Protoplanetary disks and exoplanets in scattered light

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Publication date
2017

Document Version
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We have entered an exciting era in which high-contrast imaging has enabled the direct detection of gas giant exoplanets and resolved signatures of planet formation in protoplanetary disks. Unprecedented precision is being achieved with the newest generation of dedicated imaging instruments including SPHERE at the Very Large Telescope in Chile. In parallel, transit and radial velocity surveys have revealed a great diversity in the exoplanet population at smaller separations, indicating that the formation and evolution of planetary systems is a complex process with many possible outcomes. Combined constraints from both ends of the evolutionary pathway will eventually provide a comprehensive picture which relates the initial planet formation processes with the orbital architectures and atmospheric characteristics of the exoplanets. Placing the Solar System in a cosmic context and addressing questions regarding the habitability in other planetary systems is a long-term aim of modern astronomy.

In this thesis, we undertake observational and numerical investigations of protoplanetary disks and self-luminous exoplanets for which high-contrast imaging, scattered light, polarization, and radiative transfer modeling play a central role. The principle objective is to reveal the surface morphology of nearby protoplanetary disks in scattered light by employing high-contrast imaging techniques in order to gain insight into their structure, the properties of the dust, and the physical processes driving their evolution. Quantitative constraints are obtained with numerical calculations and three-dimensional (3D) radiative transfer simulations. Scattering processes are also important in (exo)planetary atmospheres for which we developed a 3D radiative transfer code. We compute the infrared polarization signal from self-luminous exoplanets with horizontal cloud variations and circumplanetary disks.
1 Introduction

1.1 Protoplanetary disks around young stars

Protoplanetary disks around pre-main-sequence stars are the natal environment of planets (Safronov 1972; Goldreich & Ward 1973). These accretion disks form as a natural by-product of star formation by conservation of angular momentum from a collapsing core in a molecular cloud (Shakura & Sunyaev 1973; Lynden-Bell & Pringle 1974). Consequently, protoplanetary disks are built up from recycled gas and dust from their interstellar environment. Most stars form in clusters, for example in the nearby star-forming regions of Taurus-Auriga, Chameleon, and Lupus (Briceño et al. 2002; Palla & Stahler 2002), but some stars may form in isolation, for instance the family of isolated Herbig Ae/Be stars which are not connected with dark clouds or nebulae (Waters & Waelkens 1998). The formation of protoplanetary disks around young stars is a common phenomenon as observations show that the spectral energy distributions (SEDs) of most pre-main-sequence stars exhibit an infrared and millimeter excess (Strom et al. 1989; Beckwith et al. 1990; Weintraub et al. 1989, O’dell et al. 1993). However, the fraction of young, accreting stars with an infrared excess decreases exponentially within ten million years by disk evolution and dispersal (Haisch et al. 2001, Mamajek 2009, Fedele et al. 2010), setting a stringent constraint on the timescale of planet formation (Pollack et al. 1996). In this section, I will provide a background on the global structure, evolution, and appearance of protoplanetary disks, as well as substructures that are possibly related planet-disk interactions. Furthermore, I will summarize some of the important dust evolution and planet formation processes.

1.1.1 Disk structure, evolution and appearance

Star formation is initiated by the gravitational collapse of a dark and cold core in a molecular cloud when gravity is no longer balanced by the counteracting forces of gas pressure, magnetic fields, and turbulence which could be triggered by an external mechanism such as a nearby supernova explosion (Shu et al. 1987). Within several hundred thousand years, a protostar is formed in the center while part of the infalling gas and dust creates a rotationally-supported accretion disk as a result of conservation of angular momentum from the parent cloud. Protoplanetary disks consist mainly of molecular hydrogen and helium (~99% in mass) but a small fraction of the mass resides in submicron-sized dust grains inherited from the interstellar medium (Mathis et al. 1977). Most of the gas is accreted by the central star within approximately ten million years but part of the mass and angular momentum will be removed from the innermost disk regions by jets, winds, and bipolar outflows (Bally 2016). The main evolutionary stages of star- and planet formation in an isolated system of a T Tauri (\( M \lesssim 2 M_\odot \)) or Herbig Ae/Be star (2–8 \( M_\odot \)) are illustrated in Fig. 1.1.

The observational appearance of the formation and evolution stages have been categorized in four classes, based on the SED (Lada 1987, Williams & Cieza 2011). In the Class 0 phase, the cold, dense core forms in the parent cloud and radiates at far-infrared
1.1 Protoplanetary disks around young stars

Figure 1.1: Schematic overview of the star- and planet formation stages and processes of an isolated, low- or intermediate-mass star. (a) Dark cores form in clouds of molecular gas and small traces of dust grains. (b) Gravitational collapse of the core sets in when gravity exceeds the counteracting forces. (c) A central protostar is formed which is fed by the infalling envelope. An accretion disk appears by conservation of angular momentum while part of the gas and angular momentum is removed by an outflow. (d) The central star becomes visible as most of the envelope has been dispersed from or accreted by the star-disk system. (e) Gas is accreted by the star from the protoplanetary disk’s reservoir. The interstellar dust grains evolve into larger building blocks, eventually forming planetesimals, terrestrial planets, and the cores of gas giants. (f) An evolved planetary system, similar to the Solar System. (after Hogerheijde 1998; Shu et al. 1987)

wavelengths (see Fig. 1.1b). In the Class I phase (i.e., protostellar disk), the star-disk system is still embedded but the central star heats both the inner disk regions and the surrounding envelope such that the SED is dominated by the reprocessed radiation (see Fig. 1.1c). In the Class II phase (i.e., protoplanetary disk), the envelope has been accreted and dispersed such that the star and protoplanetary disk become visible (see Figs. 1.1d and 1.1e). The SED is characterized by the stellar spectrum and still a significant amount of infrared excess. In the Class III phase, most of the remaining gas and dust has been removed from the system, possibly leaving a formed planetary system and belts of debris dust (see Fig. 1.1f). This second generation of dust grains gets replenished by collisions of planetesimals such that a minor infrared signature could be present in the SED (Wyatt 2008; Matthews et al. 2014). Summarizing, the wavelength-dependent intensity of the infrared excess provides information on the disk structure and dust distribution as longer wavelengths probe cooler disk regions (see Fig. 1.2).
Once a protoplanetary disk has formed, it evolves during the course of several million years by transporting mass and angular momentum both inwards and outwards (Williams & Cieza 2011). Differential rotation of the gas causes friction such that the angular momentum of a parcel of gas changes. The inner disk regions will lose angular momentum while the outer disk regions gain angular momentum and spread outward. Some of the mass will be accreted by the central star which occurs during the protoplanetary disk phase with rates of $10^{-11} - 10^{-8} \, M_\odot \, \text{yr}^{-1}$ (Hartmann et al. 1998; Gullbring et al. 1998; Manara et al. 2016). Viscosity plays an important role in disk evolution although the source remains debated (Turner et al. 2014; Rafikov 2017). The timescale of molecular viscosity is orders of magnitude larger than the observed disk lifetimes, therefore, magneto-rotational instabilities (MRI; Balbus & Hawley 1991) have been proposed as a dominant source for turbulence. Non-ideal magnetohydrodynamical effects have to be considered while MRI is hindered in so-called dead zones where ionization is inefficient (Flock et al. 2017). However, alternative sources for turbulent viscosity are possible such as self-gravity (Gammie 2001) and baroclinic vortices (Klahr & Bodenheimer 2003).

