure 1.7: Stellar masses vs dust masses of protoplanetary disks, derived from various ALMA observations across multiple star-forming regions (Ansdell et al. 2017).

Fulton et al. 2021), which doesn't align well with the large-scale substructures seen in Class II disks. If these planets indeed formed in the outer disk regions (in association with these substructures), significant inward migration must have occurred during their evolution.

Second, super-Earths, which vastly outnumber giant gas planets, are much more commonly found around M-type stars after their formation (Howard et al. 2010, 2012). This trend is inversely correlated with stellar mass (see Fig. 1.6). van der Marel & Mulders (2021) compared the occurrence of disks with and without substructure and the known exoplanetary systems. They proposed that in systems without large-scale substructures, indicating that giant planets have not formed at wide orbits early in the disk lifetime, radial drift leads to the formation of a compact disk. These compact disks would experience a high influx of large dust grains (pebbles) in the inner regions of the disk to form the most common type of exoplanet, the close-in super-Earths with masses < 20 $M_{\oplus}$, potentially resolving the apparent discrepancy between observed disk structures and exoplanet demographics. This idea is supported by observational trends, where compact disks and close-in super-Earths are both more frequently found around M-dwarf stars (e.g., Mulders et al. 2018).

Although demographic surveys of protoplanetary disks have already provided valuable insights into disks properties and dust evolution, such as the correlation between stellar mass and dust mass, and the observed decrease in dust mass in older star-forming regions (see Fig. 1.7) (~0.25", Ansdell et al. 2016; Barenfeld et al. 2016; Cieza et al. 2019). These studies have generally been conducted at relatively low angular resolution, especially when looking at complete star-forming regions. As a result, key properties of compact disks, such as their true sizes and dust content, remain poorly constrained. Most high-resolution ALMA observations to date have focused on the brightest and therefore largest disks and only a limited number of compact disks have been observed at high resolution in recent years (Facchini et al. 2019; Long et al. 2019; Kurtovic et al. 2021; van der Marel et al. 2022; Miley et al. 2024; Shi et al. 2024). While these studies were novel, the exact connection between compact disks and the formation of super-Earths remained inconclusive.

1.4 This thesis

While it is now believed that substructures in protoplanetary disks are, directly or indirectly, essential for planet formation, their exact origin remains unclear. In this thesis, we aim to address questions about these substructures and how they relate to planet formation and dust growth. Specifically, we want to investigate how and when these substructures form by studying young disk systems such as IRAS4A and HL Tau, as well as those in a nearby star-forming region like Lupus. Can substructures be detected in optically thick environments, and even at optically thick wavelengths, assuming they are deep enough? Does the chemical structure in these embedded disks show signs of dust evolution? Are substructures only common in large, massive disks, or is their absence in the most compact disks simply a matter of resolution? And if compact disks truly lack substructures, do they still have the conditions necessary to trigger planet formation, particularly for planets like super-Earths? We will use ALMA and VLA observations at several wavelengths (8, 2.1, 1.3, 0.9, and 0.45 mm) to study these questions of protoplanetary disks. We will first focus on optically thick observations of two systems at different evolutionary stages: the Class 0 source IRAS4A and the Class I source HL Tau. We aim to constrain the dust properties and vertical structure (scale height) of both disks to better understand the dust distribution and its role in dust evolution and disk substructures. For IRAS4A, we will also analyze molecular line emission to further constrain the dust distribution and provide insights into its evolutionary stage. Finally, we will study all protoplanetary disks, including the faintest ones, at high angular resolution of 0.025" in the Lupus star-forming region, aiming to determine their true dust sizes and explore the implications for dust evolution and the formation of the most common exoplanets: super-Earths.

1.4.1 Analysis tools

For the work in this thesis, we primarily used three publicly available software packages: RADMC-3D (Dullemond et al. 2012), GALARIO (Tazzari et al. 2018), and CASSIS (developed by IRAP-UPS/CNRS (https://cassis.irap.omp.eu)). These tools were employed to analyze observations from the telescopes at sub-mm wavelengths (ALMA or VLA), using the visibility data or the molecular and continuum emission.

RADMC-3D is a publicly available radiative transfer code widely used in astrophysics and astronomy. It is primarily designed to simulate the thermal and radiative properties of environments such as protoplanetary disks, molecular clouds, and circumstellar envelopes. The code calculates the dust temperature using a Monte Carlo radiative transfer method, producing realistic dust continuum emission. For gas, line radiative transfer is performed under the assumption of local thermodynamic equilibrium (LTE). RADMC-3D acts as a post-processing tool, allowing users to generate synthetic images, spectra, and spectral energy distributions (SEDs) based on parametric input models of gas and dust density and a stellar radiation field. One of its key strengths is its flexibility: it supports fully three-dimensional geometries, making it ideal for modeling complex disk structures. Because the models are user-defined, RADMC-3D offers significant freedom in setting up custom simulations. Its output can be directly compared with observational data, such as those obtained from the ALMA telescope.

