The future of protoplanetary disk models
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ENGLISH SUMMARY

During my PhD, I have been studying protoplanetary disks: the disks of gas and dust that surround a newly-forming star. These disks slowly evolve and clump together over the course of several million years, eventually forming new planets. This chapter forms a summary of the work in this thesis, where I try to make the work that I have done and the essential conclusions of this thesis accessible to a wider audience. Sections 1 and 2 introduce briefly what a protoplanetary disk is, and give the reader a sense of where these objects fit in the Universe. In Section 3 I describe how we can observe protoplanetary disks, and finally in Sections 4 to 9 I briefly introduce the current status of protoplanetary disk research, and describe each chapter of my thesis.

1. THE ORIGIN OF PROTOPLANETARY DISKS

Within the observable Universe,\(^1\) there are perhaps up to two trillion galaxies. Within each galaxy, there might be 100 billion stars. Most of these stars are much younger than their host galaxies: they have been created from the recycled material of their predecessors, the stars that have used up all of their nuclear fuel and died in spectacular fashion.

New stars are formed from what we call the *interstellar medium*. Within the interstellar medium, there are vast clouds of gas and dust whose filaments thread their way through their host galaxy. Some regions of these clouds are more dense than others, thus their greater gravitational field allows them to collect even more of their surrounding material. Eventually, such a cloud becomes gravitationally

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\(^1\) Because the Universe itself is only 13.8 billion years old, the observable Universe is a sphere around the Earth with a radius of 13.8 billion light years. Although there is almost certainly *something* beyond this barrier, the laws of physics are such that the light from those regions has not yet had time to reach us.
unstable and begins to collapse inwards. This is the beginning of a new star. Figure A.1 shows the Pillars of Creation in the Eagle nebula (M16). M16 is an emission nebula, where the colours seen are due to many bright, young stars illuminating the surrounding clouds of gas. The dark areas are rich in dust, and the bright light emanating from the tips of the Pillars of Creation comes from newly-forming stars. The molecular clouds in nebulae such as M16 are home to many protoplanetary disks.

During the collapse of a molecular cloud, most of the matter falls inwards to the gravitational centre, where enough matter is gathered to form a new star. However, some of the matter is not immediately accreted. These star-forming clouds are not stationary objects. Not only do they orbit the galactic centre like any regular star, but they also toss and tumble: they have their own angular momentum. During the phase of gravitational collapse, the cloud is becoming more and more dense. As a result, the particles in the cloud begin to collide with each other more often.

Although every particle in the cloud has its own angular momentum, the molecular cloud as a whole also rotates in a particular direction. As all of the particles collide, the angular momentum of the cloud is gradually nullified in every direction except the average direction of the molecular cloud. Because the laws of physics dictate that the total angular momentum of the molecular cloud must be conserved, the result is a rotating disk of debris. A protoplanetary disk. Figure Fig. A.2 shows a Hubble Space Telescope image of four disks in the Orion nebula. The disks are very small compared to the size of the nebula, but we can see them with our best telescopes. These are hardly static objects, but full of interactions between the gas and dust including the growth and destruction of dust grains, the chemistry of gas molecules (and their freezing into ices), and the effects of radiation from the hot, newly-forming star at the centre of the system. Figure A.3 shows a sketch of the structure of a protoplanetary disk and the physical processes that occur within.

Over the course of several million years, the remnants of gas and dust that make up a protoplanetary disk begin to evolve. Some of the matter falls into the central star, through a process that we call accretion. Some is dissipated back into the interstellar medium through photoevaporation and disk winds, due to the intense stellar radiation. But some of it slowly clumps together to form larger bodies: comets, asteroids, moons, and planets. These planets around other stars are called exoplanets.
Figure A.1: The M16 nebula, as imaged by the William Herschel Telescope in May 2015, using narrow-band filters. Red corresponds to hydrogen emission, green is sulphur, and blue is oxygen. Stars are actively forming in the famous “Pillars of Creation” in the centre of this image.
Figure A.2: Four proplyds (ionized protoplanetary disks) in the Orion nebula, seen with the Hubble Space Telescope. This image is from a NASA press release (hubblesite.org/news_release/news/1994-24).

Figure A.3: The structure of a typical protoplanetary disk. Figure reproduced from Henning & Semenov (2013).
2. Relative Sizes

Protoplanetary disks are, by some measures, quite large: a typical protoplanetary disk around a star that is similar to our own Sun has a radius of about 600 AU (one “AU”, or astronomical unit, is equal to the average distance between the Earth and the Sun: about 150 million km). However, it is easy to get misled by distances in astronomy. Although a typical protoplanetary disk might have a diameter that is ten times the size of Pluto’s orbit, our galaxy is hundreds of millions of times bigger. In this section I describe how small these disks are compared to the larger scales of our Galaxy or the Universe.