The time-dependent gas evolution of a thin, axisymmetric disk was first formulated by Lynden-Bell & Pringle (1974). The viscosity, $\nu$, drives the evolution of the surface density of which a steady-state solution can be derived from the mass conservation equation (Pringle 1981). The viscosity is often parameterized by a dimensionless turbulence parameter, $\alpha < 1$, which relates the pressure scale height, $H_p$, and sound speed, $c_s$, to the viscosity, $\nu = \alpha H_p c_s$ (Shakura & Sunyaev 1973; Pringle 1981). Direct measurements of turbulence are challenging as it requires accurate observations of molecular line broadening (Hughes et al. 2011), however, the Atacama Large Millimeter/submillimeter Array (ALMA) may provide the required sensitivity (Flaherty et al. 2015). The heating of the disk is mostly dominated by irradiation such that the temperature is approximately described by $T \propto r^{-1/2}$, yielding a surface density distribution of $\Sigma \propto r^{-1}$ (Adams & Shu 1986; Kenyon & Hartmann 1987; Bell et al. 1997), which is less steep than what is defined by the minimum mass solar nebula, $\Sigma \propto r^{-3/2}$ (Weidenschilling 1977b).

The surface density, pressure scale height, and equation of state determine the vertical gas structure of the disk (D'Alessio et al. 1998). Locally, the gas pressure and the vertical gravity component of the central star are in hydrostatic equilibrium (Kenyon & Hartmann 1987). The vertical density distribution is described by a Gaussian profile if the thermal disk structure is assumed to be vertically isothermal (Robitaille et al. 2006; Woitke et al. 2016). In that case, the pressure scale height is given by the ratio of the sound speed and the Keplerian frequency, $H_p = c_s/\Omega$. The scale height of the gas is commonly parameterized with a power law exponent, $\beta$, which can correspond to a flaring ($\beta > 1$) or self-shadowing ($\beta < 1$) profile, depending on the radial temperature parameterization (Dullemond & Dominik 2004). The surface geometry depends on the combined effect of the radially changing surface density and pressure scale height. The amount of disk flaring is determined by the interplay between the radial temperature structure and the stellar irradiation of the disk (Chiang & Goldreich 1997). However, various physical and chemical


1.1 Protoplanetary disks around young stars

Figure 1.2: Left: Spectral energy distributions of a continuous disk and a transition disks, simulated with the continuum radiative transfer code MCMax3D (Min et al. 2009). Longer wavelengths probe cooler regions at larger distances from the star and/or closer to the midplane of the disk. Right: Artist’s rendition of a transition disk. The inner and outer disk are separated by a wide gap that is possibly opened by the gravitational interaction of forming planets. (Credit: NAO)

processes may affect both globally and locally the disk structure, for example planet-disk interactions (Baruteau et al. 2014), magnetohydrodynamical effects (Flock et al. 2011), and dust evolution processes (Testi et al. 2014). The flaring index affects the amount of infrared excess in the SED which led to the Group I/II classification of Herbig stars. This was initially interpreted as a subdivision in flaring disks (Group I) and self-shadowed disks (Group II) of which the latter disk structure was assumed to be more evolved due to dust settling (Meeus et al. 2001; Dominik et al. 2003; Dullemond & Dominik 2004). However, several studies have shown that both subclasses evolve separately, while the Group I disks are characterized by large dust gaps (Maaskant et al. 2013; Menu et al. 2015).

Transition disks are a subclass of protoplanetary disks characterized by a deficit of near- and mid-infrared excess while the far-infrared excess of their SED is similar to other Class II objects (Strom et al. 1989; Skrutskie et al. 1990). Indeed, high-resolution imaging observations have revealed inner dust cavities in many of such disks (Andrews et al. 2011), as indirectly deduced from spatially-unresolved observations, possibly coinciding with a lowering in gas density (van der Marel et al. 2016). It has been hypothesized that transition disks are in the process of evolving from the Class II to the Class III stage. Dust, and possibly gas, is removed from the central disk regions for example by planet formation processes or photoevaporative winds (Owen 2016). However, observational evidence has emerged that large dust cavities can also be present in the earlier stages of disk evolution while the cavity may still be filled with gas (Sheehan & Eisner 2017). Figure 1.2 shows an artist’s rendition of the transition disk around PDS 70 (Hashimoto et al. 2012), as well as a comparison of simulated SEDs of a continuous disk and a transition disk. In this thesis, protoplanetary disks from the transition family are studied with high-contrast scattered light observations.
1.1.2 Gaps, cavities and spiral arms

High spatial resolution observations have revealed intriguing disk morphologies (see Sect. 1.3.1), both in scattered light (Grady et al. 2013; Garufi et al. 2013; Avenhaus et al. 2014b), sensitive to micron-sized grains in the disk surface, in (sub)millimeter continuum emission (ALMA Partnership et al. 2015; Pérez et al. 2016; Loomis et al. 2017), tracing millimeter-sized pebbles in the midplane, and to a lesser extent in (sub)millimeter line emission (Christiaens et al. 2014; van der Marel et al. 2016). The populations of small and large grains evolve differently such that knowledge on both distributions provides insight into the physical and chemical disk processes responsible for the resolved substructures (Sicilia-Aguilar et al. 2016). I will highlight gaps, cavities, and spiral arms which belong to the most common subclasses of observed disk morphologies.

Sharp, radial decreases in surface brightness have been resolved both in scattered light and at (sub)millimeter wavelengths which are often interpreted as gaps (radially localized) and cavities (extending down to the star) in the surface density, both interchangeably used with an identification of ring-like emission. Planet-disk interactions are often invoked as explanation for both gaps (Dong et al. 2015b; Dipierro et al. 2016) and cavities (Zhu et al. 2012; Pinilla et al. 2012a) although alternative interpretations exist such as dust evolution (Birnstiel et al. 2015), chemical condensation fronts (Zhang et al. 2015; Okuzumi et al. 2016), dead zones (Pinilla et al. 2016), and photoevaporative winds (Clarke et al. 2001).

An annular gap is carved around the orbit of an embedded planet if the torque exerted by the planet on the disk is larger than the viscous torque responsible for the spreading of the disk (Lin & Papaloizou 1986a). The shape of the gap profile can be solved, by approximation, analytically for low-mass ($\lesssim 1 M_{\text{Jup}}$) planets (Duffell 2015) but requires hydrodynamical simulations otherwise (Papaloizou et al. 2004; Crida et al. 2006; Zhu et al. 2013). The depth and width of the gap depends on the planet-to-star mass ratio, $q$, disk aspect ratio, $H_p/r$, and turbulence parameter, $\alpha$ (Fung et al. 2014; Kanagawa et al. 2015; Dong & Fung 2017b). Simulations in which both the gas and dust evolution is solved, show that micron-sized grains remain coupled to the gas dynamics while the millimeter-sized grains drift inward as predicted by theory (Zhu et al. 2012; Pinilla et al. 2015a; Dong et al. 2015c). Planets, dead zones, and Rossby wave instabilities can induce radial and azimuthal pressure maxima, which may trap drifting particles, and give rise to axisymmetric and non-axisymmetric emission features (Pinilla et al. 2012a; Flock et al. 2015; Owen & Kollmeier 2017). The left image in Fig. 1.3 shows the effect of three embedded planets (0.2 $M_{\text{Jup}}$) on the thermal submillimeter emission (Dong et al. 2015c). The pressure maxima exterior of the planet orbits cause a pile up of large dust grains which manifest as multiple ring-like emission features.

In scattered light, a radial minimum in brightness does not necessarily relate to a decrease in micron-sized grains because self-shadowing by the disk can also mimic gap-like features (Siebenmorgen & Heymann 2012; Dong 2015). Self-shadowing has an effect on both the scattered light flux and the reprocessing of stellar radiation by the dust, therefore,
a conjunction with a reduced infrared excess is expected (Wisniewski et al. 2008, Garufi et al. 2017). Also azimuthally localized shadows have been detected on several disks (Chapter 4, Chapter 7, Mayama et al. 2012, Itoh et al. 2014). For example, a warped inner disk can produce a pair of shadow lanes (Marino et al. 2015) or an azimuthal brightness modulation (Rosenfeld et al. 2012, Debes et al. 2017). The fast dynamical timescales in the innermost disk regions may result in illumination variations of the outer disk on a timescale of days to weeks (Chapter 5).

