Radiative transfer models of protoplanetary disks: Theory vs. observations

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For thousands of generations people have looked up to the night sky at the stars. But only in the modern scientific age have we begun to understand what it is that we see in the night sky, and what we can learn from it. Most importantly, we have learned that the stars in the sky are glowing balls of gas powered by hydrogen fusion in their cores. They are located so far away that even the dim light we receive from them at night has taken years and sometimes even millenia to reach us. One thing that has become clear is that we are not the center of the universe: the Earth is but one planet among eight orbiting the Sun, the Sun is but one star among a hundred billion in the Milky Way, and the Milky Way is but one galaxy among billions.

This raises intriguing questions: if the Sun is not special, then how special is the Earth that we live on, and how special are we? Do all stars we see have planets, and what do these look like? Are any of these planets able to support life, and is there intelligent life out there? We are now starting to find answers to these questions.

It was only eighteen years ago that the first planet orbiting another star was discovered by Mayor & Queloz (1995), and the number of exoplanets found has increased ever since (Figure 1.1). The known population of exoplanets shows a large diversity: giant planets can be found much closer to their host star than any in our solar system, or much further out; a new class of super-Earths, with masses between that of the Earth and Neptune, has been discovered that will be prime candidates in the search for extraterrestrial life.

To explain this diversity of exoplanets, and to understand our own origins, we have to look into the process of their formation. Planets form from the leftover material of star formation that orbits newborn stars. This material takes the form of a protoplanetary disk, and these disks are the main subject of this thesis. Our Sun once possessed such a protoplanetary disk when it was just born, around 4.5 billion years
The disk-shape of this material explains why all solar-system planets revolve in the same direction and in the same plane around the Sun, and always cross the same constellations in the night sky. The existence of such a disk was first postulated in the 18th century by Kant (1755). Although the protoplanetary disk around the Sun has long since been dispersed, part of its history can still be reconstructed through studying the meteoritic record that traces the formation of our planetary system.

However, star and planet formation is not just something that took place only in the past: the space between the stars is not empty, but filled with gas and dust that is still forming stars today. The Sun is located near the Gould Belt, a large complex of star-forming regions where we can find thousands of young stars still surrounded by protoplanetary disks. It is here that we can catch planet formation in action. Orion (Fig. 1.2) is perhaps the most well-known of these regions and its constellation is easily identified in the night sky.

In this chapter I will give a brief overview of star formation, protoplanetary disks and planet formation. I will then discuss in detail some of the observational and modelling techniques commonly used to investigate what these disks look like and how they may form planets.
1.1 Star and planet formation

Stars form from collapsing molecular clouds of dust and gas. Although some stars form in isolation, most of them form in larger clusters such as the Orion Nebula or Taurus-Aurigae. The clouds that spawn these clusters are held together by gravity, while gas pressure, magnetic fields and turbulence may prevent them from collapsing. They have a filamentary structure, probably originating from turbulent motions within the cloud. Within these filaments, dense cores form. I will discuss the collapse of these cores as if they were isolated from their environment. The trigger for collapsing such a core, however, may well be external, for instance a nearby supernova.

1.1.1 The formation of a star-disk system

Once a core starts to collapse under its own gravity, it will form a star in the center within a hundred thousand years. If the core had no rotation, all material would fall
directly onto the forming star in the center. In reality, cores will have some rotation due to turbulent motions in the parental molecular cloud. This prevents the outer layers from falling directly onto the star: as the material falls in, conservation of angular momentum increases the angular velocity of the material, similar to how figure skaters start to rotate faster if they pull in their arms. Some of the material will rotate so fast it never reaches the star and ends up in orbit around it, forming a circumstellar disk.

These disks are essentially angular-momentum transport machines, and allow material to flow towards the central star while the disk also expands to conserve its angular momentum. The star grows by accreting material from the disk, but also starts to disperse the surrounding cloud. Young stars can drive powerful jets and outflows perpendicular to the disk, creating a cavity in the surrounding material. Because the disk is also much denser than the cloud, it can remain in place long after the cloud has dispersed, creating a star-disk system. This disk is the protoplanetary disk that will later form planets (Fig. 1.3).

1.1.2 The appearance of protostars

From an observational point of view, the transition from core to star can be described using the Lada sequence (Lada 1987; Adams et al. 1987; Andre et al. 1993). Figure 1.4 shows this sequence, which classifies protostars based on the amount of energy emitted at different wavelengths, the Spectral Energy Distribution or SED. This emission is mainly stellar light and released gravitational energy, absorbed and re-emitted
1.1 Star and planet formation

Figure 1.4: Evolutionary phases of a forming star, classified according to the Lada Sequence (see text). The left panels show the SED with the star in yellow and the envelope/disk material in red. The right panels show a sketch of the corresponding geometry. The overall shape of the SED changes as the protostar evolves from a dense core (Class 0), via an embedded star-disk system (Class I) and a protoplanetary disk phase (Class II) to a star with a planetary system and a debris disk (Class III), similar to our solar system. Figure adapted from the Encyclopedia of Astrobiology.
at a different wavelength by the dust in the system. In general, the emission at short wavelengths originates from warm regions close to the star, while emission at longer wavelengths traces colder material further away. The shape of the SED – roughly defined by the ratio of short to long wavelength emission – therefore holds important information on the evolution from a cold cloud core to a hot star.

Class 0: Before the star has formed, only a cold core is present with a temperature of around 10 Kelvin. This cold material radiates in the far-infrared at a wavelength of around 300 micrometers, creating an SED that is very red in color. When the star forms, this core will heat up, but the thick envelope around it will hide this hot core from view in the SED.

Class I: Once a star-disk system forms, the (accretion) luminosity from the central star heats up the inner regions. These will start to emit in the near-infrared, at wavelengths of roughly a micron. The now thinner outer envelope still absorbs a significant fraction of this light, re-emitting it at longer wavelengths. The SED of a class I source therefore still peaks in the far-infrared, but has a significant contribution in the near-infrared.

