The role of ice in planet formation

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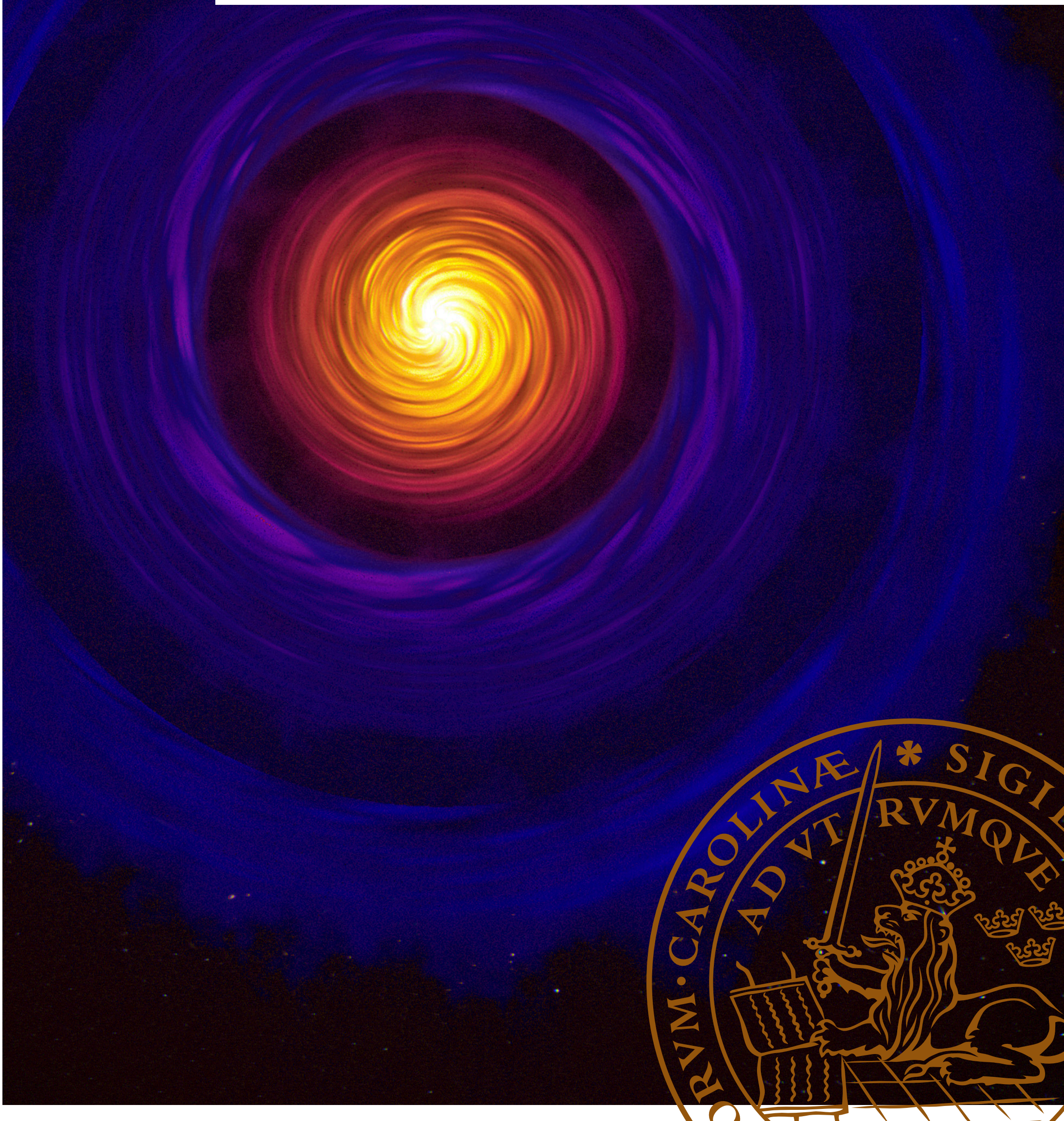

The role of ice in planet formation

Katrin Ros

Thesis for the degree of Doctor of Philosophy

Thesis advisor: Professor Anders Johansen
Co-advisor: Professor Nils Ryde
Faculty opponent: Doctor Sebastiaan Krijt

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Abstract

As stars form they are surrounded by a disc composed of gas, dust and ice – the protoplanetary disc, where solids grow from micrometer-sized dust to planets. Small dust grows readily by collisions, however, it is challenging to reach high enough particle sizes and dust-to-gas-ratios for continued growth to planetesimals – kilometre-sized and larger planetary building blocks.

In this thesis I explore the effect on ice on the growth towards pebbles, in order to investigate if the water ice line – the radial distance from the star where water undergoes a phase change from vapour to solid – can be a favourable location for the initiation of growth towards planetesimals.

In a series of papers, I numerically and experimentally investigate condensation and sublimation at the water ice line. In Paper I, we develop a numerical model where we investigate the dynamics of ice and vapour and find that condensation indeed can lead to large pebble-sized particles at the water ice line. In Paper II, we introduce the mechanism of nucleation – the distinction between forming the first ice layer on rock and continued condensation onto ice. We find that this important mechanism effectively sorts out the large amount of rocky dust present, and allows icy pebbles to grow. In Paper III, we experimentally investigate the outcome of sublimation and find that the sublimation of icy pebbles can result in relatively intact pebbles, rather than small dust. Finally, in Paper IV, we study the nucleation and condensation after accretion outbursts, that are frequent among young stars and have been observed to shift the ice line outwards with tens of astronomical units. Our results show that condensation growth after these outbursts lead to fast formation of centimetre-sized pebbles. In conclusion, we find that ice lines are important locations in protoplanetary discs, with condensation being a robust growth mechanism that can facilitate growth towards planetesimal and planets.

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Cover: Artist impression of a protoplanetary disc with substructures, edited to show the inner region where water vapour is present in red, and the outer region where water ice is frozen out in blue. Credit: NASA, ESA, CSA, Joseph Olmsted (STScI).

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Contents

List of publications

This thesis is based on the following peer-reviewed publications:

I **Ice condensation as a planet formation mechanism**
K. Ros and A. Johansen (2013)
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II **Effect of nucleation on icy pebble growth in protoplanetary discs**
K. Ros, A. Johansen, I. Riipinen, and D. Schlesinger (2019)
Astronomy & Astrophysics, Volume 629, id.A65

III **The fate of icy pebbles undergoing sublimation in protoplanetary discs**
S. Spadaccia, H. L. Capello, A. Pommerol, P. Schuetz, Y. Alibert, **K. Ros**, and N. Thomas (2022)
Monthly Notices of the Royal Astronomical Society, Volume 509, Issue 2

IV **Fast formation of large icy pebbles after FU Orionis outbursts**
K. Ros and A. Johansen
Submitted to Astronomy & Astrophysics

Popular summary

Studying how planetary systems form is not an easy task. We do have our own planetary system – the Solar System – to start from, but the formation of our Sun and its planets took place billions of years ago. Still, we can find clues to its formation processes in the final product; in its configuration, in the planets and in the minor bodies of the system. Twenty years ago, astronomers also started to find so-called exoplanetary systems, planets outside of our Solar System. Today, we know that planets are common in the Milky Way, and we can combine our knowledge of all the systems we know of to compose a more coherent view of the outcome of planet formation processes and mechanisms. Fortunately, nowadays we also have more direct information in the form of observations of planet formation taking place right now, in so-called protoplanetary discs. These are discs of gas, dust and ice surrounding young stars, and it is in these discs that planet formation happens. Initially, the solids in these discs are in the form of micrometre-sized dust and ice grains, and during the lifetime of the disc of a few million years this solid component grows into planets.