Scattered light imaging has revealed spiral arms in several protoplanetary disks (Hashimoto et al. 2012, Muto et al. 2012, Grady et al. 2013, Canovas et al. 2013, Boccaletti et al. 2013, Wagner et al. 2015a), while only a few counterparts have been resolved in CO gas (Christiaens et al. 2014, Tang et al. 2017). Higher spatial resolution is required in most cases to determine if the spiral arms can be traced down to the midplane. The origin of the detected spiral arms remains debated as it is not possible, from scattered light imagery alone, to determine if temperature and/or density perturbations are responsible (Juhász et al. 2015). The leading hypothesis for their origin are planet-disk interactions (Dong et al. 2015b, Zhu et al. 2015, Fung & Dong 2015), but alternative mechanisms have been proposed such as gravitational instabilities (Dong et al. 2015a), shadows (Montesinos et al. 2016), and light travel time effects (Kama et al. 2016).

Embedded planets and binary companions excite density waves at the Lindblad resonances of a protoplanetary disk (Goldreich & Tremaine 1979) which results, for low-mass...
planets, in a one-armed spiral feature by constructive interference (Ogilvie & Lubow 2002). For higher mass companions, $q \gtrsim (H_p/r)^3$, the perturbation of the spiral arms is non-linear which manifests in spiral arms with larger pitch angles and amplitudes, and the presence of an azimuthally-symmetric secondary component (Zhu et al. 2015; Fung & Dong 2015; Dong & Fung 2017a), resembling some of the observed spiral arms (Dong et al. 2015b; 2016). The right image in Fig. 1.3 displays a raytraced scattered light image of an hydrodynamical simulation in which a primary and secondary spiral arm emerge interior to the orbit of a massive gas giant (Dong et al. 2015b).

The interaction between embedded planets and their circumstellar environment will also affect the orbital architecture as significant variations in semi-major axis, inclination, and eccentricity may occur during the lifespan of a protoplanetary disk (Lin & Papaloizou 1986b, 2010). The dynamical evolution in the protoplanetary disk might be reflected in some of the architectural characteristics of exoplanets such as compact systems with low-mass planets at short orbital radii (Ormel et al. 2017), multi-planet systems in a (near-)resonance chains (Winn & Fabrycky 2015; Liu et al. 2017), and spin-orbit misalignment of hot Jupiters (Lai 2014; Crida & Batygin 2014).

### 1.1.3 Planet formation in a nutshell

The reservoir of initial planet building blocks in a protoplanetary disk is provided by the submicron-sized dust grains from the molecular cloud core. Approximately thirteen orders of magnitude in size have to be crossed for those grains to become terrestrial planets like Earth. The standard picture of planet formation is commonly subdivided in different processes that govern the growth from microscopic dust grains up to planetesimals and larger (Chiang & Youdin 2010; Morbidelli et al. 2012; Testi et al. 2014).

Although only $\sim 1\%$ of the disk mass resides in the dust, the high midplane density allows grains to coagulate and grow in size and mass (Weidenschilling 1980). This process occurs efficiently up to millimeter-sized pebbles, however, it is halted by the bouncing barrier (Zsom et al. 2010) and the fragmentation barrier (Brauer et al. 2008). Relative velocities above a certain threshold will cause bouncing or fragmenting interactions instead of sticking encounters (Windmark et al. 2012), in particular at smaller disk radii where the impact velocities are larger (Birnstiel et al. 2012). However, the outcome depends on the composition and structure of the dust grains. For example, icy particles or dusty aggregates tend to coagulate more efficiently than pure silicates or compact grains (Poppe et al. 2000; Gundlach et al. 2011; Kothe et al. 2013). Figure 1.4 (left) shows an interplanetary dust particle of about $10 \mu$m in size with a fluffy aggregate structure, possibly related to the early coagulation processes.

The dynamics of the dust grains is driven by the turbulent gas in the disk (Birnstiel et al. 2010). Vertically, the dust distribution will settle towards the midplane under the influence of gravity, however, turbulence will diffuse well-coupled grains upward to the disk surface (Dubrulle et al. 1995; Fromang & Nelson 2009). Scattered light observations
are sensitive to micron-sized dust grains suspended in the upper atmosphere of the disk of which the scattering opacity is large at small wavelengths (see Sect. 1.4.1). The dynamical coupling of the dust with the gas is set by the Stokes parameter, $St = \Omega t_s$, where $t_s$ is the stopping time by which the dust looses momentum to the gas. Particles with a Stokes parameter around unity enter a regime in which radial drift is important because the grains decouple from the gas. Consequently, large grains loose angular momentum by the headwind of the sub-Keplerian gas which is supported by an additional radial pressure gradient (Weidenschilling 1977a; Nakagawa et al. 1986). This generates another barrier which limits the maximum particle size as drifting pebbles are rapidly accreted by the central star (Birnstiel et al. 2012).

Several scenarios have been proposed to circumvent the radial drift barrier and grow pebbles across the size regime in which regular coagulation processes are inefficient while the gravitational interaction between particles is still small (Blum & Wurm 2008). Radial pressure maxima will trap drifting particles (Nakagawa et al. 1986), for example when a gap is opened by a forming planet (Zhu et al. 2012, Pinilla et al. 2012a) or due to MHD effects (Simon & Armitage 2014). Pebble accretion is a mechanism by which planetary embryos grow rapidly from a radial influx of drifting pebbles (Ormel & Klahr 2010, Johansen & Lacerda 2010). Particles with stopping times comparable to their orbital time are efficiently accreted by planetesimals via aerodynamically-induced settling into the planetesimal’s gravitational well. The growth timescale is significantly faster compared to a gas-free environment in which accretion by planetesimals only occurs through gravitational focussing (Lambrechts & Johansen 2012). Another promising mechanism is rapid planetesimals formation via the streaming instability which may occur when the dust-to-gas ratio is locally enhanced (Youdin & Goodman 2005, Johansen et al. 2006). The collective gravitational effect of an ensemble of particles could be important...
in pressure bumps and vortices, which are efficient dust traps, such that pebbles collapse gravitationally in planetesimals (Johansen et al. 2014; Owen & Kollmeier 2017).

Gravity governs the growth of planetesimals for which collisions do not result any longer in fragmentation (Chiang & Youdin 2010). These objects are kilometer-sized or larger such as the comet 67P/Churyumov-Gerasimenko (see Fig. 1.4, right). The largest planetesimals will grow most efficiently as their gravitational pull is strongest, sweeping up the remaining smaller planetesimals (Ida et al. 2008), such that planetary embryos are formed with typical sizes of a thousand kilometer (Greenberg et al. 1978). Planetary embryos more massive than \( \sim 10 M_\oplus \) may start to accumulate a gaseous envelope by accreting gas from the circumstellar environment (Lubow & D’Angelo 2006; Lissauer et al. 2009) which, if the disk lifetime allows, may end up in a runaway accretion process by which Jupiter-like planets could be formed (Helled et al. 2014). This two-step formation of a rocky core and gaseous envelope is know as the core accretion scenario (Pollack et al. 1996). Alternatively, gas giants may form directly through a gravitational collapse when the protoplanetary disk is gravitationally unstable (Boss 1997). Self-gravity is important when the disk mass is high and cooling efficient. A disk becomes unstable to axisymmetric perturbations when \( Q = c_s \Omega / (\pi G \Sigma) < 1 \), which is known as the Toomre’s stability criterion (Toomre 1964). Long-period exoplanets, such as those detected with direct imaging observations, might have formed through gravitational instabilities as the growing timescales are possibly too long for regular core accretion (Ma & Ge 2014; Li et al. 2015). In contrast to planets at smaller radii (\( \approx 5–10 \) au) which form more efficiently because the growing timescales are shorter (Morbidelli et al. 2012).