Class II: When the envelope has completely fallen onto the star or has been blown away, a star and its protoplanetary disk remain. The star accretes from the disk at a moderate rate, and heating from the star will be the main source of energy in the disk. The SED therefore peaks in the optical, where the star shines, but a significant infrared excess from the disk remains.

Class III: After the disk has disappeared, a star and its planetary system remain. Planets are too faint to be detected in the SED, but smaller bodies may collide and generate a dusty debris disk that can reprocess a small portion of the star light. The SED is dominated by the star, and there is only a very small infrared excess.

The protoplanetary disks that are the subject of this thesis are Class II sources: the naked star is visible without an obscuring envelope, but a significant infrared excess coming from the disk is still present. A subclass of these disks are the transitional disks (Muzerolle et al. 2004b; Calvet et al. 2005). They have less emission in the near-infrared than typical Class II sources, but similar amounts in the far-infrared. This indicates that they might be in transition from class II to III, and that this transition starts in the inner disk. A possible reason for this is that they have formed planets, which I will discuss in the next section.
1.1 Star and planet formation

Figure 1.5: Approximate size range spanned in the planet formation process. Purple regions above the scale bar indicate the size ranges currently observable outside the solar system. Indicated below are objects found in the solar system, from left to right: an interplanetary dust particle, a meteorite, asteroids, a terrestrial planet (Earth) and a gas giant planet (Jupiter). Figure based on Kees Dullemond’s lectures. Figures above the scale bar © David A. Hardy/www.astroart.org

1.1.3 The formation of planets

Unlike stars, most planets are not massive enough to form directly by a gravitational collapse. Only the most massive planets that are located far away from their host stars – such as those recently discovered in direct imaging surveys (Marois et al. 2008; Carson et al. 2013) – may be an exception to this. However, the bulk of exoplanets discovered have much lower masses and are found closer to their host stars. These planets can form through the growth of microscopic dust grains all the way up to the size of terrestrial planets (Weidenschilling 1980). If these rocky cores become massive enough, they continue to grow further by pulling in gas from the surrounding disk, forming giant planets in what is known as the core-accretion scenario (Pollack et al. 1996). This whole process spans around 40 orders of magnitude in mass or 13 orders of magnitude in radius (Figure 1.5), and presents a formidable challenge to both observers and theorists. This growth range is usually subdivided into a number of stages, in which different physics dominate the growth of dust (e.g. Chiang & Youdin 2010; Morbidelli et al. 2012).

Growth by coagulation: The initial step of planet formation is the growth of microscopic dust grains through coagulation following mutual collisions. Due to the high densities in protoplanetary disks, grains collide frequently and can grow much larger than in the interstellar medium or molecular clouds. They grow quickly from micron to millimeter sizes (Weidenschilling 1980). How-
ever, as grains grow larger, the relative velocities keep increasing, until they reach a size where the impact velocities are so high that collisions become destructive. This is called the fragmentation barrier and provides an upper limit to the size grains can grow by coagulation, ranging from roughly a meter in size in the inner disk to a millimeter in size in the outer disk. Coagulation and fragmentation are described more extensively in section 1.2.3. There are other barriers along the way as well, such as the bouncing barrier (Zsom et al. 2010) – related to decreased sticking efficiency at larger sizes – and the electrostatic barrier (Okuzumi 2009), which prevents collisions between charged dust grains. Although these barriers may temporarily stall the planet formation process, they are important because they keep a small fraction of micron-sized dust in these disks, which is observed in protoplanetary disks of all ages.

The intermediate regime: Growth of dust grains is most difficult to understand in the regime where grains are too large to grow by coagulation (Blum & Wurm 2008), but too small to grow by gravitational interaction. In addition, should particles reach one meter in size, they would feel a strong headwind from the gas and drift inwards, quickly depleting the disk of solids to form planets (Weidenschilling 1977). This barrier is called the meter-sized or radial-drift barrier. A promising mechanism to cross this regime and overcome these barriers is the collective gravitational effect of an ensemble of particles. Two centimeter-sized particles do not gravitationally attract each other, but a million might. Long lived-structures in the gas such as pressure bumps and turbulent eddies (vortices) can trap large numbers of particles, making them susceptible to gravitational collapse directly into much larger bodies (e.g. Johansen et al. 2006) before they can drift or fragment. The size distribution of asteroids in the solar system indicates that they indeed formed in this way, skipping the intermediate sizes and coalescing directly from centimeter-sized dust grains to kilometer-sized asteroids (Morbidelli et al. 2009).

Gravitational growth: Once kilometer-sized bodies, now called planetesimals, have been formed, gravity takes over as the main driver of growth. At these sizes, collisions do not lead to fragmentation, as their gravitational pull is strong enough to retain most of the material of a collision in a single body. This growth is usually subdivided into two phases. In the first phase, more massive planetesimals have a higher chance of colliding. They grow faster than the smaller ones, and this phase is therefore called runaway growth (Greenberg et al. 1978). In the second phase, the gravity of these largest bodies prevents the growth of smaller planetesimals. They continue to grow themselves by slowly capturing the less massive planetesimals. This phase is called oli-
garchic growth (Kokubo & Ida 1998), and creates planetary embryos of about a thousand kilometers, the size of Pluto.