Andromeda, the Large Magellanic Cloud, and the Small Magellanic Cloud are all nearby galaxies that we can see with the naked eye. Clusters of galaxies are very close together, at least relative to their own size: the distance separating each galaxy is often only 10 or 100 times their own diameter. Our own Milky Way galaxy is about $6.4 \times 10^9$ AU in diameter, or 100,000 light years: the distance from here to the Andromeda galaxy is about 25 times this diameter – imagine the galaxies as two ping pong balls, spaced 1 m apart. Relative to their own sizes, stars are much further away from each other than galaxies – if two nearby stars in a galaxy were ping pong balls, they might now be spaced 1000 km apart. If two galaxies collide and merge, it is very unlikely that two stars will collide with each other.

Although we can see other galaxies with the naked eye (such as Andromeda, the LMC, and the SMC), the same is unfortunately not true for protoplanetary disks and exoplanets. Protoplanetary disks are such short-lived objects that they can only be found in regions that are actively forming new stars, and the nearest star-forming regions are about 120 light years away. The distance to the nearest star-forming regions is several million times the distance between the Earth and the Sun. If the Sun were a ping pong ball, these regions would be 65,000 km away. Consequently, the angular size of a typical nearby protoplanetary disk in our sky, with a radius of 600 AU, is about two thousandths the size of the Moon. Thus, protoplanetary disks are hard to observe because they are so small.

3. Observing Protoplanetary Disks

The outer regions of these disks – much like our own Solar System – are very cold. They emit primarily not in the visible spectrum, but at infrared and mm wavelengths. As a result, it is much better to use telescopes that operate with infrared, sub-mm and mm wavelengths.

In order to observe an entire protoplanetary disk, no single telescope can cover the immense wavelength range necessary: from near-infrared wavelengths
of around 2 $\mu$m, all the way to wavelengths of a few millimetres. The mm-wavelength light that comes from the cold, sparse outer disk has a wavelength that is 1000 times longer than the near-infrared light. For comparison, there is only about a factor of two difference between the shortest wavelengths (violet) and longest wavelengths (red) that the human eye can see.

**Infrared**

Infrared observations are difficult because room temperature objects emit significant amounts of infrared light, and also because the Earth’s atmosphere easily absorbs infrared light. Additionally, the star itself is very bright in the infrared and can easily drown out the disk: we need to use a coronograph to physically block the stellar light from reaching the telescope.

The wavelength range between about 5 $\mu$m and 50 $\mu$m is known as the mid-infrared, while from about 50 $\mu$m to 1000 $\mu$m, or 1 mm, is the far-infrared. In order to observe in the mid- and far-infrared, we need to use a cryogenically-cooled space telescope. The Spitzer and Herschel space telescopes have done this job in the past, and the upcoming *James Webb Space Telescope* will further push the boundaries of our knowledge: JWST has a 6.5-meter mirror, compared to the 0.85 meter mirror of its predecessor, Spitzer. Combined with new technology in its instruments, JWST will be up to 100 times more sensitive than Spitzer.

Because the part of a protoplanetary disk that is bright in the near infrared is very small, it is difficult to spatially resolve a disk in the near infrared. However, taking the spectrum of a disk can still yield a lot of useful information. The spectra tell us about simple molecules in the disk such as hydrogen cyanide and water. There is a lot to learn from the brightness and shape of the spectral lines, such as finding out how much water there might be in the disk, and where it resides (an important consideration for forming habitable planets).

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2 $1$ $\mu$m is a micrometre, or one millionth of a metre. The range of visible light is about 0.39 $\mu$m to 0.7 $\mu$m.

3 There are a few “windows” in the atmospheric absorption that allow ground-based near- and mid-infrared observations, but to get uninterrupted wavelength coverage it is necessary to go to space.