1.2 Extrasolar planets and their atmospheres

Over two decades ago, the first extrasolar planet orbiting a main-sequence star was discovered (Mayor & Queloz 1995). Since then, research on exoplanets has become one of the most rapidly growing fields in modern astrophysics with today over 3600 exoplanet detections (http://exoplanet.eu). It has become well established that the population of discovered exoplanets is highly diverse in their orbital architectures, as well as their masses, radii, and temperatures (Fressin et al. 2013; Fabrycky et al. 2014; Winn & Fabrycky 2015). This poses challenging questions regarding the formation and evolution of planetary systems and the uniqueness of the Solar System. In this section, I will highlight some of the demographical and atmospheric characteristics of exoplanets.

1.2.1 Exoplanet demographics

The haul of exoplanet detections by the transit and radial velocity technique has provided exquisite statistics on the demographics of exoplanets in the solar neighborhood, \( \lesssim 2000 \) pc (Mayor et al. 2014; Lissauer et al. 2014). These techniques rely on an indirect inference of the presence of a planet by measuring a periodic brightness (Charbonneau
1.2 Extrasolar planets and their atmospheres

Figure 1.5: Exoplanets known on 2017 May 25 with a constraint on both their mass and semi-major axis (http://exoplanet.eu). Color coding indicate the detection methods by which the planets were discovered. Subclasses of the exoplanet population have been highlighted.

et al. 2000) or Doppler shift variation of the stellar light (Mayor & Queloz 1995). Orbital parameters (e.g., period, semi-major axis, eccentricity) and bulk parameters (mass, radius, equilibrium temperature) can be derived which has revealed a great diversity of such macroscopic parameters. Figure 1.5 shows the detected population of exoplanets with available constraints on both the semi-major axis and mass of the planets. The clustering of data points reflects both the detection biases and the underlying subclasses of the planet population.

The first exoplanet detections were achieved with the radial velocity technique which is inherently biased towards massive, short-period planet. This led to the discovery of multiple gas giants orbiting at very small separations from the central star (Mayor & Queloz 1995; Marcy & Butler 1996; Butler et al. 1997). These so-called hot Jupiters are tidally locked and strongly irradiated on the day side of their atmosphere (Seager & Sasselov 1998). In situ formation of gas giants at small disk radii is challenging such that migration mechanisms in the protoplanetary disk phase have been invoked to explain their current location (Lin et al. 1996; Rasio et al. 1996). Measurements of the Rossiter-McLaughlin effect have revealed that a fraction of the hot Jupiter population has orbits that are misaligned with the equatorial plane of their star (Albrecht et al. 2012).
Super-Earths are another class of planets which have no direct analog in the Solar System while their population dominates the size distribution of known exoplanets (Fressin et al. 2013; Petigura et al. 2013). Those planets have masses of 1–10 $M_\oplus$ and radii of $1.25–2 R_\oplus$, leaving a range of possibilities for the composition of their interior and envelope as only the bulk density can be derived from the total mass and radius (Seager et al. 2007; Valencia et al. 2007). One possibility is that super-Earths are composed of a rocky and/or icy core with an envelope of hydrogen and helium (Ikoma & Hori 2012). Distinguishing between different atmospheric compositions can be achieved with spectroscopy (Miller-Ricci et al. 2009) although high signal-to-noise atmospheric observations of super-Earths are still challenging and the presence of clouds may hinder the detection of molecular lines from deeper atmospheric layers (Kreidberg et al. 2014; Knutson et al. 2014).

While the transit and radial velocity techniques are biased towards short-period planets, direct imaging (i.e., high-contrast imaging) enables the detection of self-luminous gas giants on long-period orbits beyond 5–10 au (Oppenheimer & Hinkley 2009). Large-scale surveys of young (≤100–200 Myr) and nearby (≤100 pc) stars have been ongoing for a decade and yielded mainly null-results as the population of gas giant exoplanets on wide orbits is inherently sparse (Biller et al. 2013; Rameau et al. 2013a; Chauvin et al. 2015). Although the occurrence rate of 5–13 $M_{Jup}$ planets at orbital distances of 30–300 au is only $0.6^{+0.7}_{-0.5}\%$ (Bowler 2016), direct imaging enables detailed atmospheric characterization through photometry and low-resolution spectroscopy because the planet’s emission is spatially separated from the central star (Konopacky et al. 2013; Barman et al. 2015; Skemer et al. 2016; De Rosa et al. 2016). The detection and characterization of exoplanets with high-contrast imaging will be summarized in more detail in Sect. 1.3.2.

### 1.2.2 Exoplanet atmospheres

Planetary atmospheres are complex environments in which the thermal structure is determined by radiation transport, 3D hydrodynamical processes such as convection and advection, as well as cloud formation and photochemistry (Madhusudhan et al. 2014). Atmospheric temperatures span a wide regime from the cold ice giants in the Solar System to irradiated and young gas giant exoplanets with effective temperature of several thousand Kelvin (see Fig. 1.6). The diversity is also reflected in the elemental composition ranging from atmospheres that are H/He-dominated to composition of heavier molecules such as H$_2$O, CO$_2$, or N$_2$ (Madhusudhan et al. 2016). This variety of climates has led to intriguing observational insights beyond what is expected from the Solar System planets, at the same time challenging our theoretical understanding of planetary atmospheres.

In chemical equilibrium, the local mixing ratios can be calculated from the pressure, temperature, and composition (metallicity) by minimizing the Gibbs free energy (Tsuji 1973; Lodders & Fegley 2002). However, in the cool upper regions of an atmosphere the composition might deviate from equilibrium as the chemical reaction timescales are shorter than the dynamical timescales which might lead to chemical quenching (Prinn & Barshay...
1.2 Extrasolar planets and their atmospheres

Figure 1.6: Pressure-temperature profiles of Jupiter, and the hot Jupiters HD 189733b and WASP 12b, spanning a broad range of temperatures and chemical compositions. The chemical transition regions of CH$_4$/CO and NH$_3$/N$_2$ (dashed lines) are shown together with the condensation curves of ammonia, water, and several refractory materials (dot-dashed lines). Figure adopted from Madhusudhan et al. (2016).

Irradiated planets are also affected by photochemistry, typically at micro- and millibar levels which receive the highest ultraviolet flux, a well known process in the atmosphere of Jupiter, Saturn, and Titan (Yung et al. 1984; Gladstone et al. 1996). Clouds form by condensation when the partial pressure exceeds the saturation vapor pressure (Marley et al. 2013). The composition of the cloud condensates is determined by equilibrium chemistry. For example, NH$_3$ condenses into ice crystals in the atmospheres of Jupiter and Saturn while dust grains composed of Al$_2$O$_3$ and Mg$_2$SiO$_4$ can be present in the atmospheres of hot Jupiters (see Fig. 1.6) and young gas giants (Morley et al. 2012, 2014). The formation and sedimentation of cloud particles involves several processes such as the nucleation and growth of particles, atmospheric dynamics, and chemistry, which challenges calculations on the distribution of clouds and the sizes of the particles (Ackerman & Marley 2001; Helling et al. 2008; Lee et al. 2016). Hazes, or aerosols, form by disequilibrium processes such as photochemistry, either in-situ or from photochemically produced gas which flows dynamically towards cooler regions (Madhusudhan et al. 2016). For example, carbon is locked up in CH$_4$ in cool regions of an atmosphere, which can be sequenced to more complex hydrocarbons by photochemistry (Tomasko et al. 2005). However, there is also evidence for the presence of aerosols in the hot atmosphere of WASP-12b (Sing et al. 2013).