GALARIO (GPU Accelerated Library for Analyzing Radio Interferometer Observations) is a library package designed to accelerate the comparison between model predictions and observed visibilities from radio interferometric telescopes. With the rapid advancement of interferometric techniques and the increasing volume of data across a wide range of spatial frequencies, fast and efficient computational tools like GALARIO are essential. Rather than working with reconstructed images, GALARIO operates directly in the Fourier (uv) plane, preserving the full spatial information and avoiding biases introduced during image deconvolution. GALARIO is particularly well suited for fitting disk models, comparing visibility profiles of disks with and without substructure with observations. It is especially useful in high-resolution studies of protoplanetary disks, where exploring parameter spaces directly in the uv-plane enables robust constraints on disk geometry and emission profiles.

CASSIS is a publicly available software tool for identifying molecular transitions and modeling spectra from astronomical observations. It is valuable for interpreting data from sub-millimeter observations from radio telescopes like ALMA. CASSIS allows users to visualize, analyze and identify molecular emission lines using spectral catalogs such as CDMS and JPL. It supports both LTE modeling and non-LTE analysis through integration with RADEX. CASSIS is particularly useful in the study of protoplanetary disks, where it helps extract key physical parameters, such as gas temperature, column density, and velocity structures—from observed molecular line emission.

Chapter 2: IRAS4A1: Multiwavelength continuum analysis of a very flared Class 0 disk.

In this chapter, we analyze the continuum dust emission of the protobinary system NGC1333-IRAS4A (IRAS4A), a well-studied Class 0 system located in the Perseus molecular cloud at a distance of 293 parsecs (Zucker et al. 2018). IRAS4A consists of two Class 0 protostars, IRAS4A1 and IRAS4A2, with a separation of 1.8" (Tobin et al. 2018). We obtained high-resolution ALMA and VLA observations (78 mas) of this protobinary system, which allowed us to create dust continuum images of IRAS4A1. From these images, we derived radial profiles of the spectral index and brightness temperature. Our analysis focuses exclusively on IRAS4A1, as IRAS4A2 remains unresolved at the resolution of our current dataset.

We modeled and fitted the emission at each wavelength using radiative transfer equations and Markov Chain Monte Carlo (MCMC) methods to infer the dust properties that better reproduce the observed brightness temperatures across the disk. Our results suggest that, while IRAS4A1 is significantly more massive than typical Class II disks, the characteristic dust grain sizes are already of millimeter sizes.

To investigate the presence of substructures in IRAS4A1, we used the radiative transfer code RADMC-3D to simulate disks with varying scale heights and flaring angles. Our models show that substructures, such as rings or gaps, can remain hidden in optically thick disks if the vertical scale height is large and the disk is moderately inclined. Using the mass estimates derived from our dust parameters, we specifically modeled IRAS4A1 and found that certain features in the emission, such as shoulders, could only be reproduced by introducing substructures into the models. This suggests that substructures could indeed be present at these early stages but remain concealed within optically thick regions, a scenario that could plausibly extend to other Class 0 sources as well.

Chapter 3: From large-scale outflows to compact line emission in IRAS4A2.

In Chapter 3, we focus our analysis on IRAS4A2, as unlike IRAS4A1, its molecular content is not hidden by optically thick dust. Although a multi-wavelength continuum analysis could not be performed for this source, IRAS4A2 is believed to be more evolved than IRAS4A1. This motivated a comprehensive study of its molecular emission and what it reveals about dust distribution and the embedded disk conditions.

IRAS4A2 is one of the first hot corinos ever discovered (Bottinelli et al. 2004). As previously mentioned, it is part of a binary system that shows significant interaction in both the millimeter continuum and line outflow emission. Its molecular content has been extensively studied (e.g., Taquet et al. 2015; López-Sepulcre et al. 2017; De Simone et al. 2017), although only very recently at high resolution of 0.2" (Frediani et al. 2025). Here, we present observations at even higher angular resolution (~0.15") and over a broader frequency range (140.7319–140.8512 GHz and 265.8214–267.6103 GHz).