4 This will be possible with the E-ELT, due to its huge 39 m mirror and adaptive optics that combat blurring due to atmospheric turbulence.
Microwave wavelengths

The wavelength range between 1 mm and 1 m is the microwave range. At the short end of this range, around 1 mm, ground-based telescopes such as the ALMA observatory in Chile are very successful in observing protoplanetary disks. There is no life-limiting supply of cryogenic coolant to worry about, and the sparse, dry air of the high-altitude Atacama desert reduces the effects of water in the atmosphere absorbing the light. However, there is an unfortunate complication: the angular resolution of an image is given by the Rayleigh criterion, \( \theta = \frac{1.22 \lambda}{D} \), where \( \lambda \) is the wavelength of light and \( D \) is the telescope diameter. As the wavelength increases by a factor of 1000 from near-infrared to mm wavelengths, the sharpness of an image drops by a factor of 1000. To make up for this, the ALMA observatory is what we call an interferometer: there are over 50 separate dishes with a 12 m diameter, and twelve 7 m dishes. By spreading the large 12 m dishes out over a large distance (up to 10 km apart) and using a specialized computer called a correlator\(^5\) to combine their signals together, the telescope array now has the resolving power of a 10 km dish and the light-gathering capability of a 44 m dish. The smaller dishes remain more closely spaced, in order to combat the loss of large-scale detail that can otherwise occur using interferometry. This technique allows us to capture incredible images of protoplanetary disks, such as the image of TW Hydrae seen in Fig. A.4.

We can also obtain spectra with ALMA that allow us to detect simple molecules and trace where they occur in the disk, helping us to understand the chemistry in protoplanetary disks and determine physical conditions such as where water vapour freezes into ice (the pressure in a protoplanetary disk is much too low for liquid water to exist). Recently, Pinte et al. (2018b) have even suggested that kinematic information obtained from observations of carbon monoxide provides evidence for an embedded, invisible protoplanet (see Fig. A.5).

4. The state of today’s research

We are reasonably certain in our broad knowledge of the formation of stars and planetary systems. We know that stars form in the dense star-forming regions of the molecular clouds which thread their way through our galaxy. We also know that over the course of several million years, new planets can form in protoplanetary disks and that these disks generally dissipate not long afterwards. However, many of the finer details are still uncertain. Much of today’s research involves investigating individual pieces of the larger scale: it is much too difficult (and our computers are not fast enough) to study and simulate everything at once. We have to pick small pieces of the puzzle to study, one at a time. For example, running hydrodynamical simulations of molecular clouds and protoplanetary

\(^5\) The ALMA correlator is one of the fastest computers in the world. However, its application-specific integrated circuits cannot do anything else.
Figure A.4: The protoplanetary disk around the young star TW Hydrae. In the inset image, we see a gap at approximately the same radius from the star as the Earth is from the Sun: this gap may have been carved by a newly-forming planet. Other gaps are visible in the main image, at much larger radii comparable to the distance of Uranus or Pluto in our own Solar System. This image is from an ESO press release (eso.org/public/news/eso1611/), accompanying the scientific paper by Andrews et al. (2016).

Figure A.5: Carbon monoxide emission from the disk around the star HD 163296, captured with ALMA (Pinte et al. 2018b). The data trace a subset of the CO emission, at a relative velocity of 1 km s$^{-1}$. Most of the CO gas is travelling either faster or slower than 1 km s$^{-1}$, because the entire disk is rotating: this is why it does not look like a disk. The data look like we would expect them to, but with one exception: a small kink in the surface, outlined by the dotted circle. The blue dot indicates the location of the potential planet that could cause this kink.
disks, to study their formation and physical evolution over time. Some researchers look towards our own Solar System for clues: studying the structure of meteorites and the orbits and compositions of comets, to gain insight into what our Solar System might have looked like back when it was a protoplanetary disk.\footnote{For example, we currently do not know exactly how Earth got its water: did the Earth form further away from the Sun than it now orbits, gathering water at the same time? Or did the Earth form closer to where it is now, with much of its water being delivered by comets and small protoplanets from the outer Solar System?}

Another major branch of research is in the chemistry and structure of protoplanetary disks: what does a protoplanetary disk look like in detail, at an instantaneous point in time? Protoplanetary disks generally change and evolve too slowly to directly observe these changes with our telescopes (although we can observe the kinematics of gas and dust in disks (Teague et al. 2018), the long-term evolution happens over millions of years). This is where we try to match computer models to images from telescopes such as the ALMA array in Chile, or to spectra from the Spitzer space telescope. Because every disk is different, each individual disk has the potential to tell us something new about protoplanetary disks.

5. **MY THESIS**

My research involves understanding the structure and chemistry of protoplanetary disks, using a purpose-built computer code called ProDiMo. Within the code, there is a large number of parameters that can be adjusted: simple adjustments might include changing the size and mass of the disk, the luminosity of the central star, or changing the size, distribution, and composition of the dust particles.