**Final stages of assembly:** In the final stages of planet formation, the protoplanetary disk is seeded with planetary embryos or protoplanets that have collected most of the solid materials (‘dust’) in their direct vicinity. They are too tightly packed to form stable planetary systems, and will continue to collide and grow to do so. Whether these embryos will form terrestrial planets or gas giants depends on a number of factors, most importantly their mass and the available amount of gas. If a protoplanet reaches a mass of about ten Earth masses while the disk still has plenty of gas, it can accrete significant amounts of this gas to become a gas giant like Jupiter in our solar system (Pollack et al. 1996). If this size is reached after most of the gas has been dispersed, an object with the mass of Neptune or a super-Earth will remain. Cores that never reach the size will form terrestrial planets, which slowly assemble in the years after all the gas has been dispersed to form the exoplanetary systems that we observe today. These core accretion models provide a good match to the observed population of exoplanets (Mordasini et al. 2012).

## 1.2 Physics and observations of protoplanetary disks

In the last decades it has been firmly established by observations that most young stars, once they have accreted or dispersed their natal envelope, are surrounded by protoplanetary disks (e.g. Sargent & Beckwith 1987; Strom et al. 1989; O’Dell & Wen 1994). Over the course of a few million years, the fraction of stars that have disks steadily drops, until most disks are dispersed by the age of ten million years (Haisch et al. 2001, Figure 1.6). Because this timescale is too long to be followed by any human observer, we have to reconstruct the disk evolution from the disks that we can observe today. In this section, I will describe the basic physics of protoplanetary disks, and how they tie in with current observations.

### 1.2.1 Global disk evolution

Like the planets in our solar system, the gas and dust in protoplanetary disks is in orbit around its host star. To first order, these orbits are stable, and the typical disk persists over thousands to millions of orbits. However, there are additional processes acting on the dust and gas in these disks that make the disk evolve and eventually form planets.

Most importantly, these disks are observed to accrete gas onto the central star, at a rate of approximately $10^{-8} M_\odot/\text{yr}$ (Solar masses per year) for classical T Tauri stars,
the precursors of Sun-like stars (Hartmann et al. 1998). This means that during the disk’s few-million year lifetime, they accrete about one hundredth of a solar mass of gas, a significant amount of the total disk mass. Because most of this mass resides in the outer disk, this requires an efficient mass transport mechanism throughout the entire disk. What drives this accretion and mass transport within protoplanetary disks?

If the gas is on Keplerian orbits, material close to the star will rotate faster than gas further out, a process known as differential rotation. If there is some sort of friction between orbits, or the gas at different radii is otherwise coupled, the inner gas will slow down while the outer gas will speed up. To conserve angular momentum, the inner gas that was slowed down will end up in a lower orbit, while the outer gas that was sped up will move to a higher orbit. The net effect of this coupling is that gas will spread radially in both directions, a phenomenon called viscous spreading. The question as to why disks accrete is therefore equivalent to asking what provides the coupling of gas at different radii, i.e. what is the viscosity of the gas.
Because disks are geometrically thin (see next section), the equations describing the radial structure can be decoupled from those describing the vertical structure. For an axisymmetric disk, the evolution can be described in terms of the surface density $\Sigma$ – which is the amount of material in a column perpendicular to the disk, at a certain distance from the star, $r$. The time-dependent evolution of this gas was first derived by Lynden-Bell & Pringle (1974), who show that the bulk of the gas in a viscous disk accretes onto the star, while a small amount of gas at larger radii carries away the angular momentum. The evolution of the surface density under the influence of a viscosity $\nu$ at a time $t$ is given by Pringle (1981):

$$\frac{\partial}{\partial t} \Sigma(r, t) = \frac{3}{r} \frac{\partial}{\partial r} \left( r^{1/2} \frac{\partial}{\partial r} \left[ \nu \Sigma(r, t) r^{1/2} \right] \right).$$

(1.1)

If the initial and boundary conditions for the surface density are known, the disk evolution is determined solely by the viscosity.

However, the magnitude of the viscosity, and how it varies with the location in the disk, remains one of the largest uncertainties in understanding disk evolution (see Armitage (2011) for an excellent review of this topic). Direct measurements of the turbulent velocity in protoplanetary disks have only recently become possible (Hughes et al. 2011), and to date have not been able to characterize the viscosity in the entire disk. From a theoretical point of view, the molecular viscosity of the gas is insufficient to explain the observed accretion rates and disk lifetimes, and hence another mechanism is needed.

Pending the identification and characterization of such a mechanism, the viscosity is often parametrized using either a power law in radius, or following the ideas of Shakura & Sunyaev (1973). In the latter case, the scaling of the viscosity is based on subsonic turbulent motions and dimensional arguments: the viscosity $\nu$ has units $[m^2/s]$, i.e. a length scale $[m]$ times a velocity $[m/s]$. Taking the pressure scale height of the disk $H_p$ as the maximum size of turbulent eddies and the sound speed $c_s$ as their maximum velocity, the viscosity is given – again in the form of Pringle (1981) – by:

$$\nu = \alpha H_p c_s,$$

(1.2)

where $\alpha < 1$ is a dimensionless parameter that describes the overall strength of the viscosity.

We can get a good estimate of the surface density profile by looking at the steady state solution for an infinite disk – i.e. ignoring boundary conditions. Assuming the scale height and sound speed can be described by power-laws, eq. 1.1 has an analytic solution. A steady-state disk ($\frac{\partial}{\partial t} \Sigma(r, t) = 0$), with an irradiated ($c_s \propto r^{-0.25}$), flaring surface ($H_p \propto r^{1.25}$, see section 1.2.2), yields $\Sigma(r) \propto r^{-1}$. Relaxing the boundary condition at the outer edge adds an exponential taper, but retains the power-
law behaviour away from the outer edge (e.g. Hartmann et al. 1998; Hughes et al. 2011).

These $\alpha$ disk models are reasonably successful in explaining disk observations. Looking at accretion rates, and comparing disk lifetimes to sizes and radii, yields a typical value of $\alpha = 0.01$ (Hartmann et al. 1998). In addition the observed surface density profiles in the outer regions of protoplanetary disks match those predicted by $\alpha$-type models reasonably well (Andrews & Williams 2007, figure 1.7). However, some disks possess surface density profiles that are not well matched by $\alpha$-type models (Hueso & Guillot 2005; Isella et al. 2009), or alternatively formulated, require an $\alpha$ that varies with radius.