My thesis is about understanding the growth of disc solids to make further growth towards planets possible, and in particular how water ice helps in the growth process. Initially, the disc solids are in the form of micrometre-sized ice and dust grains. These grains can grow via collisions, but only until a certain size, around millimetres, when collisions result in fragmentation or bouncing instead of growth. The next growth step is when pebbles are concentrating in the disc until reaching they form a clump of a critical concentration and size where self-gravity takes over and the clump collapses into a solid object, that we call a planetesimal. We see such leftover planetesimals in the form of asteroids, comets and other minor bodies in our Solar System. However, there is an issue here. For such clumping mechanisms to be effective, the pebbles in the clump must reach a large enough size and concentration, and these conditions are not readily met anywhere in the protoplanetary disc. Therefore, we look for sweet-spots in the disc, where particles either can grow extra large, or can concentrate more than elsewhere, or both.

The water ice line has the potential to be such a sweet-spot, and this is what I am investigating in this thesis. Since the disc is hotter and denser towards the star, and colder and more sparse further out, we find water in vapour form close to the star and in the form of ice further out. The location where the transition between vapour and ice happens is called the ice line. In the early Solar System the ice line was located just between Mars and Jupiter, and it is thought to be precisely the existence of the ice line there that has shaped the Solar System such that the

smaller planets are found inside of it and the more massive ones on the outside.

At the ice line, planetesimal formation, and therefore planet formation, can be facilitated both because the amount of solid material increases sharply there, and because it adds one more dust growth mechanism, in addition to collisions: condensation. Icy particles crossing the ice line sublimate, and when the resulting vapour goes back across it, the vapour condenses onto already existing particles. This is the mechanism I have studied in this thesis, through numerical simulations and laboratory experiments.

We have investigated both a quiescent disc, and a disc cooling down after an outburst, something which frequently occurs for young stars. In both cases we have found that condensation can contribute to a fast growth to pebbles, with the potential of increasing the concentration of solids enough for continued growth towards planetesimals. Our results also highlight that it is important to take nucleation – the fact that vapour condenses easier onto ice than rock – into account. Due to this, already icy pebbles can grow to larger sizes locally at the ice line, whereas small dust grains tend to stay small and diffuse out over the disc. In conclusion, our results show that condensation indeed is an important growth mechanism, making the ice line a potential sweet-spot where planet formation can be initialised.

Populärvetenskaplig sammanfattning

Att ta reda på hur planetsystem bildas är ingen lätt uppgift. Vi har vårt eget planetsystem – solsystemet – att utgå ifrån, men vår sol och dess planeter var färdiga med att bildas redan för flera miljarder år sedan. Trots det kan vi hitta ledtrådar till hur bildningsprocessen gick till i slutprodukten: själva planetsystemet som vi bor i. För tjugo år sedan fick vi också tillgång till fler ledtrådar till planetbildningsprocessen då den första exoplaneten, det vill säga den första planeten utanför vårt solsystem, hittades. Idag vet vi att exoplaneter är vanliga i Vintergatan, och vi kan kombinera vår kunskap om alla de system vi känner till för att skapa en mer sammanhängande bild av resultatet av planetbildningsprocesserna. Som tur är har vi numera också mer direkt information i form av observationer av planetbildning såsom den sker just nu, i så kallade protoplanetära skivor. Dessa är skivor av gas, stoft och is som omger unga stjärnor, och det är i dessa skivor som planetbildning sker. Till en början är de fasta ämnena i dessa skivor i form av mikrometerstora damm och iskorn, och under skivans livstid på några miljoner år växer denna fasta komponent till planeter.

Min avhandling handlar om att förstå hur den fasta komponenten i de protoplanetära skivorna går från små mikrometerstora stoft- och iskorn till större kroppar, som sedan kan bilda planeter. Medan de fortfarande är små, kan kornen växa genom kollisioner, men när de passerat ungefär millimeterstorlek resulterar kollisioner inte längre i tillväxt, utan istället i att de slås sönder eller studsar mot varandra.

Därefter är nästa steg i tillväxtprocessen att partiklar klumpas ihop till en större klump med en kritisk koncentration och storlek, där den kollapsar av sin egen gravitation. Detta resulterar i en kilometerstor fast kropp som vi kallar planetesimal. Sådana planetesimaler kan ses än idag i solsystemet i form av till exempel asteroider och kometer, som helt enkelt är överblivna planetesimaler från när solsystemet bildades.

Det finns dock ett problem här. För att dessa planetesimaler ska kunna bildas genom att partiklar koncentreras och klumpas ihop, måste dessa partiklar först både bli tillräckligt stora, och uppnå en tillräckligt hög koncentration. Dessa villkor uppfylls tyvärr inte hur som helst eller var som helst i den protoplanetära skivan. Därför letar vi efter speciella platser i skivan, där antingen partikeltillväxten är extra gynnsam eller där partikelkoncentrationen kan bli extra hög.

En plats som har potential att vara just en sådan extra gynnsam plats är den så kallade frostlinjen eller islinjen. Eftersom det är varmare närmre stjärnan än längre ut från den hittar vi vatten i form av ånga längst in mot stjärnan och i form av is längre ut. Avståndet från stjärnan där övergången mellan vattenånga och is sker är det vi kallar för islinjen. I det tidiga solsystemet låg islinjen mitt emellan Mars och Jupiter, och man tror att det är just islinjen som bidragit till att de mindre planeterna alla ligger innanför denna position, medan de större ligger utanför. Vid islinjen är det lättare för planetesimaler att bildas, både för att andelen fast material ökar där, och för att partiklar där kan växa även genom kondensation och inte bara genom kollisioner. När partiklar med ett ishölje passerar islinjen blir isen till vattenånga genom sublimation. Ångan kan passera tillbaka till den kallare delen av den protoplanetära skivan, där den kondenserar då den möter fasta partiklar. Detta leder till att de partiklar som befinner sig där kan växa större.

I min avhandling har jag studerat just denna mekanism i datorsimuleringar och i laboratorieexperiment. Vi har undersökt både en lugn protoplanetär skiva och en skiva som just har genomgått ett stjärnutbrott, där temperaturen plötsligt höjts i den omgivande skivan. Sådana utbrott är vanliga hos unga stjärnor och resulterar i att islinjen tillfälligt förflyttas utåt. I båda fallen visar våra resultat att kondensation kan bidra till att partiklar snabbt växer till ungefär centimeterstorlek. Vi har också sett att det är möjligt att koncentrationen av partiklar blir tillräckligt hög för att planetesimaler skulle kunna bildas. Dessutom har vi visat att ånga kondenserar lättare på partiklar som redan har ett ishölje än på partiklar utan ishölje i protoplanetära skivor. Detta resulterar i att isiga partiklar kan växa sig stora lokalt vid islinjen, medan stoftpartiklar utan ishölje tenderar att stanna vid stoftstorlek och sprids därmed lättare ut i den omgivande gasen. För att sammanfatta, visar våra resultat att kondensation är en viktig tillväxtmekanism för stoftpartiklar i protoplanetära skivor, vilket gör islinjen till en potentiellt gynnsam plats för fortsatt tillväxt mot planetesimaler och planeter.

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Most importantly, of course, Anders. Many years ago, I thought I wanted to do a project on exoplanets and was pointed to ”the new Danish guy”. It turned out the new Danish guy was also a fantastic scientist, excellent at finding the coolest and most interesting questions to work on, and someone who could also actually explain the most complicated things in ways so they became understandable. I have learned so much during these years, and I feel super privileged to have gotten to work with you—thank you.

During this time, I have had the opportunity to attend and present my work at many conferences and also organised meetings here in Lund. Going to meetings and being part of the planet formation community has been a very important part of research for me, and I have met a lot of amazing people all over the world. I will not even try to name you all, but instead, I simply say thank you to the planet formation community which I have been very happy to be a part of.

I would like to thank my collaborators outside of Lund: Ilona and Daniel for doing the hard work of communicating between different scientific fields. Holly and Stefano for inviting me to their research group and showing me a bit of the exciting world of experiments, and just how hard it can be to make the right kind of icy pebbles.