In order to run a ProDiMo disk model, we begin by defining how the dust particles in the disk are distributed. For example, the total dust mass is normally defined as 1% of the gas mass, and dust particles may vary in size between 0.05 $\mu$m and 3000 $\mu$m. Dust is very important for the radiative transfer – the way in which light is propagated through the disk – because it is very efficient at scattering and absorbing light. Thus, after the dust distribution has been defined, we run a radiative transfer algorithm that determines how much light from the central star reaches every part of the disk. The midplane\footnote{The midplane is our term for the middle of the disk, in a vertical sense. If you cut a piece of pita bread in half to make a sandwich, you have sliced along the midplane.} of the disk is typically very cold and dark (about 10 K), because dust tends to concentrate itself there.\footnote{In astronomy, we always use the Kelvin scale: it is like the Celsius scale, but shifted so that 0 K is absolute zero ($−273.15^\circ$C). Thus, 0$^\circ$C is 273.15 K.} As seen in Fig. A.3, disks also tend to curve upwards at larger distances from the star. These upper layers have relatively little dust and receive much more stellar radiation, so they are much hotter (between a few hundred to a few thousand degrees Kelvin).
Once the radiative transfer calculations have finished, we calculate the chemistry. We begin with a mixture of light elements: hydrogen, helium, carbon, and so on (heavy elements such as iron are also included, but they exist mostly in the dust). These initial abundances are fed into a chemical network: a large set of chemical reactions that can occur, so that more complex molecular species such as water and hydrogen cyanide can form (usually, we allow a total of 235 different species to form). Once the chemistry algorithm has found a steady-state solution, the disk model is complete and it now describes how each of the molecular species is distributed throughout the disk. Because each species forms in a different way and is sensitive to different temperatures and types of stellar radiation, we can learn a lot from analyzing the chemistry of these models and comparing them to observed disks.\(^9\)

Each of the three science chapters of my thesis uses these disk models in order to answer a different question.

6. **Brown Dwarf Protoplanetary Disks**

In the first science chapter, I calculate the most detailed models yet of a protoplanetary disk around a brown dwarf star. A brown dwarf is a “failed star” – a star which is not massive enough to fuse hydrogen into helium. A star that is less massive than 0.08 times the mass of our Sun is a brown dwarf. Relatively little is known about brown dwarfs, because they are so small and faint. Despite the thousands of exoplanets that have been detected around other stars, we have not yet managed to detect an exoplanet around a confirmed brown dwarf.\(^10\)

However, we have observed many exoplanets around stars that are just above this mass threshold, for example the TRAPPIST-1 system. Thus, the question: are brown dwarf disks fundamentally different to the disks around higher-mass stars? Or is the lack of observed planets simply because our telescopes have not been sensitive enough to detect small, rocky planets?

In this chapter, I take a model of a larger, higher-mass “T Tauri” type disk and scale it down to the size of a brown dwarf: that is, I take the same set of model input parameters, change the central star to a brown dwarf, and significantly reduce the mass and radius of the disk – these model parameters were guided by predictions from previous literature. We find that our model compares well to the observations of a known brown dwarf disk, and that there do not appear to be any discontinuous differences between brown dwarf and T Tauri disks: the model looks very similar to a T Tauri disk that has only been shrunken in size and mass.

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9 For example, Pinte et al. (2018a) have directly imaged the emission from $^{12}$CO, $^{13}$CO, and C$^{18}$O in the disk around the star IM Lupi. Because the emission from each species comes from different vertical layers in the disk, the authors managed to locate the vertical CO “snow line”: the height in the disk at which CO freezes from a gas directly into a solid.

10 Excluding some questionable cases such as a planet that is too massive to have formed in a disk and most likely formed at the same time as the star, or the host star has not been confirmed as a brown dwarf.
The significant result of this chapter is that we can expect brown dwarf disks to be dominated by the same chemical processes as their more massive T Tauri counterparts. For example, our models still have a water snow line, which is the threshold across which water can exist as solid ice. This threshold is thought to be an important catalyst for planet formation. Finally, our models predict that chemical species which had never been observed before in a brown dwarf disk using ALMA, such as HCN or HCO$^+$, should be detectable given enough observing time.

7. **Infrared Spectra of T Tauri Disks**

The second science chapter focuses on the infrared spectra of T Tauri disks. These are the disks around stars which are very similar to our own Sun. The infrared spectrum is rich with emission lines from species such as CO$_2$ and H$_2$O, which can tell us a lot about the inner few AU of the disk. I use a new computer code called FLiTs to produce infrared spectra of a series of disk models, in order to understand how these spectra respond to changes in the radiation environment (such as increased UV radiation, or the upwards curve of the outer disk that increases the amount of stellar radiation that hits the disk surface). Once JWST launches, we expect many such spectra also from all types of disks, including brown dwarfs: hence, we need to calibrate and test our models against existing observations.