1.2.2 The vertical structure

Because protoplanetary disks are heated by the central star, their vertical structure determines to a large extent the amount of radiation they can absorb and re-emit. After the launch of the Infrared Astronomy Satellite (IRAS) in the eighties, it became
clear that protoplanetary disks produce more far-infrared emission than was predicted by a flat disk geometry (Adams et al. 1987). Kenyon & Hartmann (1987) suggested that the required thickness of the disk follows naturally when the gas is in vertical hydrostatic equilibrium. The authors show that such a disk has a flaring geometry, in which the upward curvature of the disk surface increases with distance from the star (Figure 1.8). This allows a flared disk to intercept and reprocess a significant fraction of starlight at large radii where the disk is cold, thus boosting far-infrared emission.

Flared disk models have been further improved both analytically and numerically (e.g. Chiang & Goldreich 1997; D’Alessio et al. 1998), and still form the basis of disk models used today and in this thesis. The degree of flaring of the disk surface – and therefore the observational appearance of the disk – depends on the vertical structure of both gas and dust. The latter is discussed in the next section, while the former follows from vertical hydrostatic equilibrium discussed below.

Let’s consider gas in the disk at a radius $r$ from the star and at a height $z$ above the midplane of the disk. Assuming the radial pressure gradient is negligible and the gas is on a Keplerian orbit, the gas only feels the vertical component of the gravitational

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**Figure 1.8:** Spectral energy distribution and corresponding geometrical model of a flaring disk. The surface layers of the disk, displayed in light gray, are directly exposed to the stellar radiation and radiate in the near to mid-infrared. The material in the midplane of the disk, displayed in darker gray, is well shielded from stellar radiation and therefore colder, radiating at longer wavelengths. Figure adapted from the review by Dullemond et al. (2007).
Introduction

field of the star, given by:

\[ g_z = \frac{GM}{r^2} \frac{z}{r} = \Omega_k^2 z, \]

where \( g_z \) is the gravitational acceleration in the \( z \)-direction, \( G \) is the gravitational constant, \( M \) is the mass of the star and \( \Omega_k = GM/r^3 \) is the Keplerian frequency. To achieve equilibrium, this acceleration must be balanced by the pressure from the gas below it minus the pressure from the gas above it, i.e. the pressure gradient

\[ \frac{dp}{dz} = -\rho g_z, \]

where \( p \) is the pressure and \( \rho \) is the gas density. Combined with the equation of state that relates the pressure to the density for an ideal gas \( (p = \rho c_s^2) \) and reordering variables, we find

\[ \frac{dp}{p} = -\frac{\Omega_k^2}{c_s^2} z \, dz, \]

which can be directly integrated to find the vertical pressure and corresponding density structure of the gas. Assuming the sound speed is independent of \( z \), i.e. there is no vertical temperature gradient, this equation has the analytic solution

\[ \rho = \rho_0 e^{-z^2/(2H_p^2)}, \]

where \( \rho_0 \) is a normalisation constant that can be scaled to the surface density and \( H_p = c_s/\Omega_k \) is the pressure scale height. This isothermal vertical structure with a constant vertical scale height is commonly used in radiative transfer models (e.g. Robitaille et al. 2006).

The radial dependence of this pressure scale height determines the flaring of the gas, and is often parametrized as \( H_p \propto r^\beta \), where \( \beta \) is referred to as the flaring index. The main uncertainty in calculating this index comes from the radial dependence of the temperature. Taking the temperature profile for an optically thin \( (T \propto r^{-0.5}) \) and flat \( (T \propto r^{-0.75}) \) disk as extremes, Kenyon & Hartmann (1987) found that disks are indeed flaring, with the scale height varying between \( H_p \propto r^{1.25} \) and \( H_p \propto r^{1.125} \), respectively. However, the temperature structure of the disk itself depends on the disk flaring, and the derived solutions need not be self-consistent. This issue is addressed in the seminal paper by Chiang & Goldreich (1997), who take the feedback of the scale height profile on the temperature structure into account. The authors find a slightly more flaring scale height profile \( H_p \propto r^{9/7} \), corresponding to a shallower temperature profile \( T \propto r^{-3/7} \).

In reality, disks are not vertically isothermal due to high optical depth, and the real vertical structure will deviate from the Gaussian distribution of equation 1.6. Chiang
1.2 Physics and observations of protoplanetary disks

Figure 1.9: Interplanetary dust particle, from Jessberger et al. (2001). Its aggregate shape is consistent with being formed by coagulation of smaller dust particles in the protoplanetary disk around the Sun.

& Goldreich (1997) divided the disk in two zones: a radially optically thick, but vertically optically thin surface layer and an optically thick midplane (see figure 1.8). This surface layer absorbs the impinging stellar radiation and heats up. It radiates equal amounts of energy away into space and into the optically thick interior, where it is absorbed. The interior will therefore be colder than the surface layer, giving rise to a silicate feature in emission (see also Calvet et al. (1992) and section 1.2.4). Abandoning the two-layer approach altogether and solving for the detailed temperature structure using radiative transfer, a similar behaviour is found with a smooth temperature gradient from a cold midplane to a warm surface layer (e.g. D’Alessio et al. 1998). The vertical structure of the gas then follows from integrating equation 1.5. More details on vertical structure calculations in radiative transfer models can be found in section 1.3.3.