Our observations revealed that the molecular environment spans from large-scale outflows, traced by HCN, H_2CO, and HCO^+, to the innermost regions of the IRAS4A2 system. Using CASSIS, a spectral analysis tool (Vastel et al. 2015), we detected numerous complex organic molecules (COMs), confirming the presence of at least 4 (e.g., $C_2H_3CN_{v=0}$, $CH_2(OH)CHO$, CH_3OCHO, and $CH_3C^{15}N$), with several additional tentative detections. These molecules appear to trace multiple components of the system simultaneously, increasing the challenge of the analysis.

Through analysis of the zero-moment maps (integrated emission of the molecules), we identified four distinct regions: the bipolar outflows, a large flattened envelope structure, a disk, and a warm inner envelope. Some emission lines also show strong absorption, particularly in the regions associated with the warm inner envelope.

Position–velocity (PV) diagrams, combined with upper-state energy levels and emission area estimates, indicate that many molecules, including sulfur-bearing species that are likely tracing accretion shocks too, trace stratified layers in the disk, as well as mid-plane emission near the central star. The mid-plane emission appears to be partially absorbed for many molecules, though not for all, suggesting that the envelope has either dissipated in the outer regions, has become optically thin in most areas, or has shrunk and moved closer to the star and the mid-plane, pointing towards settling processes still ongoing. This, combined with continuous dust radial drift, affects the location at which sublimation temperatures for different COMs are reached, altering both the radius and scale height where they are observed. These findings indicate that the radial and vertical chemical structure and emission in young stellar objects are more complex than previously anticipated and that the dust keeps rapidly evolving within the system.

Chapter 4: Into the thick of it: ALMA 0.45 mm observations of HL Tau at a resolution of 2 au.

In Chapter 4, we analyzed the protostellar system of HL Tau, one of the most well-known and extensively studied protoplanetary disks. HL Tau is a young stellar object located in the Taurus-Auriga molecular cloud (~147 pc; Galli et al. 2018). It is classified as a Class I disk transitioning to Class II (Furlan et al. 2008), with an estimated age of less than 1 Myr (Liu et al. 2017). HL Tau was among the first protoplanetary disks observed at high resolution with ALMA that revealed bright and dark ring features (ALMA Partnership et al. 2015).

For this work, we analyze optically thick emission using ALMA Band 9 observations. Despite the high optical depth, Band 9 data offers valuable insights due to its unprecedented angular resolution. In the case of HL Tau, we achieved a resolution of 13 milliarcseconds, the highest ever obtained for a protoplanetary disk with ALMA. This unprecedented resolution allowed us to probe the innermost regions of the disk, where we identified a previously undetected substructure at ~2.5 au. This feature, shown as an increase in the brightness temperature, is likely caused by an increase in the surface density of small dust particles, potentially linked to the effects of the water snowline.

Additionally, we identified a notable asymmetry within the inner 32 au of the disk. We argue that this asymmetry arises from a combination of optically thick emission, a significant dust scale height, and a certain disk inclination. Using radiative transfer modeling, we found that the HL Tau disk exhibits a dust dimensionless scale height (h/r) of approximately 0.08 at the observed wavelengths, and that the observed asymmetry is degenerate with the dust mass. This suggests that millimeter-sized grains may be less settled than previously assumed, and that the dust scale height may vary with radius in protoplanetary disks.

Finally, we revisited the multi-wavelength analysis from Carrasco-González et al. (2019), this time incorporating the optically thick Band

9 data. The addition of this high-frequency dataset allowed us to better constrain the dust temperature profile, which in turn influenced all other model parameters. We derived grain sizes up to an order of magnitude larger within 60 au, along with consistently lower dust temperatures at all radii.

Altogether, this work emphasizes the importance of studying the smallest observable wavelengths with ALMA. Despite observational challenges, these data are essential for revealing the detailed dust properties and structures within protoplanetary disks, demonstrating that deep substructures can still exist in optically thick and unsettled environments.

Chapter 5: A high-resolution survey of protoplanetary disks in Lupus and the nature of compact disks.

To better understand planet formation and its connection to protoplanetary disks, specifically around M-dwarfs, we obtained high-resolution observations of all Class II disks in the Lupus star-forming region. Lupus is a nearby (∼160 pc; Lombardi et al. 2008; Galli et al. 2020), young (1–2 Myr), low-mass star-forming region in the Scorpius-Centaurus association, comprised of several molecular cloud complexes (Lupus 1–9).

With resolved observations of nearly all disks within this single region, we constructed a comprehensive image gallery of Lupus disks at high resolution, gathering data from both our observations and existing literature. This enabled a complete analysis of the full sample of 74 Class II disks around low-mass (M-type) stars.

We found that 67% of the disks in Lupus are compact, with dust radii smaller than 30 au. Notably, we measured dust sizes down to 0.58 au and discovered previously undetected substructures, primarily cavities, in 11 of these compact disks.