I also analyze the regions from which each chemical species emits infrared light. For example, I find that each of the species tends to emit from regions where the gas is warmer than the dust (by between 50 K and a few hundred K). This is because the infrared line emission comes from regions in the upper disk, that are *optically thin* (stellar radiation easily penetrates these regions). Chemical heating from exothermic reactions acts to heat up the gas significantly, while the densities of both gas and dust in these upper regions are low enough that the gas and dust temperatures can be decoupled from each other.

The combination of FLiTs and ProDiMo produces the most advanced models yet of protoplanetary disk spectra, and my results also highlight the complexity of trying to model these objects. In the past, we had sometimes used approximations such as assuming the gas and dust temperature to be equal to each other, or running “slab models” that do not encompass any spatial information. However, we know that fundamental properties such as the gas temperature and abundances of different species can vary across the line-emitting region: to correctly interpret observations is a difficult task.\(^\text{11}\) On the horizon, we have JWST which will deliver much better quality spectra than ever before, and E-ELT which will be able to spatially resolve the inner few AU of protoplanetary disks.

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\(^\text{11}\) The line-emitting region is the part of the disk where a specific spectral line is emitted from. For example, the mid-infrared CO$_2$ lines come from a region between 0.1 AU and 1 AU away from the star.
In order to make the most of these capabilities, we need to continue improving our understanding of how to create accurate, highly-detailed models.

8. THE EFFECTS OF DUST EVOLUTION ON INFRARED SPECTRA

The final chapter analyzes the effects that dust evolution can have on infrared spectra. Because dust is the main opacity carrier (determining how much stellar radiation reaches different parts of the disk), it is also very influential on the infrared light emitted from gaseous molecules. As a protoplanetary disk evolves through the course of its several-million-year lifetime, the dust evolves too. Some of the dust is dragged into the central star, because the viscosity of the disk causes some of the dust to lose angular momentum. Dust may also grow in size, to eventually become asteroids or planets. Thus, as the dust changes, we expect the infrared spectra to change as well.

In this chapter, we use a dust evolution code called two-pop-py to simulate this evolution. We create snapshots of the dust at several different disk ages, and then compute a ProDiMo model based upon these predetermined dust structure snapshots. The result is a description of how a protoplanetary disk might respond to changes in the dust structure. One important difference in these models, as compared to the models in previous chapters of this thesis, is that the manner in which dust is allowed to settle towards the midplane is likely more realistic. Dust settling more efficiently clears the upper disk layers of small sub-micron dust grains, reducing opacities and helping to increase molecular line fluxes (the brightness of a particular spectral line).

In the past, we have struggled to use models to reproduce the line fluxes seen by Spitzer: our models are not bright enough. The quick solution has been to increase the total mass ratio between gas and dust in the disk, from 100:1 to 1000:1 (so by mass, there is 1000 times more gas than dust). However, this does not remove the dust using a physical process. Combined, the new methods of dust settling and evolution are able to reduce the gas-to-dust ratio in the line-emitting regions enough to accomplish the same effect, while keeping the initial overall gas-to-dust ratio (before the dust evolution begins) at 100.

The main result of this chapter is that dust evolution can affect the brightness of mid-infrared lines by a factor of 100, as the disk model ages from 0.018 to 10 million years old. The ages themselves are rather uncertain – exactly how quickly dust evolution happens in reality is difficult to ascertain – but the potential for dramatic changes is clearly there, and it is now easy to create disk models with bright enough mid-infrared lines to match any observed spectrum. We also find that the gas temperature of the line-emitting regions does not appear to change significantly until the dust is very highly evolved and has almost disappeared entirely from the disk. For example, the CO\textsubscript{2} emission always comes from a temperature of about 300 K, even as the line flux increases by a factor of 10.
Results such as these are a valuable contribution towards our understanding of how to interpret mid-infrared spectra.

9. CONCLUSION

In this thesis, I have explored a variety of different ways in which we can further our understanding of protoplanetary disks and how to model them. We now know that we can model brown dwarf disks without needing significantly to modify our existing tools. Our results on infrared spectra show that the sheer amount of detail in these models is both a blessing and a curse: although we can learn a lot from them, we do not fully understand all of the details in our models. Preparing for JWST and E-ELT, and knowing how to make the most of the revolutionary data that these observatories will deliver, is of great importance to the disk modelling community. This thesis both answers some questions relating to this goal, and opens new questions to provide direction for future research.