1.2.3 Grain growth and dust settling

Although the vertical structure of the gas is set by hydrostatic equilibrium, the vertical structure of the dust can deviate significantly from it. From comparing observations that probe the thickness of the dust disk to hydrostatic radiative transfer models, we know that the dust disk is usually thinner than the gas disk (D’Alessio et al. 1999). These observations include not only the amount of infrared excess in the SED, but also the thickness of the dust lane in edge-on disks and the number ratio of face-on and edge-on disks. This indicates that the surface of these disks are depleted of small dust grains, due to the combined effects of dust settling and grain growth (D’Alessio

Grains grow by coagulation. When they collide, they stick together to form larger dust grains (Fig 1.9, Weidenschilling 1980). When grains grow larger, they feel less friction from the gas and their collision velocity increases. Grains keep growing until these velocities are so high that they start fragmenting upon colliding, replenishing the supply of small dust grains (Dullemond & Dominik 2005). This leads to a grain size distribution where both the smallest (<\(\mu\)m) and largest (>mm) grains are present (Fig. 1.10).

Such a size distribution is required to explain disk observations. Smaller grains need to be present at the disk surface to explain the presence of a silicate feature in emission (Cohen & Witteborn 1985), which is only produced by grains less than a few micron in size (van Boekel et al. 2003). Large millimeter-sized grains are required to explain the fluxes and the slope of the SED at millimeter wavelengths (Weintraub et al. 1989; Andrews & Williams 2007). The details of the size distribution depend on the microphysics of the dust and the global disk properties (e.g. Brauer et al. 2008; Birnstiel et al. 2010a). In practice, grain size distributions are often approximated by a power law in size, similar to that of the interstellar medium (Mathis et al. 1977), but extended to millimeter sizes (e.g. D’Alessio et al. 2001). Because intermediate-sized\(^1\) grains have no direct observational signature, two-component models with only a small and large grain population are also commonly used (e.g. Dullemond & Dominik 2004a).

The dynamical decoupling of dust and gas also affect the vertical structure of the dust disk in a process called dust settling. The coupling of the dust and gas is given by the Stokes number

\[
St = \frac{a_{gr} \rho_s \Omega_k}{4 \rho_{gas} c_s},
\]

where \(a_{gr}\) is the grain size, \(\rho_s\) is the density of a dust grain and \(\rho_{gas}\) is the local gas density. A Stokes number smaller than one means the dust is dynamically coupled to the gas, a number larger than one means they are decoupled. If dust grains grow beyond a Stokes number of one, the pressure gradient of the gas can no longer support the gravitational pull of the star (see eq 1.4). The dust will settle towards the midplane of the disk where the gas densities are higher (eq 1.6), decreasing the Stokes number until the dust re-couples to the gas. For each grain size, there will be a typical height above which the dust is severely depleted (Dullemond & Dominik 2004b). This size-sorting process, called stratification, has been observed in the disk of GG Tau (Pinte et al. 2007).

The timescale for both dust settling and grain growth is shorter than the disk life-

\(^1\)Grains much larger than the micron-sized dust observed in the surface layers, but much smaller than the millimeter-sized dust grains observed in the radio.
1.2 Physics and observations of protoplanetary disks

Figure 1.10: Grain size distribution from a numerical simulation including growth and fragmentation, from Dullemond & Dominik (2005). Darker lines correspond to later times (0, 10^2, 10^3, 10^4, 10^5, and 10^6 years, respectively). In this particular model, at 1 AU in the midplane of the disk, the fragmentation barrier occurs around 1 to 10 cm (10^4...10^5 \(\mu\)m). A quasi steady-state is reached before 10^5 years for grain sizes below this barrier.

time (Dullemond & Dominik 2004b, 2005). Because we do not see flat disks with only large grains, this implies an additional mechanism is necessary to replenish the supply of small grains and move them back to the disk surface. These mechanisms are fragmentation and turbulence. The turbulence of the gas provides random velocities to the dust particles, which tend to diffuse the smallest dust grains produced by fragmentation back up to the disk surface. The consequence of these processes is that dust settling and grain growth reach an equilibrium or steady-state. Therefore, the grain sizes and degree of settling we observe now are not a proxy of disk evolution, but rather reflect the internal physics in the disk (Mulders & Dominik 2012, Chapter 3).

1.2.4 Dust opacities and mineralogy

Dust carries the bulk of the opacity in protoplanetary disks. Together with the geometry it is an important factor in determining the temperature structure of the disk, and therefore also the observational appearance in the SED and other disk observations. The opacity depends on the mineralogy (chemical composition and lattice structure), size and structure of the dust. Mid-infrared spectroscopy has revealed a set of solid-state features that can serve as a diagnostic of these properties, and they can serve as a tracer of the evolution of dust in protoplanetary disks.
Mid-infrared observations of the dust in protoplanetary disks, especially with the Infrared Space Observatory and later with the Spitzer Space Telescope, have provided strong constraints on the dust properties in protoplanetary disks (e.g. Watson 2009). The ubiquitous presence of broad solid state features at 10 and 20 µm indicates the presence of (sub)micron-sized amorphous silicate grains in the upper layers of protoplanetary disks (see figures 1.8 and 1.11). They are mostly olivines ([MgFe]_2SiO_4) and pyroxenes ([MgFe]SiO_3), and tend to be magnesium-rich and iron-poor (Juhász et al. 2010). The shape of these features is sensitive to a limited size range, roughly between 0.1 and 5 µm, and different grain sizes are observed in protoplanetary disks (van Boekel et al. 2003).

A set of narrower features, belonging to crystalline silicates, is observed in a subset of these disks (e.g. Waelkens et al. 1996; Malfait et al. 1998; van Boekel et al. 2005). They are mainly enstatite and forsterite, with the same chemical composition as the amorphous silicates, but with their atoms ordered in a lattice, producing stronger and narrower features. These features are more sensitive to the iron content, and are observed to be iron-poor (Sturm et al. 2010; Mulders et al. 2011). Why some disks possess dust crystals and others do not remains unclear. The dust in the interstellar medium is mostly amorphous (Kemper et al. 2004), so the dust must have crystallized during the disk lifetime. Crystals are formed by heating them close to their sublimation temperature, but at their current observed location, temperatures are too low (~ 100 K) to do this. Either efficient radial mixing from warmer regions in the inner disk, or a local process such as shocks or parent body processing must be responsible. Unfortunately, there are few observed correlations with stellar and disk parameters that could guide the way to identifying these mechanisms (Bouwman et al. 2001; van Boekel et al. 2005; Oliveira et al. 2013), though local production of crystals in an outburst has been observed (Ábrahám et al. 2009).