Here in Lund, I want to thank the many people at our division of astrophysics for a great work atmosphere and for a lunchroom filled with discussions on all kinds of topics. To all my office mates during this time, Alexey, Asli, Noemi, Simona, Madeleine and Anna, thanks for all the conversation on everything from unicorns to relationships – it has been a pleasure to share an office with all of you! Specifically for this thesis, I would like to thank Brian for sharing the thesis template, and Rebecca and Johan for all the help with everything practical that weirdly enough can never be found in writing when you need it, and of course, for cheering me on the past weeks. And thank you, Eva, for knowing everything administration-related, reminding me every time I forgot something, and helping out with every question that I have asked you.

I am also very happy to have been part of the planet formation group here in Lund, and later in Copenhagen-Lund. It has been really cool to see this group grow from just a handful of us to a big and very active research group. Thanks to everyone for all the discussions and presentations of interesting work. Michiel, we were both part of the first mini-small planet formation group – thanks for all the help and support during the writing of my first papers, and also for all the work you have done to make the group grow and thrive.

Wow, this became longer than I expected, but I guess so did the time I have been a PhD student. Before ending this acknowledgement section, I would of course also like to thank my family with all of my heart. Thank you for being there, always. Thanks for supporting me, both practically and emotionally, and for always having encouraged me to find my own way.

Thomas, thanks for believing in me also on the days when I don't believe in myself, for having the magic to make me happy when I am sad, and also the magic to make good things even better.

Och sist men inte minst – Anton och Klara, mina gullisar: Ja, NU är jag färdig med min bok. Nu vänder vi blad.

Part I

Research context

Chapter 1

Gathering clues to planet formation

This thesis is about the formation of planets – our own home planet Earth and its siblings in the Solar System, but also all the distant planets orbiting stars other than the Sun; extrasolar planets, or just exoplanets.

Planet formation is not one single process, but rather a series of different physical and chemical mechanisms and reactions spanning over a wide range of particle sizes, from the tiniest micrometre-sized dust to giant planets with radii of tens of thousands kilometres. My research, and therefore this thesis, has been focused on the growth of dust-sized to pebble-sized particles and the role that water ice plays in this step. However, before we actually get to the details of planet formation and particle growth, I want to start by discussing how we can even know anything about how planets form at all.

1.1 The Solar System

Understanding how planets form starts with understanding our own planetary system. The Solar System with the Sun as its central star, its eight planets, numerous moons and minor bodies, is the result of a planet formation process that took place approximately 4.5 billion years ago. Unfortunately, we cannot go back in time and observe what actually happened here then. However what we can do is gather clues to the formation process from its outcome – the Solar System as it is today.

Already in the 18th century, without much more information than the fact that the Sun is in the centre and surrounded by planets, the so-called Nebular hypothesis was formulated; the first parts of it by Swedish scientist and philosopher Emmanuel Swedenborg, and it was later completed by Immanuel Kant and independently by Pierre Simon Laplace. According to this hypothesis, the Sun's atmosphere was once significantly larger before cooling and contracting. From this cooled gas, planets were believed to have condensed and begun orbiting the Sun, driven by the conservation of angular momentum. This early theory laid the groundwork for understanding planet formation as a natural consequence of star formation, forming the basis of modern theories on the origin of planetary systems (Dunér, 2016).

Taking one step further, and looking at the architecture of the Solar System, the planets can be divided into different groups. Closest to the Sun we find the small, terrestrial planets; Mercury, Venus, Earth and Mars, rocky planets with at most a thin gas atmosphere surrounding them. Further out we find giant planets; the gas giants, Jupiter and Saturn, that are dominated by their massive gaseous envelope, and the ice giants, with thinner envelopes surrounding their cores. This distinction between terrestrial planets in the inner Solar System and giant planets in the outer part already suggests that the outcome of planet formation in part depend on the distance from the central star.

However, maybe unintuitively it is the minor bodies in the Solar System that come with the most direct clues to the planet formation process. Recognition of the importance of planetesimals, kilometre-sized or larger planetary building blocks held together by gravity, is often attributed to Viktor Safronov, who published his theory of planetary accretion already in 1969 (Safronov, 1969). The minor bodies in the Solar System, such as asteroids, Kuiper belt objects and comets, are thought to be such remnant planetesimals – planetary building blocks that did not make it into larger bodies. Asteroids are located closer to the Sun, where the number densities are higher and orbital time scales shorter, and therefore they have undergone collisions since their formation, which means that they have been processed and therefore altered since formation (Bottke et al., 2005; Morbidelli et al., 2009). Bodies in the outer Solar System such as Kuiper Belt objects and comets do not have this disadvantage and are believed to have remained primordial since the formation of the Solar System (Gomes et al., 2018). Thus, from a planet formation perspective, these outer bodies are a great source of information. From their sizes and shapes we can draw conclusions about their most likely formation mechanisms (Morbidelli et al., 2009; Johansen et al., 2015; McKinnon et al., 2020). Sending space probes to explore these bodies in detail has given us

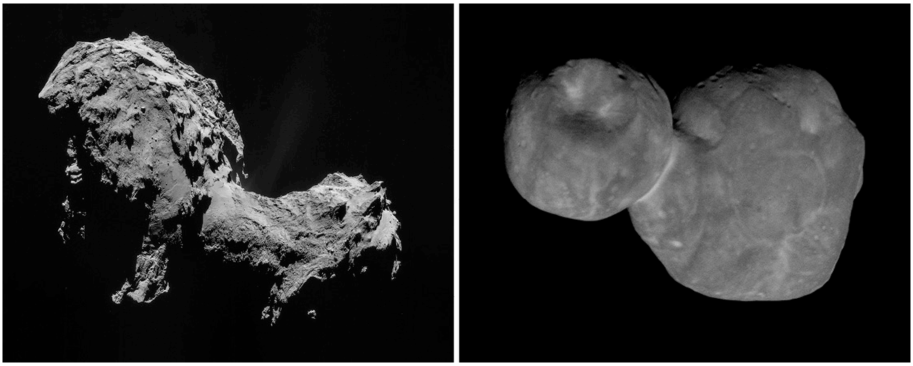

Figure 1.1: Two of the minor bodies, or leftover planetesimals, of the Solar System that have been explored by space probes. **Left:** Comet 67P/Churyumov-Gerasimenko imaged by ESA space probe Rosetta in 2015. **Right:** Kuiper belt object Arrokoth imaged by NASA mission New Horizon in 2019. Credit left image: ESA/Rosetta/MPS. Credit right image: NASA/Johns Hopkins University Applied Physics Laboratory/Southwest Research Institute/National Optical Astronomy Observatory.

information on their composition, and thereby the composition of the dust and ice particles that were present during formation. For example, the results from the ESA space probe Rosetta that visited the comet 67P/Churyumov-Gerasimenko in 2015 showed that it seems to be composed of millimetre-sized to centimetre-sized pebbles and has a porous interior, consistent with formation by a gentle gravitational collapse (Blum et al., 2017). For Kuiper Belt objects, the presence of binaries and contact binaries give clues to planetesimal formation that point in the same direction (Nesvorný et al., 2019).

1.2 Exoplanets

Despite all we can learn from the Solar System, it still has the drawback of being one single planetary system. This makes it difficult – if not impossible – to make generalised theories as we are working with one data point only. It was not until 1995 that the first planet orbiting a solar-type star outside our own Solar system was found, a proof that planet formation has taken place around other stars than our own (Mayor & Queloz, 1995). This first extrasolar planet, or exoplanet in short, was named 51 Pegasi b, a naming convention that tells us both the star it orbits (51 Pegasi) and that it was the first planet discovered around it (b), as we count alphabetically from the star in order of discovery.

This first discovery has since then been followed by many, many more. Nowadays, new exoplanets are routinely being observed, and at the moment of writing this, the count is at over 5600 confirmed exoplanets and rising (see Winn & Fabrycky, 2015, for a review). Even though we are far from having found them all, we can still say with high certainty that exoplanets are about as common as stars in our galaxy (Winn & Fabrycky, 2015). Already this hints as something that is a cornerstone in the context of planet formation – planet formation really does seem to be a natural consequence of star formation, something that we will explore more later on.