By plotting the size–luminosity relation, we found that the majority of disks follow a trend consistent with a drift-dominated evolutionary scenario. Through radiative transfer modeling, we estimated the dust masses of the compact disks to be relatively low (ranging from 0.3 to 26.3 $M_\oplus$), corresponding to optically thin emission in most cases. This suggests either that current observations probe only a surface layer of the total dust mass or that we are witnessing the remnants of dust material left after the bulk of planet formation has already taken place.

Finally, our results show that one-third of the total disk population in Lupus is smooth, and only large disks commonly show substructure at the current resolution. Taken together, these findings highlight compact disks as promising birthplaces with the ideal conditions for forming super-Earths, the most common type of exoplanet observed.

1.4.2 Main conclusions

- By showing the possibility of substructures in a system like IRAS4A1 and the chemical distribution in IRAS4A2, we suggest that planet formation may already be well underway, or even completely finished by the Class II phase in protoplanetary disks. This suggests that it must begin very early in the disk lifetime, during the Class 0/I phase, or happen rapidly during the transition from Class 0/I to Class II. Understanding these early formation stages is therefore critical for constraining planet formation mechanisms. One way to investigate this is by exploring the connection between disk substructures and the occurrence of planets. By identifying substructures in the earliest stages of disk evolution or linking their presence, or absence, to known and distinct types of exoplanets, these studies can provide valuable insights into how and when planets are most likely to form.

- There is much scientific value in looking beyond the more common wavelengths of 0.8-1.3mm with ALMA and the brightest protoplanetary disks. Small disks and optically thick regions with ALMA can offer equally valuable insights about disk structure and evolution. Moreover, high-resolution molecular line observations, combined with dust continuum data, are essential to fully understand the distribution of solids and the conditions that drive planet formation. Future efforts should focus on studying the most common disks in our galaxy, compact disks, as they are crucial for building a more representative and comprehensive picture of protoplanetary disk evolution.

- The vertical distribution of dust (i.e., dust settling) is just as important as the radial distribution (i.e., radial drift) in shaping protoplanetary disk structure. These processes must be studied together to gain a comprehensive understanding of disk evolution. Furthermore, radial variations in the vertical structure of disks appear to be more common than previously thought, and their characterization in disk substructures may hold the key to understanding the initial conditions for planet formation.
- Most disks in low-mass star-forming regions are compact (less than 30 au), with substructures commonly observed only in larger disks. However, substructures may remain hidden in the innermost regions of these compact protoplanetary disks, or some other mechanism, still unknown, might be slowing down radial drift. The fact that most compact disks have relatively low dust masses and optically thin emission could also suggest, again, very early planet formation (during Class 0/I), with ideal conditions for forming the most common exoplanet, super-Earths.

1.4.3 Future science

Despite the remarkable progress made in recent years, there is still much to uncover with ALMA using its current capabilities. Investigating dust and CO emission at high resolution in older star-forming regions, such as Upper Scorpius, will provide valuable insights into the evolution of dust and gas, helping us build a more complete picture of disk evolution in the latter stages of protoplanetary disks. Moreover, one major instrument upgrade is on the horizon for ALMA. The Wideband Sensitivity Upgrade will increase the spectral bandwidth by a factor of four without compromising spectral resolution. This will come with a full upgrade of ALMA's receivers and digitizers, which will significantly increase its overall sensitivity as well as much wider bandwidth for simultaneous line observations. These upgrades will improve our ability to study dust and molecular emission in compact disks by making such observations much less time-consuming.

The arrival of JWST was a groundbreaking moment for astronomy, offering a revolutionary view of the universe. Many new opportunities have arisen with this powerful telescope in many fields, including in the study of protoplanetary disks. In particular, future observations of compact protoplanetary disks with JWST are expected to uncover their inner chemical compositions and provide a detailed infrared perspective of these small, faint systems.

Looking ahead, the next-generation Very Large Array (ngVLA) will define the future of radio astronomy (expected 2035). With unprecedented angular resolution down to 1 milliarcsecond and sensitivity an order of magnitude greater than the current Jansky VLA, the ngVLA will allow us to observe the innermost regions of protoplanetary disks and some of the most compact ones, with exceptional detail. Operating over a frequency range from 1.2 GHz (21 cm) to 116 GHz (2.6 mm), the ngVLA will probe the optically thin regions of disks where the largest dust grains and the fundamental building blocks of planet formation (dust growth) are found. The advanced capabilities of ngVLA will also make it possible to detect new COMs, which are those predicted but not yet observed. This will provide clues about the chemical initial conditions of many planetary systems.