Although the identification of silicates has narrowed down the range of possible dust compositions, not all types of dust have observable features. Especially iron (outside of silicates) and carbon (apart from Polycyclic Aromatic Hydrocarbons) have no strong features, but can contribute significantly to the continuum opacity in the optical and near-infrared (see Fig. 1.11). They are found in solar system meteorites, and are probably present in some form in the dust of protoplanetary disks. Their presence or absence provides one of the largest uncertainties in modelling the dust in protoplanetary disks, which may lead to degeneracies with the derived disk structure.

Besides chemical composition, grain size is an important factor in determining the dust opacity. For a given refractive index (which depends on composition and is measured in the lab), the absorption and extinction opacities can be calculated for a given grain size. A common approach is to use Mie Theory, a series of analytical
1.2 Physics and observations of protoplanetary disks

Figure 1.11: Dust opacities of small and large compact spheres, with and without a continuum opacity source. The solid line shows a 1 \( \mu m \) pyroxene grain with 20\% amorphous carbon, the dotted line shows the same particle without carbon. The dashed line shows a 100 \( \mu m \) particle. The gray dotted and dashed lines show the approximate location of the resonance regime (\( \lambda \sim 2\pi a_{gr} \)) for the small and large particle, respectively.

solutions to the Maxwell equations for light interacting with the electric field of a compact spherical particle (Mie 1908). It is also possible to use other particle shapes, such as a distribution of hollow spheres (Min et al. 2005a). Their opacities mimic those of particles with an irregular shape, and provide a better fit to the observed spectral features. Dust is likely present in the form of aggregates, but computing their optical properties is computationally expensive. If they are present in the surface layers of the disk, it is possible that grain sizes are systematically underestimated because we measure the size of the monomers, rather than the whole aggregate (Min et al. 2006).

A few examples of dust opacities illustrating their general behaviour as a function of wavelength are shown in figure 1.11. The figure shows three different regimes, determined by the particle size in comparison to the wavelength: the Rayleigh regime (\( 2\pi a_{gr} < \lambda \)), the resonance regime (\( 2\pi a_{gr} \sim \lambda \)) and the geometrical optics regime (\( 2\pi a_{gr} > \lambda \)). In general, the opacities are flat in the geometrical optics regime, and drop off with \( 1/\lambda^2 \) in the Rayleigh regime. Because the opacity in the geometrical optics regime scales with the surface to mass ratio as \( 1/a_{gr} \), the opacity in the optical and near-infrared is dominated by the smallest grains (< \( 1 \mu m \)). The larger grains are only visible at the wavelength where they are in the resonance regime, and dominate the opacity over grains of other sizes. At (sub)millimeter wavelengths, the shape of the opacity is dominated by such large grains (0.1...10 mm, Draine 2006), and
measuring the slope of the SED at these wavelengths has revealed that most protoplanetary disks indeed contain grains of these sizes (Weintraub et al. 1989; Andrews & Williams 2007).

Aside from the absorption efficiency, the scattering efficiency can also be used as a diagnostic of the dust content in disks. Direct observations of scattered light have become possible through spatially resolved imaging using the Hubble Space Telescope in the optical and using ground-based telescopes with adaptive optics in the near-infrared. Because real grains scatter light in an anisotropic way, the brightness asymmetry of an inclined disk can serve as a proxy for the grain size (Pantin et al. 2000; Pinte et al. 2008b). The scattering color and brightness can provide additional constraints on the grain size (Mulders et al. 2013, Chapter 4).

1.2.5 Transitional disks

A small fraction of protoplanetary disks has a smaller excess in the near-infrared, but still significant excess at longer wavelengths (Strom et al. 1989; Najita et al. 2007). This may indicate that the inner regions are depleted of material, while the outer disk remains. These depleted inner regions are also seen as (partly) empty gaps or inner holes in resolved images (e.g. Andrews et al. 2011). These disks are believed to be in transition from class II to III (see section 1.1.2), and are therefore called transition disks or transitional disks (Muzerolle et al. 2004a; Calvet et al. 2005). The mechanism that creates a transitional disk remains unclear, but is likely connected to...
planet formation and disk evolution. Several mechanisms have been proposed, the most important ones being photo-evaporation and dynamical interaction with giant planets. The recent detection of a planetary candidate inside the gap of the transitional disk LkCa 15 lends support to this last hypothesis (Kraus & Ireland 2012).

Photo-evaporation is driven by UV photons and X-rays. These photons heat up the gas in the upper layers of the disk, and when the gas thermal velocity approaches the local escape velocity, start driving a disk wind. The strength of the wind depends on the photon energy. Extreme-UV photons can drive mass loss rates of the order $10^{-9}$...$10 M_\odot/yr$ (e.g. Hollenbach et al. 1994), which is much lower than the typical accretion rate. Far-UV photons and X-rays penetrate deeper into the disk, and can drive more substantial outflow rates, on the order of $10^{-7}$...$8 M_\odot/yr$ (Gorti & Hollenbach 2009; Owen et al. 2010). Because UV and X-rays are strongest close to the star, while the escape velocity is lower further away, photo-evaporation mainly acts to open gaps at intermediate radii of 1 to 10 AU (Gorti et al. 2009; Owen et al. 2010). When the accretion rate in the disk drops below the photo-evaporative mass-loss rate, a gap is carved out. The inner disk can no longer be refilled and quickly drains onto the star, creating a transitional disk geometry (figure 1.12). This mechanism can explain transitional disks with low accretion rates and small holes, but not the strongest accretors with the largest holes (Owen et al. 2012).