Naively, one could have expected that all of these new planetary systems would be mirror worlds of our own. Instead, we have found a rich diversity in planetary system architectures, with types of planets that do not even have counterparts in the Solar System (Batalha et al., 2013). For planet formation purposes, this means that we need to expand the original theories modelled only from our own planetary system, to account also for these new-found exoplanets and the architecture of their systems.

In the Solar System there is a lack of planets in the mass range between the terrestrial planets – Mercury, Venus, Earth and Mars – and the giant planets – Jupiter, Saturn, Uranus and Neptune. This, slightly confusing, fact is however not mirrored by the exoplanet population, where Super-Earths, with a mass of a few Earths, and Sub-Neptunes, just below the mass range of our giant planets, are common.

In exoplanetary systems we also find exoplanets more massive than anything in our own Solar System. One specific example is the so-called Hot Jupiters – giant planets with a mass similar to that of Jupiter, or even higher, but that are in very tight orbits around their host stars. These planets are generally quite rare and make up about 1% of all giant exoplanets, however they are over-represented in exoplanet surveys simply because large planets close to their stars are easier to detect than smaller planets further out in the system (Beleznay & Kunimoto, 2022). Nevertheless, the existence of the Hot Jupiters pose an important constraint on planet formation theories: Since there likely is not enough mass for forming this type of planet where they are presently located, it is likely that they must have migrated through the disc during their formation process (Lin et al., 1996; Kley & Nelson, 2012).

1.3 Protoplanetary discs

Finally, apart from studying the outcomes of planet formation, we can also observe planet formation in action through protoplanetary discs. These are dusty and icy gas discs surrounding young stars, where solids grow to eventually reach planet sizes.

In the last decade, high-resolution observations of protoplanetary discs have been possible with the commissioning of the Atacama Large Millimeter/submillimeter Array (ALMA), resulting in a huge step forward in our understanding of planet formation (Andrews et al., 2018). The amount of information we have been able to gather through such observations is huge, and in this section I will only briefly introduce a few observables that are important for setting the initial conditions for the formation of planets.

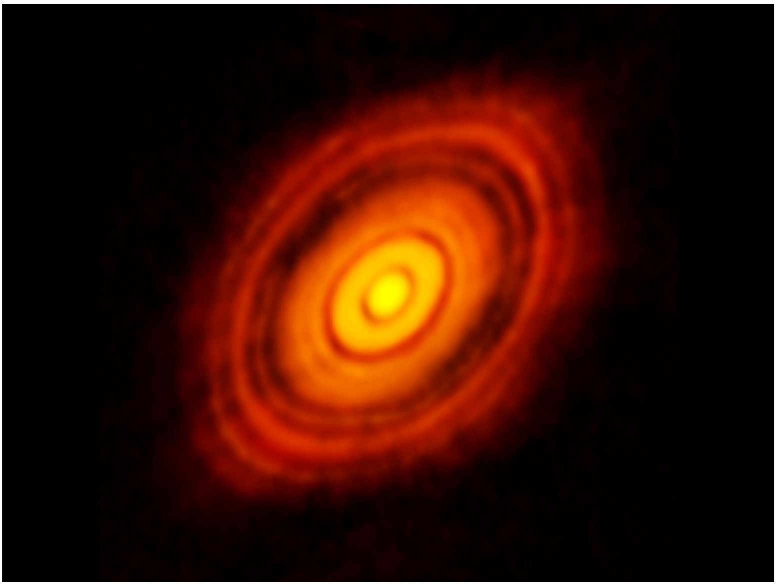

Figure 1.2: The protoplanetary disc surrounding the young star HL Tau as observed by ALMA at a wavelength of 1.3 mm, showcasing several rings and gaps. HL Tau is one of the best studied protoplanetary discs, located in the Taurus star forming region, approximately 140 pc from Earth. The dust disc, which we see in this image, has a radius of approximately 120 au. Credit: ALMA (ESO/NAOJ/NRAO)

A fundamental fact that we need to take into account when modelling planet formation is that their birthplaces, the protoplanetary discs, have limited lifetimes – a fact that places hard time constraints on any process taking place here. The expected disc lifetime is typically estimated by measuring the fraction of stars that are surrounded by discs in active star-forming regions, and places the lifetime somewhere in the range of a few to several million years. Earlier result tended towards shorter values of 2-3 million years (e.g. Haisch et al., 2001), whereas newer estimates with updated selection criteria give values as high as 6-8 million years (Michel et al., 2021).

Furthermore, the amount of solid material in the disc can be constrained by observations. This is important since the solid material makes up terrestrial planets and the cores of giant planets. Disc dust masses are typically estimated from the disc flux at millimetre to centimetre wavelengths and typically result in dust masses of 1-10 Earth masses in the late stages of protoplanetary disc evolution, although much higher dust masses of 50 to several hundred Earth masses in earlier disc stages where the main planetary accretion may occur (Tychoniec et al., 2020).

During the past decade, the view on protoplanetary discs has changed from seeing them as fairly smooth discs to being able to image discs full of substructures on all scales, down to the resolution limit (Andrews et al., 2018). The substructures come in various forms and shapes, displaying rings, gaps and spiral structures. These structures should likely be seen as signs that protoplanetary discs are dynamic structures with various ongoing processes, rather than signposts of one specific physical mechanism. Both underlying physical conditions in the disc, such as locations where volatile material freezes out (Zhang et al., 2015), and ongoing planet formation, has indeed been shown to be able to produce substructures in protoplanetary discs (Walsh et al., 2014; Zhang et al., 2018).

Chapter 2

From dust to planetary building blocks

2.1 Setting the stage for the formation of planets

Even though this thesis is about the formation of planets, we are going to briefly talk about stars as well. The formation of a planetary system is a process tightly intertwined with the formation of its host star, and consists of the build-up of solid bodies from the left-over material that did not make it into the central star. Thus, without the formation of a star we would not have planets. And conversely, when a star forms, there will typically be planets as well.

Star formation takes place in molecular clouds – cold, dark and dense regions of predominantly hydrogen gas and dust in the interstellar medium (ISM). Water is also present in these regions, mostly as ice but in a minor amount also as vapour (e.g. Wirström et al., 2014; van Dishoeck et al., 2021). These molecular clouds are not homogeneous, but instead the material is clustered into denser filaments and regions that we call dark cores – the precursors to stars. As long as the dark core is not too massive, there is a balance between the internal gas pressure of the core that keeps it stable, and gravity that holds it together. However, when the core becomes massive enough, it reaches a tip-over point where its internal gas pressure can no longer support it from collapsing. Gravity wins and the core starts to collapse – a star has started to form. However, before these forming stars have evolved enough for us to actually start calling them stars, we refer to them as young stellar objects.

During the collapse of the core the material is redistributed from a large envelope surrounding a central point, through what we call an accretion disc, and on towards the central protostar. The surrounding envelope is eventually dispersed and most of the mass is concentrated in the forming star, whereas some of the mass in the disc forms a planetary system (Shu et al., 1987). Now, in order to find where the work in this thesis fits in, let us take a closer look at this collapse sequence.

The young stellar objects that are evolving from a collapsing core towards a star and planetary system are typically divided into class 0, I, II, and III, based on observational characteristics (Adams et al., 1987; Lada, 1987; Andre et al., 1993). From an evolutionary perspective, these classes represent different stages in the life of a forming planetary system. In the collapse stage, class 0, the central protostellar object is formed and rapidly grows, embedded in a large gas envelope. From the perspective of planet formation, something very important happens already here in the early stage of class 0: The accretion disc, a disc consisting of gaseous and solid material in orbital motion around the center, forms (Tobin et al., 2012). This accretion disc will be the place of action in this thesis – it is where planets are actually formed, and therefore we typically refer to it as the protoplanetary disc. During class I the envelope is dispersing, and once we enter class II the envelope surrounding the forming star and disc is completely dispersed. We now have a system consisting of a young star and a protoplanetary disc, and this is the stage that I will be focussing on in this thesis – the actual planet formation stage. In the final stage, class III, the accretion disc is essentially gone and we are left with a more or less final system consisting of the central star, surrounded by a so-called debris disc (leftover solid material) and orbited by planets and other solid bodies.