During the recent years, the field of exoplanetary science has gained momentum beyond planet detections into the direction of atmospheric characterization (Seager & Deming 2010; Madhusudhan et al. 2014, 2016). Spectral observations are so far limited...
to mainly gas giants with high temperatures and large scale heights, either by a strong irradiation field from their host star (see right image in Fig. 1.7) or because of their young age which makes them self-luminous. Obtaining spectra of exoplanet atmospheres requires highly accurate measurements such that typically space telescopes and large, ground-based telescopes are employed (Crossfield 2015).

The wavelength-dependent size of a planet can be measured during a primary transit (Charbonneau et al. 2002), a so-called transmission spectrum (Seager et al. 2000), which is sensitive to the absorption features of the chemical species in the upper part of the atmosphere along the day-night terminator (Pont et al. 2013; Sing et al. 2016). The top left panel in Fig. 1.7 displays a near-infrared transmission spectrum of WASP-12b, a hot Jupiter with an orbital period of 1.1 days and an equilibrium temperature of 2500 K (Kreidberg et al. 2015). The secondary eclipse can be used to measure an emission spectrum in the infrared which probes the thermal structure and composition from the day side of the planet, revealing absorption (or emission in case of a thermal inversion) features from deeper atmospheric layers (Charbonneau et al. 2008; Grillmair et al. 2008; Swain et al. 2009). The phases of a planet provide spatial information about the atmosphere as the amount of reflected (optical) and thermal (infrared) radiation changes with the orbit of the planet. A 1D longitudinal brightness map can be created of short-period planets (Knutson
et al. 2007; Stevenson et al. 2014) which are expected to be tidally locked with their host star (Bodenheimer et al. 2001). Such phase curves yield insight into the atmospheric dynamics (Showman et al. 2009; Zellem et al. 2014) and presence of inhomogeneous clouds (Demory et al. 2013). The bottom left panel of Fig. 1.7 shows a phase curve of the hot super-Earth 55 Cancri e. The brightness of the planet’s thermal emission changes along its orbit with a maximum shortly before the secondary eclipse, that is, eastward shifted with respect to the substellar point by efficient energy circulation (Demory et al. 2016). The detection of molecules and orbital motion is also possible at high resolution with Doppler spectroscopy (Brogi et al. 2012; Birkby et al. 2013), revealing imprints of the atmospheric dynamics (Snellen et al. 2010) and rotation of a planet (Snellen et al. 2014). Emission spectra of long-period, self-luminous planets are accessible with high-contrast observations which are the topic of the next section.

1.3 High-contrast observations

For decades, the inference about the structure and evolution of protoplanetary disks, as well as the distribution and properties of the building blocks of planets was largely based on observational constraints from spatially-unresolved observations such as photometry and spectroscopy, or low-spatial resolution imaging. Also the detection of exoplanets has been mostly achieved via indirect observations. During the years, tremendous advances have been made in the development and construction of large, ground-based telescope facilities and state-of-the-art instrumentation (Oppenheimer & Hinkley 2009; Traub & Oppenheimer 2010; Mawet et al. 2012). This has opened a pathway to resolve substructures in nearby (≲ 200 pc) protoplanetary disks and characterize the direct light coming from gas giant exoplanets (Absil & Mawet 2010; Quanz 2015; Crossfield 2015). In Chapters 3 till 7, we use scattered light images obtained with VLT/SPHERE to study the structure of four protoplanetary disks, as well as the dust properties in their surface layers. In this section, I will highlight some of the recent scientific output of high spatial resolution observations, with a focus on high-contrast imaging of disks and planets. Furthermore, I will provide a brief description of the SPHERE instrument and the related differential imaging techniques.

1.3.1 The era of high-resolution disk observations

High-resolution observations of scattered light in the optical and near-infrared, as well as the dust continuum and molecular lines in the (sub)millimeter, are currently revolutionizing our understanding on physical and chemical processes occurring in protoplanetary disks. So far, the scientific haul of spatially-resolved observations has revealed substructures in most disks whereas smooth distributions of dust and gas seem exceptional. Gaps, cavities, spiral arms, and vortices have been commonly detected (van der Marel et al. 2013; Grady et al. 2013; Quanz et al. 2013b; ALMA Partnership et al. 2015) which are possibly related to disk and dust evolution processes (see Sect. 1.1.2).
Protoplanetary disks are optically thick at short wavelengths, therefore, scattered light observations trace the distribution of micron-sized dust grains in the surface layer of the disk which are dynamically coupled to the gas. Continuum (sub)millimeter observations on the other hand are sensitive to the millimeter-sized pebbles in the midplane because at those wavelengths the disk is largely optically thin. High spatial resolution is achieved by employing large, optical telescopes or long-baseline interferometers. The extreme adaptive optics system of VLT/SPHERE yields a typical angular resolution of 40 mas in the $J$ band (Chapter 5), close to the diffraction limit (38 mas) of a 8.2 m aperture. The diffraction limit of a circular aperture is formulated by the Rayleigh criterion, $\theta = 1.22\lambda/D$ with $\lambda$ the photon wavelength and $D$ the mirror diameter.

The newest generation of high-contrast imaging instruments enable a spatial resolution of 4–10 au in the nearest star-forming regions (Avenhaus et al. 2017), similar to the long-baseline capabilities of ALMA (ALMA Partnership et al. 2015). Combining spatially-resolved scattered light and (sub)millimeter observations provides a detailed map of the radial and vertical disk structure through the different dust populations, as well as molecular gas species. Figure 1.8 displays two protoplanetary disks that have been observed with high spatial resolution, both revealing a wealth of radial substructure. The left panel shows the protoplanetary disk around the nearest T Tauri star (59.5 pc), TW Hya, in polarized scattered light (van Boekel et al. 2017). This Class II disk is in a relatively evolved stage ($\sim 8$ Myr), in contrast to the Class I-II disk around HL Tau (140 pc), displayed in the right panel, which is still embedded in an extended envelope such that the disk structure is only accessible at (sub)millimeter wavelengths (ALMA Partnership et al. 2015).

The interpretation of scattered light images can be non-trivial as the surface brightness

Figure 1.8: High spatial resolution observations of radial substructures in protoplanetary disks. Left: VLT/SPHERE polarized scattered light image of TW Hya (59.5 pc) in the $H$ band (van Boekel et al. 2017). Right: ALMA continuum image of HL Tau (140 pc) at 1.3 mm (ALMA Partnership et al. 2015).
is determined by a combination of the disk structure, dust properties, and illumination/shadowing effects. The vertical distribution of dust is mainly set by the local surface density, temperature, and turbulence (see Sect. 1.1.1). These parameters depend on the radial position in the disk, consequently they affect the radial variation in the height of the scattering surface, that is, where the stellar photons reach an optical depth of unity. Increasing the dust mass, flaring of the pressure scale height, or the turbulence will increase the geometrical cross section of the disk surface and thereby the scattered light flux. For inclined disks, the scattering properties of the dust grains are also important because both the angular scattering probability and the polarization efficiency depend on the local scattering angle (West et al. 1997; Min et al. 2005; Hovenier & Muñoz 2009). While the phase function typically peaks in forward direction, the single scattering polarization of silicate grains peaks at a scattering angle of 90° (Mishchenko et al. 2000; Volten et al. 2001; Min et al. 2016). Finally, the surface brightness is affected by illumination/shadowing effects as the stellar light might traverse a region of locally enhanced optical depth before scattering of the disk surface further outward (Dullemond & Monnier 2010). Extinction of the stellar radiation can occur both in the innermost disk regions and at larger radii, depending on the radial and vertical disk structure (Chapter 5; Wisniewski et al. 2008).