A forming planet in a protoplanetary disk exerts a gravitational torque on the disk.
A sufficiently massive planet can open an annular gap if this torque is larger than the viscous and pressure torques in the disk (e.g. Lin & Papaloizou 1979, 1986, Fig. 1.13). However, these gaps span a relatively small radial range, and may be visible in imaging, but hardly in the SED (Steinacker & Henning 2003; Varnière et al. 2006; Wolf et al. 2007). To explain the low near-infrared excess, an additional mechanism is needed. This mechanism also needs to meet three additional observational criteria to explain transitional disks:

- They have large inner holes in their population of millimeter-sized grains, as traced by resolved millimeter imaging (Andrews et al. 2011).

- Most of them have no apparent holes when imaged in near-infrared scattered light (Dong et al. 2012), indicating that these gaps or holes are not devoid of micron-sized grains.

- Most transitional disks accrete at a ten times lower, but still substantial rate of around $10^{-9} \mathcal{M}_\odot$/yr (Najita et al. 2007), with individual disks as high as $10^{-8} \mathcal{M}_\odot$/yr (See figure 17 of Owen et al. 2012 and references therein).

Multiple giant planets are necessary to explain the radial extent of these holes, but also block the accretion flow onto the star (Zhu et al. 2011). A single planet may let some of the gas through, but needs an additional mechanism to explain the depletion of the disk inside the planet’s orbit. The most promising mechanism is dust filtration: a planet in the gap also creates a pressure bump in the disk that may block large millimeter-sized grains, but allows passage of some of the small grains (Zhu et al. 2012; Pinilla et al. 2012). Observations of the dust and gas with the Atacama Large Millimeter Array will probably shed new light on the origins of transitional disks, by imaging them at much higher spatial resolution and with better sensitivity than was previously possible.

### 1.3 Radiative transfer

There are no analytic solutions to the equations of radiative transfer in an arbitrary geometry. Therefore, numerical radiative transfer codes are necessary to map the dust geometry and composition of protoplanetary disks to observable quantities such as the SED. There are different types of radiative transfer codes, ranging from the 2-layer models from Chiang & Goldreich (1997) that were discussed before, 1+1D models that split the radial and vertical transport of energy (D’Alessio et al. 1998), 2D models that perform 3D radiative transfer in a 2D geometry (Dullemond & Dominik 2004a; Pinte et al. 2006; Woitke et al. 2009) and even 3D codes for non-axisymmetric disks (Wolf et al. 1999; Robitaille 2011). Over the last decades,
increase in computational power and improvements in radiative transfer algorithms have led to an increased use of 2D radiative transfer codes.

For this thesis, I have used the radiative transfer code MCMa, written by Michiel Min (Min et al. 2009). It performs 3D Monte Carlo radiative transfer in a 2D axisymmetric geometry, and hence I will refer to it as 2D radiative transfer. In addition to determining the dust temperature, MCMa also solves for the vertical structure iteratively, and includes different disk physics such as dust settling (Chapter 4), dust sublimation (Kama et al. 2009), viscous heating (Min et al. 2011) and temperature-dependent opacities (Chapter 3). In this section, I will briefly describe this code. For a comparison with other 2D radiative transfer codes, see Pinte et al. (2009).

1.3.1 Monte Carlo radiative transfer: MCMa

A Monte Carlo code takes a probabilistic approach in order to solve the equation of radiative transfer. The radiation field from the central star is subdivided into a number of chromatic photon packages, which are propagated through the disk to set its temperature (figure 1.14). First, the code draws a random number to decide into which direction the photon is emitted. As it travels along its path, it has a certain probability to be absorbed, scattered or not interact in every grid cell it encounters. The code draws another random number to decide in which grid cell the photon package will interact according to this probability.
If the photon package is absorbed, its energy is added to the cell, increasing the cell temperature. If this is the first photon to be absorbed in this cell, a new photon will be emitted with a spectrum corresponding to this temperature and the local dust opacity. If the cell has absorbed and emitted photon packages before, it will emit a photon with the difference spectrum between the temperature before and after absorption (figure 1.15). This way, the total emitted spectrum of all photons remains consistent with the final cell temperature. This procedure was introduced by Bjorkman & Wood (2001) and is called immediate temperature correction (or sometimes immediate re-emission).

After re-emission (or scattering), new random numbers are drawn to decide into which direction the photon package will propagate and where its next interaction will take place. This whole procedure is repeated until the photon package leaves the disk. Once all photon packages have been propagated through the disk, the temperature structure of the disk has been calculated. For an infinite number of photon packages, all possible photon paths are covered and the temperature structure is exact. For a realistic number of photons package (on the order of a million), not all paths are covered and there is a stochastic error on the temperature in each cell. This is the
random noise inherent to all Monte Carlo approaches. This error is well characterized by the number of photon interactions in each grid cell, and can be reduced by simply increasing the number of photons, at a computational cost.

1.3.2 Gaining speed: regions of high optical depth

The largest computational challenge for Monte Carlo radiative transfer codes is formed by regions of high optical depth $\tau$, as run time scales roughly with $\tau^2$. A large number of photon packages is necessary to ensure that enough of them reach these regions to get a low statistical error on the temperature. MCMax includes two approximations to reduce the overall run time and improve the temperature structure in these regions. These are a partial diffusion approximation and a modified random walk approximation (Min et al. 2009).

The modified random walk approximation reduces the run time for a given number of photon packages. In regions of high optical depth, photon packages effectively start a random walk with many interactions in the same regions, which takes a disproportionate amount of computation time. This time can be significantly reduced by treating interactions in the same region with a single computational step using the modified random walk approximation from Fleck & Canfield (1984).