2.2 The protoplanetary disc – the place where planets form

In this section we will look more closely at the birth places of planets, and in particular their characteristics that place some of the constraints we have on the processes of planet formation, from a modelling perspective.

As we saw in the previous section, the material in the disc is inherited from the interstellar medium and reprocessed through the envelope surrounding the star and disc. Therefore the composition of the disc is similar to that of the surrounding space. Most of the disc is gaseous, with the main components being molecular hydrogen (H_2) and helium (He). A smaller component, of the order of 1%, is in solid form, with the material being predominantly submicron-sized silicate and carbonaceous grains formed in supernova explosions and AGB stars (Draine, 2003;

Andersen et al., 2003), and solid ice grains.

As we saw in the previous chapter, some information to be used can be gained from the Solar System, some from observing other planetary systems, and some from observations of current protoplanetary discs, but in the end we need to collect the different bits and pieces together in a model that we can use to make predictions.

There are many ways this can be done, but a classical model is the Minimum Mass Solar Nebula, MMSN in short (Hayashi, 1981). This model is essentially constructed by extrapolating backwards from the present Solar System, and just as the name implies it gives us the minimum amount of material that would have been needed in order to build all the planets that we see orbiting the Sun today. Constructing this model consists of two steps: Firstly, we take the known mass of solids for each planet and add hydrogen and helium to reach solar composition. This, we assume, is the minimum mass that was needed at each planet's location. Secondly, we divide the Solar System into annuli centered at each planet's location and smear the mass found in step 1) over each annulus. And there, we have a model of our planetary system's protoplanetary disc.

The result is not to be seen as a precise initial condition, but rather as a useful standard model that is both easy to understand and works well as a baseline to compare other models and results to. In particular, in this model all solids in the disc are assumed to end up as planets, something which in reality is not very likely. Also, all planets are expected to stay where they were formed, whereas nowadays it is generally accepted that planets migrate through the disc during the late formation stages.

From the MMSN we can extract a total disc mass of $M_{\text{disc}} \approx 0.01\, M_{\odot}$, where $M_{\odot} \approx 2 \times 10^{33}$ g is the solar mass, consistent with observed values. The surface density profile gives us the distribution of mass in the radial direction and can be written as

$$\Sigma(r) = 1700\,\text{g}\,\text{cm}^2 \left(\frac{r}{\text{au}}\right)^{3/2}, \tag{2.1}$$

where 1 au $\approx 1.5\ \times 10^{13}$ cm is the distance between the Earth and the Sun. The temperature profile, with temperature decreasing with the distance from the Sun, can be written as

$$T(r) = 280\,\text{K} \left(\frac{r}{\text{au}}\right)^{-1/2}. \tag{2.2}$$

The sound speed in the disc is a function of temperature, and is given by

$$c_{\rm s} = 9.9 \times 10^4 \, {\rm cm\,s^{-1}} \left(\frac{2.34}{\mu} \frac{T}{280\,K} \right)^{1/2} , \tag{2.3}$$

where $\mu = 3.9 \times 10^{-24}$ g is the mean molecular weight of molecular hydrogen, the most common species in the disc (Nakagawa et al., 1986). Typical discs are thin. The gas scale height gives the distance over which the gas pressure decreases with a factor e and scales as

$$H/r \propto \left(\frac{r}{\rm AU} \right)^{1/4} \tag{2.4}$$

according to the MMSN estimate.

Protoplanetary discs are turbulent, an important characteristic that allows for mixing and interaction between particles. Following Shakura & Sunyaev (1973), the strength of turbulence is typically parameterised by a dimensionless α-value, defined as

$$\nu = \alpha c_{\rm s} H \, , \tag{2.5}$$

where ν is the turbulent viscosity. The α-value can theoretically range from 0, meaning no turbulence, to 1, and can be constrained by different observational methods. Earlier estimates from observations of accretion rates onto young stellar objects indicated a high turbulence with $\alpha \approx 10^{-2}$ (Hartmann et al., 1998). However, newer, more precise methods, suggest lower values of $\alpha \approx 10^{-4} - 10^{-3}$, with agreement between measurements of non-thermal broadening of molecular emission lines (e.g. Flaherty et al., 2017, 2018, 2020) and geometrical arguments from analysing disc scale heights (Pinte et al., 2016), dust ring widths (Dullemond et al., 2018) and disc sizes (Trapman et al., 2020).

2.3 From dust to pebbles

The first step in the growth towards planets, and the step that is the focus of this thesis, is that of sub-micrometre-sized ice and dust grains to pebbles. Pebbles, in the context of planet formation, are approximately millimetre-sized to centimetre-sized particles, better defined by the fact that these sizes are marginally coupled to the surrounding disc gas. In the next subsection we will examine this concept in the context of dust dynamics a bit closer.

Dust dynamics

In order to understand particle growth in the disc, we first need to discuss the dynamics of dust and pebbles, as this governs any interaction that can lead to growth. The dynamic behaviour of these particles is set by their coupling to the turbulent gas via drag forces. We can write the acceleration felt by a solid particle due to drag forces as

$$\dot{\mathbf{v}} = -\frac{1}{\tau_\mathrm{f}}(\mathbf{v} - \mathbf{u}) \,, \tag{2.6}$$

where **v** is the particle velocity and **u** is the local gas velocity. τ_f is the friction time, the time-scale over which the particle decreases its velocity with a factor of e with respect to the gas (Whipple, 1972; Weidenschilling, 1977).

The exact form of the friction time depends on the relation between the particle radius, a, and the mean free path of the gas, λ. The two drag regimes most relevant for dust to pebbles in protoplanetary discs are the Epstein drag regime for $a < (9/4)\lambda$ and Stokes drag regime for $a \geq (9/4)\lambda$ and are given by

$$\tau_\mathrm{f}^\mathrm{E} = \frac{a\rho_\bullet}{c_\mathrm{s}\rho_\mathrm{g}} \tag{2.7}$$

$$\tau_\mathrm{f}^\mathrm{St} = \frac{a\rho_\bullet}{c_\mathrm{s}\rho_\mathrm{g}}\frac{4}{9}\frac{a}{\lambda} \,, \tag{2.8}$$

where a is the radius of a spherical particle, $\rho_\bullet$ the material density, c_s the local sound speed and ρ_g the gas density. In the majority of cases, particles in protoplanetary discs that are in the dust-to-pebbles-growth range will be covered by the Epstein regime.

Typically, friction time is used in its dimensionless form, the dimensionless friction time or the Stokes number,

$$\mathrm{St} = \Omega\tau_\mathrm{f} \,, \tag{2.9}$$

where we have multiplied it with the orbital frequency, Ω, at the position of the particle. Small dust grains thus have low Stokes numbers, $\mathrm{St} \ll 1$ and are strongly coupled to the gas, whereas large bodies have high Stokes numbers $\mathrm{St} \gg 1$ and move independently of the gas motion. Pebbles are loosely defined as particles that are marginally coupled to the gas, which corresponds to Stokes numbers between $10^{-3} - 10^{-2}$ and 1.

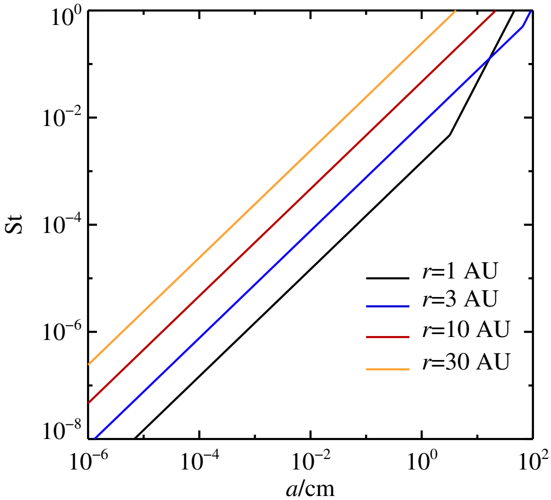

Figure 2.1: Stokes number as a function of particle radius, for spherical, icy particles with $\rho_\bullet \approx 1\,\mathrm{g\,cm^{-3}}$. The colours denote the radial distance from the star. For $r = 1$ au and $r = 3$ au the transition from Epstein to Stokes drag regime can be seen as a change in the slopes towards larger particles.