Combined constraints from the spectral energy distribution (SED), scattered light imagery, and the resolved thermal (sub)millimeter continuum yield a detailed inference about the disk structure, dust distribution, and grain properties, thereby providing constraints on the origin of resolved substructures and the driving disk processes. For example, the discrepancy of a cavity radius resolved in the (sub)millimeter continuum and in scattered light may point to the effect of planet-induced dust filtration (Zhu et al. 2012; Garufi et al. 2013) which can be used as an indirect diagnostic of the related planet mass (de Juan Ovelar et al. 2013). The disk height can be measured by fitting ellipses to concentric substructures such as rings and gaps in the scattering surface of inclined disks (Chapter 6; de Boer et al. 2016) while the thickness of a warped inner disk can be determined from the width of the casted shadow lanes (Chapter 7). Scattered light gaps that have been opened by forming planets provide indirect constraints on the planet mass and disk structure through their location, width, and depth (van Boekel et al. 2017; Dong & Fung 2017b). The wavelength-dependent scattering efficiency of the disk yields information on the dust properties in the disk surface (Chapter 4; Mulders et al. 2013a) while an azimuthal modulation of the surface brightness could be imprinted by the scattering phase function, possibly intertwined with the polarization efficiency (Murakawa 2010; Min et al. 2012). For inclined disks, the phase function can be measured by taking into account the geometry of the disk surface (Chapter 3).

1.3.2 Direct detection and characterization of exoplanets

About a dozen of self-luminous exoplanets have been directly detected (Chauvin et al. 2004; Marois et al. 2008; Lagrange et al. 2009) and even more companions near the
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Figure 1.9: Left: Emission spectrum of 51 Eri b, a self-luminous gas giant with a mass of $\sim 9 M_{\text{Jup}}$ and a projected separation of 13 au. The Y- to K$_s$-band data points are obtained with VLT/SPHERE, revealing several water and methane absorption bands. Best-fit model and randomly drawn samples from the posterior probability distribution are shown for comparison. Figure adapted from Samland et al. (2017). Right: Four gas giant exoplanets orbiting HR 8799 (39.4 pc). The central star is subtracted with a combination of the angular differential imaging technique and image post-processing, revealing the planets in the L’ band with a typical planet-to-star contrast of $10^{-4}$. The orbital distances from the star range from 15 au to 68 au. Figure adapted from Marois et al. (2010).

deuterium-burning limit (Bowler 2016). Direct imaging provides observational clues on the occurrence rate, formation and evolution, and atmospheric structure and composition of long-period companions. The four gas giants orbiting HR 8799 (see right image in Fig. 1.9) were the first directly imaged exoplanets of a main-sequence star (Marois et al. 2008, 2010). Since then, the system has been subjected to detailed atmospheric and orbital characterization (Skemer et al. 2014, Bonnefoy et al. 2016, Wertz et al. 2017). The left panel of Fig. 1.9 shows the spectral energy distribution of 51 Eri b (Samland et al. 2017), a directly imaged gas giant discovered by Macintosh et al. (2015).

The main challenges are the small angular separations involved and the large brightness contrast between planet and star. Therefore, direct imaging observations are limited to young gas giants because those planets are still luminous in the near-infrared by gravitational contraction which releases heat into their atmospheric envelope. The first directly imaged exoplanet was detected in a brown dwarf system at a separation of 778 mas ($\Delta H = 5.7$ mag; Chauvin et al. 2004). Tremendous progress has been made since then, allowing for the detection of fainter companions at smaller separations such as the brown dwarf HD 206893 B at a separation of 270 mas from the primary ($\Delta H = 11.1$ mag; Milli et al. 2017a). From a technical perspective, the brightness of the central star is also important to ensure a sufficient wavefront correction by the adaptive optics system such that a high Strehl ratio is reached in the near-infrared.

Planet masses can not be measured in most cases and have to be estimated by comparing the observed luminosity with those from evolutionary models which requires a handle on the age of the system (Bowler 2016). The cooling of a planet over time depends on its formation mechanism and the efficiency by which the accretion entropy is radiated.
away. Hot-start models represent the most luminous cases (Baraffe et al. 2003, Saumon & Marley 2008), corresponding to the most optimistically low mass estimates, thereby mimicking the evolution of planets formed through gravitational instabilities or cloud fragmentation. Cold-start models invoke a rapid loss of initial entropy, as expected for planets formed through core accretion which radiate the gravitational potential energy of the infalling gas away via accretion shocks (Marley et al. 2007, Fortney et al. 2008). Uncertainty in the formation mechanism and system’s age reflect often in a large range of possible planet masses (Macintosh et al. 2015, Skemer et al. 2016).

A few gas giants have been directly detected in their early formation stage (Quanz et al. 2013a, 2015). These protoplanets are still embedded in a protoplanetary disks with ongoing accretion of gas and dust from their environment. The thermal radiation from their atmosphere peaks at near-infrared wavelengths, yet, the photometry has revealed red colors which may hint at additional radiation from circumplanetary material (Zhu 2015). Another way to search for forming planets is with high-contrast Hα imaging. Shocks of accreting gas on the protoplanet atmosphere will ionize the hydrogen gas and Hα radiation is emitted on recombination, similar to low-mass stars, of which a first detection has been claimed in the protoplanetary disk surrounding LkCa 15 (Sallum et al. 2015).

Scattered light from planetary atmospheres is linearly polarized due to scattering of molecules and cloud particles (Hansen & Travis 1974). Polarization is a complementary diagnostic for atmospheric characterization which has been demonstrated for the planets in the Solar System (Hansen & Hovenier 1974, Schmid et al. 2006). The unique optical capabilities of SPHERE/ZIMPOL provide the opportunity to search for the polarized reflected light signature of gas giants orbiting the nearest and brightest stars. The ratio of the polarized and total flux changes with the orbital phase and wavelength, a potential pathway for the characterization of clouds and hazes in exoplanet atmospheres (Stam et al. 2004, Karalidi & Stam 2012). High-contrast polarimetric imaging in the near-infrared may probe the presence of horizontal asymmetries in the atmospheres of self-luminous planets for example due to oblateness, non-uniform clouds, or a circumplanetary disk (Chapter 2, Marley & Sengupta 2011, de Kok et al. 2011). Although both methods are still awaiting a positive detection because direct polarimetric imaging of exoplanets is a highly challenging endeavor, the newest generation of high-contrast imaging instruments may provide the required contrast, angular resolution, and sensitivity to successfully achieve this goal.

### 1.3.3 The SPHERE instrument at the Very Large Telescope

The installment of a new generation of high-contrast imaging instruments at the largest ground-based telescopes in the world is providing the field of direct imaging with a tremendous leap forward. Dedicated imagers for planets and disks such as SPHERE at the Very Large Telescope (Beuzit et al. 2008), GPI at the Gemini South Telescope (Macintosh et al. 2008), and SCExAO at Subaru (Guyon et al. 2010) employ extreme adaptive optics.
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Figure 1.10: Left: European Southern Observatory’s Very Large Telescope facility at Cerro Paranal in Chile. The picture shows the four unit telescopes (UTs) of which the primary mirrors are 8.2 m. (Credit: ESO) Right: The SPHERE instrument mounted at the Nasmyth A focus of UT3. (Credit: ESO)

(AO) systems and deliver unprecedented point spread function (PSF) stability and contrast performance (Macintosh et al. 2014; Fusco et al. 2014).

The SPHERE instrument was commissioned at the Very Large Telescope (VLT) in the Chilean winter of 2014 (see Fig. 1.10). This high-contrast imaging instrument is dedicated for the search and characterization of young gas giant and brown dwarf companions on long-period orbits. However, it is also an excellent instrument to spatially resolve the morphology of circumstellar disks in scattered light (Boccaletti et al. 2015; Thalmann et al. 2016). Light entering the instrument can be branched to three different subinstruments which are ZIMPOL (Thalmann et al. 2008), an optical imaging polarimeter, IRDIS (Dohlen et al. 2008), a near-infrared imager and spectrograph, and the IFS (Claudi et al. 2008), an integral field spectrograph. The complexity of the instrument allows for a wide range of setups such as dual-band imaging, polarimetry, and long-slit spectroscopy, as well as a variety of narrowband and broadband filters, and coronagraphs (Boccaletti et al. 2008). Apart from innovative instrumentation, an important aspect of high-contrast imaging relates to the observing strategy and post-processing of the data.