The partial diffusion approximation improves the accuracy of the temperature structure in regions of high optical depth where photon statistics are low. In these regions, energy transport takes place mainly by radiative diffusion. MCMax recalculates the temperature in these regions by applying the diffusion equation from Wehrse et al. (2000), with the Monte Carlo temperature just outside these regions (i.e. with good photon statistics), as a boundary condition. This reduces the required number of photon packages to get an accurate midplane temperature, typically by a factor 100.

1.3.3 Calculating the vertical structure

MCMax calculates the vertical structure of the disk in an iterative manner, assuming the gas is in vertical hydrostatic equilibrium, and the gas temperature equals the dust temperature. The initial vertical structure is calculated according to equation 1.6, where the sound speed is calculated from the optically thin temperature. The vertical structure of the dust is then calculated under the influence of dust settling and turbulent mixing as discussed in section 1.2.3, and described in more detail in Chapter 4. Alternatively, dust settling can be mimicked by scaling the dust scale height with respect to the gas scale height, or the dust distribution is assumed to be equal to that of the gas for a well-mixed model. After the calculation of the dust temperature as outlined above, MCMax re-calculates the vertical structure of the gas by directly integrating equation 1.5. This calculation carries the implicit assumption that the dust
temperature is equal to the gas temperature, which is true below the disk surface\(^2\) (Jonkheid et al. 2004; Kamp & Dullemond 2004). This recalculted vertical structure will deviate from the initial guess for the vertical structure, and hence the solution is not yet self-consistent. Therefore the dust temperature and vertical structure calculations of dust and gas are iterated until the density and temperature structure converge to a self-consistent solution, typically after five iterations. A schematic representation of this iteration process is shown in figure 1.16.

There are two ways of comparing this density and temperature structure to observations. By keeping track of the energy and directions of photon packages that leave the disk, the spectrum at every inclination can be reconstructed. Although these Monte Carlo spectra are inherently noisy due to the stochastic nature of the simulation, MCMax includes a multi-wavelength approach that takes into account the full energy spectrum of photon packages that leave the disk, producing smoother spectra compared to when only the energy at a single wavelength is used. Another method is to use the formal solution to the equation of radiative transfer along the line of sight through the disk. This produces an image of the disk at every wavelength, and can therefore be used to compare the model with spatially resolved images and

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\(^2\)Above the disk surface – defined as the location where the bulk of the stellar photons is absorbed – the gas temperature may be significantly higher than the dust temperature through UV and X-ray heating. Although this affects the structure of gas and emission lines coming from these regions, it does not affect the structure of the dust disk below, and has no significant impact on the SED.
interferometric data, as well as the SED.

### 1.4 Summary: thesis outline

In this thesis, we use the radiative transfer code MCMaX (section 1.3) to connect the physics of protoplanetary disks to observations (section 1.2).

In Chapter 2, we explore the effects of the vertical structure of the inner disk on the overall disk geometry in the transitional disk LkCa 15. This disk has a small amount of material close to the star, separated by a wide annular gap from the outer disk. Based on SED fitting, we constrain the vertical structure of this inner material to be either in an optically thick disk, or an optically thin halo. The illumination of the outer disk differs between both scenarios, affecting the entire disk geometry.

In Chapter 3, we constrain the location and abundance of dust crystals in the disk of HD 100546 by modelling medium resolution spectroscopic observations from the Spitzer and Herschel Space Telescopes. Crystalline forsterite has a solid-state feature at 69 µm, which has the unique property that its shape is temperature-dependent, and can therefore function like a dust thermometer. However, previous models had difficulty constraining the exact location due to a degeneracy in feature shape between dust temperature and iron content. Using 2D radiative transfer with temperature-dependent opacities and modelling both the 69 µm and shorter wavelength features simultaneously, we can break this degeneracy and locate the dust crystals. We find that they are located at the far end of the disk gap present in this system, with high local abundance. This is highly suggestive of an origin connected to the formation of the gap and the planet that may have carved it out.

In Chapter 4, we improve upon previous vertical structure calculations in radiative transfer codes and compare these models to observations to constrain the underlying physics. One of the main processes that affects the infrared excess of the disk is turbulent mixing, which is also an important driver of disk evolution and planet formation. By fitting this excess of disks around stars of different masses, we find that the turbulent mixing strength is constant along the stellar mass range. In addition, we find that the first steps of planet formation — the growth of small dust grains — are also independent of stellar mass.

In Chapter 5, we explore the role of grain size and anisotropic scattering on the brightness and color of scattered light images of circumstellar disks. We find that particles larger than the wavelength of light become extremely forward-scattering, reducing the amount of light scattered towards the observer. The strength of this effect is wavelength-dependent, and produces red scattering colors that cannot be produced by smaller particles. We apply this method to scattered light images of HD 100546, both archival and new observations from the Hubble Space Telescope. We find that
the color and intensity of these images are best fitted by grains at least an order of magnitude larger in size than previously estimated. Combining this grain size with the vertical structure calculations from Chapter 4, we find that these grains are most likely present in the form of aggregates. We speculate that the faintness in scattered light of all circumstellar disks can be explained by extreme forward scattering on large dust aggregates.

In Chapter 6, we study planet-disk interactions in the transitional disk of HD 100546, in which a giant planet is believed to be responsible for carving out the gap. By combining hydrodynamical simulations with radiative transfer, we investigate how planet and disk properties influence the gap structure. In particular, we find that the shape of the disk wall at the far end of the gap depends on the degree of turbulence in the disk and the planet mass. We measure this shape using mid-infrared interferometry, and find the disk wall to be rounded-off, corresponds to a very turbulent disk with a heavy planet. Its estimated mass is above the deuterium burning limit, making this companion most likely a brown dwarf.