Dust evolution

The best studied growth mechanism for small particles is by far that of coagulation of silicate dust. Coagulation occurs when particles in the turbulent regions of a disc collide with each other and stick together, and is efficient for small particles with moderate relative velocities. The velocity is set by a combination of Brownian motion (dominant only for the smallest particles), turbulent stirring, sedimentation towards the midplane, and radial and azimuthal drift (Brauer et al., 2008). Particles in the size range of dust to pebbles are not massive enough to stick by gravitational forces, but are instead held together upon collision by contact forces, such as van der Waals forces (Heim et al., 1999; Gundlach et al., 2011).

Both laboratory experiments and numerical simulations show that particles in typical protoplanetary disc conditions quite easily can coagulate up to millimetre-sizes (e.g. Blum & Wurm, 2008). However, for larger particles collisions instead lead to bouncing or fragmentation, which stalls or counteracts growth, typically referred to as the bouncing and fragmentation barriers (Güttler et al., 2010; Zsom et al., 2010).

In addition to bouncing and fragmentation, there is another limitation in that particles drift inwards due to aerodynamic drag – the drift barrier. The orbital motion of the gas disc is slightly sub-Keplerian due to pressure support, as the disc is hotter and denser in the inner regions, leading to a radial pressure gradient directed inwards (Nakagawa et al., 1986). Solid particles therefore face a headwind and lose angular momentum as they orbit the central star. The loss of angular momentum causes these particles to spiral in towards the star (Whipple, 1972; Weidenschilling, 1977). In the inner disc this effect is the most severe for decimetre to metre-sized particles, whereas in the outer regions millimetre to centimetre-sized pebbles are the fastest drifters. Expressed in Stokes number we get the drift time-scale as

$$t_{\text{drift}} = \frac{r}{\mathrm{v}_{\text{drift}}} \approx \frac{100}{\mathrm{St}} \frac{r}{\mathrm{au}} \ \mathrm{yr} \tag{2.10}$$

for particles of $\mathrm{St} \lesssim 1$ in the MMSN (Brauer et al., 2008). This short drift time-scale means that particles are lost to sublimation as they approach the central star before reaching sizes of about a metre, effectively limiting a complete bottom-up growth towards larger sizes, even if we could somehow surpass the bouncing and fragmentation barriers.

Different pathways to stretch coagulation growth to reach larger particle sizes have been explored, but so far none of them have been entirely successful. It has been suggested that growth to larger sizes is possible via mass transfer when a relatively large particle collides with much smaller ones (Windmark et al., 2012; Garaud et al., 2013). However, such growth is slow compared to the disc life time, and growth beyond the bouncing barrier in this scenario have been found unlikely also in later works (Estrada et al., 2016; Booth et al., 2018).

Another possibility that has been explored is the potential of icy particles being stickier than the typically investigated silicate particles. Typically, silicate particles are assumed to stick together up until collisional velocities of about $1\ \mathrm{m\,s^{-1}}$, whereas the larger surface energy of particles covered in water ice might lead to these particles being able to stick up to relative velocities of about $10\,\mathrm{m\,s^{-1}}$, as supported by some experimental work (Wada et al., 2009; Gundlach et al., 2011; Gundlach & Blum, 2015). However, other laboratory experiments suggest that the coagulation efficiencies of ice are instead similar to those typically adopted for silicates (Gundlach et al., 2018; Musiolik & Wurm, 2019). Hence, it seems fair to say that there is not enough experimental evidence to support the statement that icy particles have an advantage over silicates in collisional growth.

It has also been proposed that porous growth, where fluffy ice aggregates collides, could lead to growth to larger particle sizes (Okuzumi et al., 2012; Kataoka et al., 2013). However, in addition to relying on the questionable higher stickiness of ice, such growth is limited by erosion, and more recent models do not find growth past the fragmentation and drift barriers (Krijt et al., 2015; Estrada et al., 2022).

In conclusion, laboratory experiments and computer simulations give robust evidence for bottom-up-growth from dust to millimetre-sized pebbles, however this type of collisional growth is not possible for growth towards larger bodies. To move past the barriers due to bouncing, fragmentation and radial drift, towards planets, other mechanisms are needed.

2.4 From pebbles to planetesimals

After pebbles, the next intermediate step towards planets is the formation of approximately kilometre-sized bodies held together by self-gravity, so-called planetesimals. As we have seen in the previous section, the formation of planetesimals cannot take place by subsequent collisions of smaller particles. Instead, direct growth mechanisms, where the concentration of small particles is large enough to collapse by its own self-gravity, are invoked. These mechanisms have the advantages of not relying on growth past bouncing and fragmentation, and of being fast enough that the radial drift barrier becomes unimportant.

Several ways of concentrating particles enough for a collapse to take place have been suggested and investigated, for example through efficient sedimentation (Goldreich & Ward, 1973) and in turbulent vortices (Cuzzi et al., 2001). However, the former is counteracted by disc turbulence and the latter does not seem to lead to a high enough concentration for planetesimals to form (see Johansen et al., 2014, for a review). The leading, and most studied mechanism, for the formation of planetesimals is instead that of clumping via the streaming instability, which arises from the back-reaction of the dust onto the gas (Youdin & Goodman, 2005; Johansen et al., 2007). In this mechanism, an initially small over-density of dust locally increases the gas orbital motion through drag, and thereby slows down its radial drift, which allows particles radially outside of the clump to catch up with it and increase its density. Streaming instability followed by gravitational collapse holds up well in regards to observations of minor bodies in the Solar System, which are leftover planetesimals from our own past protoplanetary disc – both the size distribution of minor bodies (Morbidelli et al., 2009) and observational properties of the comet 67P/Churyumov-Gerasimenko (Blum et al., 2017), as gathered by the Rosetta mission, are consistent with models of planetesimal formation by the streaming instability.

For the streaming instability to work, a combination of high enough dust-to-gas ratio and large enough Stokes numbers are needed. Clumping is most efficient for a local dust-to-gas ratio above unity, where particles can concentrate further down to even small Stokes numbers of $\mathrm{St} \approx 10^{-3}$ (Youdin & Goodman, 2005). High-resolution simulations performed to analyse under which conditions the streaming instability is active have shown that it can be triggered down to lower local metallicities as well. However, this instead requires higher Stokes numbers in the range of $\mathrm{St} \approx 10^{-1}$ (Carrera et al., 2015; Yang et al., 2017; Li & Youdin, 2021). This means that even though streaming instability is an efficient mechanism for concentrating particles enough for collapse into planetesimals, the right conditions for are not met at all times and all locations in the disc. Rather, this suggests that planetesimal formation is likely not efficient everywhere in protoplanetary disks but instead restricted to localised regions, where formation of planets could be initialised (Drążkowska et al., 2016; Schoonenberg & Ormel, 2017; Drążkowska & Alibert, 2017).

Chapter 3

Particle growth at the water ice line

As we have seen in the previous chapter, growth to planetesimals relies on the solid material in the disc, initially in the form of micrometre-sized dust and ice grains, to both reach pebble-sizes and a high enough solid-to-gas ratio for collapse into planetesimals – something which does not occur simply by collisional growth mechanisms anywhere in the disc. Instead, we need specific sweet spot, where growth and concentration of particles can be boosted. In this chapter I will discuss what is maybe the most promising potential sweet spot: the water ice line, the location in the disc where water vapour condenses out to solid ice.