A powerful technique for the direct detection of circumstellar disks in scattered light is polarimetric differential imaging (PDI; Kuhn et al. 2001; Apai et al. 2004a). The technique relies on the scattering properties of the dust grains in the disk atmosphere which causes the scattered stellar light to be linearly polarized (see Sect. 1.4.1). Polarimetry requires a measurement of two orthogonal polarization directions of the light’s electric field which can be achieved with a Wollaston prism (Lenzen et al. 2003) or a pair of orthogonal polarizers (Langlois et al. 2014). While the scattered light is partially polarized, the direct stellar light is typically unpolarized (Kemp et al. 1987) such that a quasi-simultaneous measurement of the orthogonal polarization states allows for subtraction of the stellar light, as well as unpolarized diffraction residuals. In this way, the large disk-to-star flux contrast (typically $10^{-3}$–$10^{-2}$ for a protoplanetary disk) can be overcome thereby revealing
the morphology of the circumstellar disk (Hashimoto et al. 2011; Quanz et al. 2011). The Stokes $Q$ and $U$ images are obtained during post-processing, for example with the double-difference method (Hinkley et al. 2009), which requires a careful treatment of the centering of the frames and a correction of the instrumental polarization (Canovas et al. 2011; Avenhaus et al. 2014b).

The direct detection of self-luminous exoplanets is typically achieved with the angular differential imaging (ADI; Marois et al. 2006b) technique by switching-off the derotator of an altitude/azimuth telescope. The field of view of the instrument will rotate with the parallactic angle of the star while the PSF and quasi-static speckles remain stabilized in the pupil plane. Therefore, a possible companion will appear at a slightly rotated position with respect to the central star after each detector integration. The star can be used as reference PSF which is subtracted with sophisticated post-processing techniques such as a locally optimized combination of images (LOCI; Lafrenière et al. 2007) and principle component analysis (PCA; Soummer et al. 2012; Amara & Quanz 2012), thereby revealing the faint thermal emission from young gas giants at high-contrast ($10^{-4}$–$10^{-6}$) and small angular separations ($\gtrsim 100$ mas). Also circumstellar disks are routinely detected in scattered light with ADI but the interpretation can be challenging due to self-subtraction of centrosymmetric disk signal during post-processing (Milli et al. 2012). Inclined or azimuthally asymmetric disks suffer least from flux losses, providing access to the Stokes $I$ scattered light flux (Chapter 6; Janson et al. 2016; Maire et al. 2016; Milli et al. 2017b).

1.4 Radiative transfer simulations

Observations of disks and planets rely on measuring the intensity of light captured by a telescope. Spatial, spectral, and temporal variations reflect the characteristics of the observed target but a quantification of its physical properties often requires radiative transfer modeling. Solving the radiative transfer equation in a multidimensional environment is analytically not possible as the underlying physical processes combine to a nonlocal, nonlinear problem (Steinacker et al. 2013). Therefore, numerical radiative transfer codes are commonly used to compute observables such as the spatial- and wavelength-dependent fluxes and polarization (de Haan et al. 1987; Witt & Gordon 1996; Wood et al. 1996).

The Monte Carlo radiative transfer technique is commonly applied on protoplanetary disks (Pascucci et al. 2004; Pinte et al. 2009) as it is not limited by the complexity of the density distribution, computes simultaneously the thermal structure and the observables, and naturally includes multiple scattering of photons (Whitney 2011; Steinacker et al. 2013). Although the bulk mass of a protoplanetary disk resides in the gas, the dust content dominates the opacities such that the gas is safely neglected with continuum radiative transfer. In Chapters 4, 5, and 7 I use a Monte Carlo continuum radiative transfer code, MCMax3D, that is optimized for the high optical depths of protoplanetary disks (Min et al. 2009).
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The gas plays a prominent role in planetary atmospheres which introduces an additional complication as many millions of temperature-dependent molecular lines have to be considered (Sharp & Burrows 2007; Freedman et al. 2008). There are two subclasses of radiative transfer models for (exo)planetary atmospheres: forward models that apply self-consistent physics and chemistry to solve the 1D structure of the atmosphere including the pressure-temperature ($P$-$T$) profile, molecular mixing ratios, and cloud properties (Burrows et al. 1997; Marley & Robinson 2015), and retrieval models which apply a statistic framework to constrain the atmospheric properties backwards from the data while setting priors that allow for a less restricted, not necessarily physical, atmospheric structure (Madhusudhan & Seager 2009; Line et al. 2013). In Chapter 2, we undertake a semi-forward approach to investigate the effect of non-uniform clouds and circumplanetary disks on the spatially-integrated polarization signal from self-luminous exoplanets.

In this section, I will provide a basic background on scattering, polarization, and opacities, as well as the Monte Carlo radiative transfer technique.

1.4.1 Scattering, polarization and opacities

Light is an electromagnetic field that is described by the Maxwell equations (Jackson 1962). Its state is characterized by the four Stokes parameters which are the total intensity (Stokes $I$), linearly polarized intensity (Stokes $Q$ and $U$), and circularly polarized intensity (Stokes $V$) (Chandrasekhar 1960). The linear and circular component are zero when the light is unpolarized, for example the light coming from a distant star (Gehrels 1974). Elastic scattering by molecules, dust grains, or cloud particles will change the polarization state by introducing a partially fixed direction in which the electric field oscillates (Hovenier et al. 2004). The fraction of linearly polarized light with respect to the total amount of light is referred to as the degree of polarization, $P = \sqrt{Q^2 + U^2}/I$, which reflects the microscopic properties of the scatterers (Bohren & Huffman 1983; Mishchenko et al. 2000, 2002).

The angular probability distribution of the light after scattering is described by the scattering phase function of the particle (Hovenier & Muñoz 2009; Muñoz et al. 2012). Particles much smaller than the wavelength scatter in the Rayleigh limit which means that the angular distribution is close to isotropic (Bohren & Huffman 1983). The Rayleigh scattering cross section decreases as a power law with wavelength, $\sigma \propto \lambda^{-4}$, such that scattering of stellar photons by molecules is mainly important at visible wavelengths. Particles comparable to or larger than the wavelength scatter light anisotropically with the strength of the forward (and backward) peak depending on the relative size of the particle (Mishchenko et al. 2000; Min et al. 2016). Forward scattering by dust grains in a circumstellar disk manifests as a brightness asymmetry of the near and far side of an inclined disk (Chapter 6; Thalmann et al. 2014).

In polarized light, the additional effect of the single scattering polarization has to be considered which describes the scattering angle dependent polarization efficiency. The
fractional polarization peaks often at a scattering angle of 90° (West et al. 1997; Petrova et al. 2000; Hadamcik et al. 2002), however, the efficiency depends on the composition, size, and structure of the particles. In the Rayleigh limit, the efficiency is bell-shaped with 100% polarization at a scattering angle of 90° (Bohren & Huffman 1983). The single scattering polarization of silicate-rich particles is described by an approximate bell-shaped curve (Volten et al. 2001; Min et al. 2005), but the peak polarization is typically lower for larger particles (White 1979). The polarization is also sensitive to the scatterer’s composition (Muñoz et al. 2006) and structure (Min et al. 2016; Tazaki et al. 2016).