3.1 Ice lines in protoplanetary discs

An ice line, or more generally, a condensation front, is the distance from the star where the temperature and pressure is such that a volatile species undergoes a phase change from gas to solid form. When I discuss this phase change in general it is referred to as *condensation* in this thesis, following the convention in astrophysics, in contrast to *deposition*, which widely used in atmospheric physics. I will however in later sections use the words *nucleation* and *deposition* to distinguish between the formation of the first ice layer on rock and the subsequent condensation onto an already icy particle. The reverse process, where solids change into gas form, is referred to as *sublimation*.

The concept of condensation fronts relies on temperature and pressure gradients being present in the disc. The thermal properties of the disc are regulated by heating from the central star and viscous heating from the disc itself, with the heating from the central star being the dominating heat source (Mori et al., 2019, 2021). Protoplanetary discs are therefore hotter and denser towards the star and have a temperature decreasing outwards, with the temperature going from $T > 1000\,\mathrm{K}$ in the innermost part of the disc to only tens of Kelvins in the outer regions (Hayashi, 1981). The temperature also varies with height above the midplane. The disc atmosphere is hotter as it is irradiated by the central star, whereas the midplane, to where the stellar light cannot penetrate, is colder (Dullemond & Dominik, 2004). Therefore volatile elements in the disc can be in either solid or vapour form, depending on the radial and vertical distance from the star and the midplane, respectively.

All elements in the disc have specific condensation fronts. Silicates, which makes up most of the rocky material in the disc, condenses out in the very inner parts of the disc, inwards of 1 au (Johansen & Dorn, 2022). Further out we find condensation fronts of more volatile disc species, with water being the innermost one. All ice lines are expected to move radially as the disc evolves and the luminosity of star decreases with time in the early evolution (Martin & Livio, 2012, 2014), however the water ice line is typically assumed located at around $r_{\mathrm{H_2O}} \approx 2 - 3\,\mathrm{au}$, which in the early Solar System corresponds to just inwards of Jupiter (Lecar et al., 2006). Further out in the disc we find the ice lines of the ultravolatile species, with carbon dioxide and carbon monoxide at $r_{\mathrm{CO_2}} \approx 10\,\mathrm{au}$ and $r_{\mathrm{CO}} \approx 30\,\mathrm{au}$, respectively, being two of the most important ones.

3.2 The water ice line in planet formation

In this thesis, I focus on the water ice line, which is the most interesting volatile ice line for planet formation processes, for several reasons. Water is the most abundant volatile element in the protoplanetary disc, allowing the solid density of the disc to double at this location (Hayashi, 1981; Abod et al., 2019). Also, it is the volatile whose ice line is located closest to the star, and thus water is in its solid form throughout a major part of the protoplanetary disc. The location in the inner part of the protoplanetary disc also allows dynamical processes to take place on shorter time-scales than in the outer disc regions.

In the architecture of our own Solar System, we likely see the influence of the water ice line in the fact that the small, rocky planets all are positioned inwards of the water ice line, whereas the giant planets are found farther out. In particular, the position of Jupiter, the most massive planet in the Solar System, is thought to

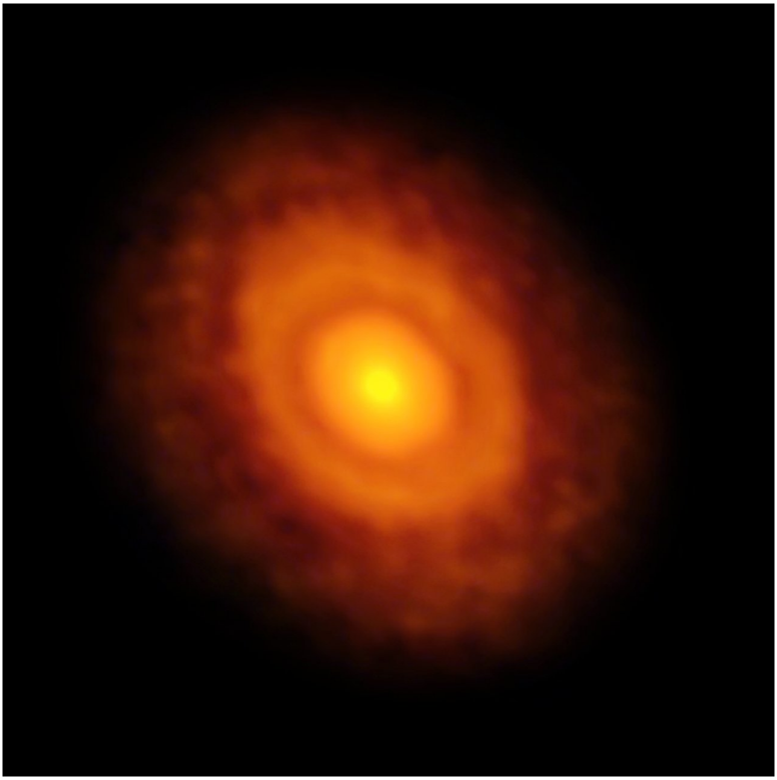

Figure 3.1: The first image of the water ice line in a protoplanetary disc, obtained by ALMA. The disc of V883 Orionis is currently in outburst mode, so that the water ice line has been pushed outwards from the star. The water ice line can be seen as the dark ring surrounding the star midway through the bright disc. Credit: ALMA (ESO/NAOJ/NRAO)/L. Cieza.

be directly linked to the position of the ice line (Stevenson & Lunine, 1988). The water gradient in the bodies making up the asteroid belt is considered a further clue that the ice line was located in this region during the formation period of the system (Pontoppidan et al., 2014). Farther out, the varying amount of CO in comets has been interpreted as to give a formation location around the CO condensation front for these icy bodies (A'Hearn et al., 2012). Similarly, the bulk composition of exoplanets should be a function of their formation location relative to ice lines (Öberg et al., 2011; Madhusudhan et al., 2017).

The water ice line influences particle growth in several ways that can increase planet formation efficiencies. Firstly, as mentioned earlier the solid density outside of the water ice line approximately doubles. This means that planet formation processes can be catalysed, as the number of particle interactions increases, and planetesimal formation by concentration mechanisms such as the streaming instability that require high solid-to-gas ratios is facilitated. Secondly, particle growth close to ice lines can, in addition to by coagulation, also proceed by vapour condensing onto particles (Stevenson & Lunine, 1988). As vapour does not condense out to form new particles under protoplanetary disc conditions (Tielens & Hagen, 1982), but instead condenses onto existing solid material, this can lead to significant growth of particles in sizes from dust to pebbles.

Finally, sublimation and recondensation at ice lines effectively halt the radial particle drift inwards. Radial drift is highly dependent on particle size, with the fastest drift occurring for particles of $\mathrm{St} \approx 1$. When the size of the particle significantly decreases at an ice line particle drift is thus slowed down and we instead get a pile-up of material around the ice line (Cuzzi & Zahnle, 2004; Ida & Guillot, 2016).

In the following sections I will focus on particle growth due to condensation and related processes, highlighting the most important results from my research.

3.3 Particle growth by condensation

In 2013, when Paper I was published, particle growth by coagulation had already been studied extensively, both in laboratory experiments and computer simulations. However, condensation as a growth mechanism was largely overlooked. Earlier works, in particular those by Stevenson & Lunine (1988) and Cuzzi & Zahnle (2004), had pointed out the potential of ice condensation, but not investigated the mechanism in full detail. Our aim for Paper I thus became to isolate condensation at the water ice line as a growth mechanism, while taking detailed particle dynamics into account, in order to qualitatively understand the importance of condensation for dust growth.

The mechanism can be outlined as follows. Around the ice line, turbulent diffusion of vapour and small particles and radial drift of solids allow water to cross the ice line and enable interaction between vapour and solids. When icy particles cross the ice line towards the star, they sublimate. Some of the resulting water vapour then diffuses back into the colder, outer region and condenses onto already existing particles, which then grow larger.