The left panel of Fig. 1.11 shows numerically calculated phase functions and polarization efficiencies in the $H$-band (1.6 $\mu$m) for different size distributions. A mixture or amorphous silicates and carbon is considered with a porous and irregular grain structure (Woitke et al. 2016; Dorschner et al. 1995; Zubko et al. 1996) of which the opacities and scattering matrices are computed by using a distribution of hollow spheres (DHS; Min et al. 2005). Scattering occurs in the Rayleigh limit when $2\pi a \ll \lambda$ (with $a$ the particle size and $\lambda$ the wavelength) and in the limit of geometric optics when $2\pi a \gg \lambda$. The extinction opacity, $\kappa_{\text{ext}}$, and single scattering albedo, $\omega = \kappa_{\text{scat}}/\kappa_{\text{ext}}$ (with $\kappa_{\text{scat}}$ the scattering opacity), are displayed in the right panel of Fig. 1.11. The opacity decreases at short wavelengths with increasing particle size while the color changes from blue to gray. Around 10 $\mu$m, a characteristic silicate feature is present (Draine & Lee 1984; Jäger et al. 2003) which is routinely detected as a broad emission band in the SEDs of protoplanetary disks (Meeus et al. 2001; van Boekel et al. 2004).

### 1.4.2 Monte Carlo radiative transfer

Monte Carlo radiative transfer relies on the stochastic nature of photon interactions. The radiation field is subdivided into many photon packages which all carry an equal amount...
of energy and propagate through the grid cells of the density structure, for example a protoplanetary disk or planetary atmosphere. The probability that a photon traverses an optical depth, \( \tau \), without any interaction to a next cell boundary is \( e^{-\tau} \) such that its fate can be sampled with a random number generator from a probability distribution (Whitney 2011). Similarly, the scattering probability and the angular distribution of the scattered light can be sampled by considering the single scattering albedo and scattering matrix, respectively. The scattering matrix is also used to calculate the photon’s polarization state after a scattering event (Chandrasekhar 1960).

Photons leaving the grid are projected onto a detector at infinity from which observables are computed such as spectral energy distributions, images, and phase curves. Alternatively, the formal solution to the radiative transfer equation can be calculated by tracing rays along the line of sight if the source function of each grid cell is obtained with the Monte Carlo photons. The thermal structure can be simultaneously calculated in case the opacities are temperature independent, following the method by Bjorkman & Wood (2001). An absorbed photon will supply energy to its grid cells after which a new photon is directly reemitted at a longer wavelength with an immediate temperature correction. The energy of the emitted photon matches the temperature and opacity of the grid cell for which the spectral difference with the cell temperature of the previously absorbed photon is used. The precision of the thermal structure and the observables is provided by the Poisson noise which decreases with increasing number of photons, in trade off with an increase in computation time.

Protoplanetary disks are optically thick at short wavelengths which is a challenge for the Monte Carlo technique as the number of photon interaction rapidly increases with
optical depth. Min et al. (2009) introduced two methods that decrease the computation time in high optical depth regions. The modified random walk approximation can be used to diffuse photons outward in a small number of computational steps instead of letting the photon follow an inefficient random walk of many steps. The partial diffusion approximation improves the accuracy of the thermal structure in high optical depth regions by extrapolating the thermal structure with the diffusion equation from regions with high photon statistics.

Monte Carlo radiative transfer allows for arbitrary density structures, for example, protoplanetary disks with gaps, inner disk warps, and spiral arms (Chapter 4; Chapter 7). The left image in Fig. 1.12 shows a raytraced image of the \( J \)-band polarized scattered light flux from a protoplanetary disk with two radial gaps in its density structure, calculated with MCMax3D (Min et al. 2009). The image is superimposed with contours of the scattering angle which are calculated with the method described in Chapter 3, taking into account the inclination (50\(^\circ\)) and flaring geometry of the scattering surface. The intertwined effect of the phase function and single scattering polarization of the dust is visible, which peak in forward direction and around the major axis, respectively. The right image in Figure 1.12 shows a scattered light image of a planet at a phase angle of 76\(^\circ\) which has been simulated with ARTES (Chapter 2). The reflected light from the clouds and circumplanetary ring is polarized in parallel and perpendicular direction, respectively, due to the difference in sign of the particle’s single scattering polarization.

1.5 Outline of this thesis

The work presented in this thesis aims to investigate protoplanetary disks and self-luminous exoplanets in scattered light. High-contrast observations are used to probe the surface morphology of protoplanetary disks, thereby revealing with high-spatial resolution various substructures that provide insight into the physical processes occurring in protoplanetary disks, possibly related to planet-disk interactions and other disk evolution processes (Chapters 4, 5, 6, and 7). Three-dimensional radiative transfer simulations are used to obtain quantitative constraints on the disk structure and dust properties (Chapters 4, 5, and 7). The phase function of the dust can be retrieved from a scattered light image of an inclined protoplanetary disk if the underlying surface geometry is known (Chapter 3). Polarized scattered light yields also information about horizontal variations in the atmospheres of self-luminous exoplanets, possibly detectable with the latest generation of high-contrast imaging instruments, which we explore with a new scattering radiative transfer code for (exo)planetary atmospheres (Chapter 2).

In Chapter 2, we present a 3D Monte Carlo radiative transfer code, ARTES, that is developed for scattering simulations in (exo)planetary atmospheres. Spectra, phase curves, and images can be calculated for reflected and thermal radiation from an atmospheric structures with an arbitrary opacity distribution. We calculate the disk-integrated degree
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and direction of polarization for self-luminous exoplanets with horizontal cloud variations and circumplanetary disks by using a parameterized atmospheric structure but a full treatment of multiple scattering and polarization.

In Chapter 3, we lay out a numerical method to map scattered light images of inclined and flaring protoplanetary disks to physical quantities. Projection effects of the scattering surface are important for the calculation of stellar irradiation corrected images and the retrieval of dust phase functions. The method is applied on archival SPHERE and NACO data of the protoplanetary disk around HD 100546, yielding new insights about the grain properties in the disk surface.

In Chapter 4, we present multiwavelength polarized scattered light imagery of the transition disk around HD 135344B, obtained with VLT/SPHERE. Several localized shadows are discovered, likely related to asymmetries in the innermost disk regions. We explore the effect of shadowing by an inner disk warp with a radiative transfer model. A measurement of the disk color yields an estimate of the typical grain sizes in the disk surface. The origin of the spiral arms and the asymmetric submillimeter emission are also analyzed and discussed.

In Chapter 5, we continue with a multi-epoch followup study on HD 135344B in which the variability of the shadows is in detail investigated by combining scattered light imagery, photometry, and near-infrared interferometry. The azimuthal and temporal variations of the scattered light flux provide insight into the geometry and dynamics of the inner disk and we discuss several mechanisms that could be attributed to the casted shadows. A grid of radiative transfer models provides a quantification of the required scale height variations in the inner disk.

In Chapter 6, we report on VLT/SPHERE scattered light observations of the flaring protoplanetary disk around HD 97048. Multiple gaps are detected which we discuss in the context of forming planets. The inclination of the disk allows for a measurement of the disk height and the dust phase function. Total intensity images are obtained with angular differential imaging which we additionally use to search for the direct emission from embedded planets.

In Chapter 7, we present optical and near-infrared scattered light imagery of the protoplanetary disk around HD 100453. Several substructures and brightness asymmetries are resolved, including two shadow lanes located close to the onset of the spiral arms. We construct a radiative transfer model to quantify the misalignment of the inner disk, the dust properties, and a possible disk truncation. The M dwarf companion might be responsible for some of the disk features, but we also discuss the possible effect of temperature and pressure variations induced by the shadows.

Acknowledgments

Based on observations collected at the European Organisation for Astronomical Research in the Southern Hemisphere under ESO programmes 095.C-0273(D), 095.C-0298, and 096.C-0241. This chapter makes use of the following ALMA data:
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ADS/JAO.ALMA#2011.0.000015.SV. ALMA is a partnership of ESO (representing its member states), NSF (USA) and NINS (Japan), together with NRC (Canada), NSC and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO and NAOJ.