The mass change of a particle subjected only to condensation and sublimation can be written as

$$\frac{\mathrm{d}m}{\mathrm{d}t} = 4\pi a^2 v_{\mathrm{th}} \rho_{\mathrm{v}} \left(1 - \frac{P_{\mathrm{sat}}}{P_{\mathrm{v}}}\right) \tag{3.1}$$

(Supulver & Lin, 2000). The particle radius is denoted by a, the thermal velocity of vapour by v_{th}, the vapour density by ρ_{v} and the saturated vapour pressure and the vapour pressure by P_{sat} and P_{v}, respectively. This equation can be rewritten using vapour densities instead of pressures. By using the ideal gas law we find

$$P_{\mathrm{sat}} = \frac{k_{\mathrm{B}} T}{m_{\mathrm{v}}} \rho_{\mathrm{sat}},\ P_{\mathrm{v}} = \frac{k_{\mathrm{B}} T}{m_{\mathrm{v}}} \rho_{\mathrm{v}}, \tag{3.2}$$

with k_{B} being the Boltzmann constant, T the temperature and m_{v} the mass of one vapour particle. We can thus rewrite Eq. 3.1 as

$$\frac{\mathrm{d}a}{\mathrm{d}t} = \frac{v_{\mathrm{th}}}{\rho_{\bullet}} \left(\rho_{\mathrm{v}} - \rho_{\mathrm{sat}}\right), \tag{3.3}$$

where $\rho_{\bullet} \approx 1\,\mathrm{g\,cm^{-3}}$ is the material density of ice and we have assumed spherical ice particles. From this we can recover the condensation and sublimation time-scales. When $\rho_{\mathrm{v}} \ll \rho_{\mathrm{sat}}$ sublimation dominates, and we can write the sublimation time-scale as

$$\tau_{\mathrm{s}} = \frac{a \rho_{\bullet}}{v_{\mathrm{th}} \rho_{\mathrm{sat}}}. \tag{3.4}$$

Conversely, condensation dominates when $\rho_{\mathrm{v}} \gg \rho_{\mathrm{sat}}$, with a condensation time-scale of

$$\tau_{\mathrm{c}} = \frac{a \rho_{\bullet}}{v_{\mathrm{th}} \rho_{\mathrm{v}}}. \tag{3.5}$$

We modelled particle motions in a disc as composed by several different contributions. Small particles are completely coupled to the turbulent gas via drag forces and thus move in a turbulent diffusion. For larger particles, additional effects need to be taken into account. As particles grow, they decouple from the background gas motions. Additionally, gravity becomes more important as particles grow larger, letting particles of approximately millimetre-sizes sediment towards the mid-plane. In the radial direction, larger particles drift inwards due to the velocity difference with the slightly sub-Keplerian orbiting gas. In our simulations, we modelled this as a random walk mimicking turbulent motions, adding size-dependent effects as additional terms.

The main result of Paper I was the finding that condensation alone can be responsible for growth from dust to pebbles. The time-scale of this process is short compared to the life-time of the disc, with pebbles forming within $t \approx 10^4$ yr for a turbulent disc with $\alpha = 10^{-2}$ and within $t \approx 10^5$ yr for a disc with a lower turbulence level with $\alpha = 10^{-5}$. The resulting particle sizes are large enough (on the order of centimetres) to initiate streaming instabilities and thereby lead to planetesimal formation. We did not in this work investigate if the resulting solid-to-gas ratio is high enough for this process. However, both Schoonenberg & Ormel (2017) and Drążkowska & Alibert (2017) modelled particle growth at the water ice line, including growth by condensation, and found an increased local metallicity that could trigger the streaming instability.

3.4 Nucleation – vapour prefers ice over rock

From atmospheric physics it is known that water vapour does not condense out equally easily on rocky particles as on those that already have an icy mantle. This has however been ignored in astrophysical models, including in our Paper I.

To model condensation properly we need to make a distinction between *nucleation* and *deposition*, where nucleation is the formation of the first icy layer on a rocky seed particle and deposition is the continued vapour condensation on the now icy particle. Including this distinction in a model of particle growth by condensation at the water ice line was our aim for Paper II. By doing this, we also address the question of whether including the large amount of rocky dust present at the ice line would hinder growth, something that we did not explore in Paper I.

Nucleation can be described by classical nucleation theory (CNT; Vehkamäki, 2006), and experiments performed to understand ice clouds in the Martian atmosphere confirm the theoretical prediction that the formation of a new ice layer on a silicate surface requires a substantially higher water vapour pressure than the deposition of water vapour on an existing ice surface (Iraci et al., 2010). In Paper II we used these experimental results, which cover a temperature and pressure range relevant also for protoplanetary discs, in order to understand the impact of nucleation on particle growth at the water ice line.

In our model, we therefore implement a critical saturation ratio (S) for deposition and nucleation, where

$$S = \frac{P_{\rm v}}{P_{\rm sat}} \,. \tag{3.6}$$

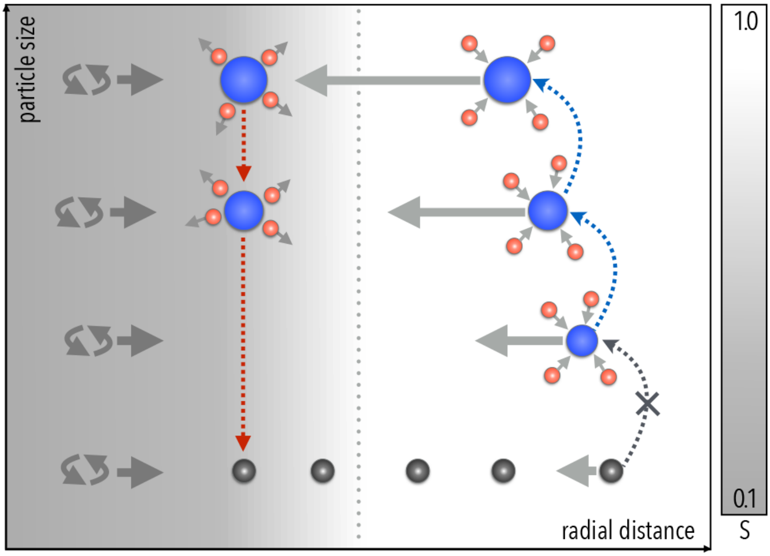

Figure 3.2: Sketch of the physical processes included in the model in Paper II. Ice-covered particles (blue) grow by the deposition of vapour (red) in a region where the saturation ratio is unity. Ice particles crossing into a region where the saturation ratio is lower than unity sublimate and, if they stay in this region long enough, eventually leave behind their silicate cores (grey) in addition to the sublimated vapour. Bare dust grains cannot acquire a new ice mantle since the saturation ratio does not reach the critical saturation ratio required for nucleation. Dynamical processes are represented by grey arrows, with the left-directed arrows representing the size-dependent radial drift, and the arrows pointing to the right representing the outwards-directed part of the turbulent diffusion.

For deposition

$$S_{\text{crit,dep}} = 1 \,, \tag{3.7}$$

meaning that as soon as we reach super-saturation vapour condenses out on icy particles. For nucleation we use the experimentally found temperature-dependent critical saturation ratio of

$$S_{\text{crit,nuc}} = -0.0026\,T + 13.0 \tag{3.8}$$

as found by Iraci et al. (2010). Thus, nucleation needs a substantially higher super-saturation than deposition in order to occur.

This reflects clearly on the results in our paper: When we include both rocky and icy particles in our model, but ignore the different saturation ratios needed for nucleation and deposition, growth is inhibited. A large amount of particles grow, but only by a minor amount each, resulting in a sea of ice-covered micrometre-sized dust grains. However, when we do include the distinction between nucleation and deposition, we find growth to larger particles, with icy pebbles of several centimetres in size in the region just outside the ice line. Meanwhile, the silicate dust stays small and diffuse out over the disc. The reason for the larger sizes in this case is that only the fraction of particles that nucleates can grow, and thereby the available vapour is shared amongst fewer particles, and not by all the small dust grains. Including nucleation in our model, we thus recover the potential of the ice line as being beneficial for growth to larger sizes than elsewhere in the disc, also when we account for the rocky dust present in the disc.

3.5 The outcome of sublimation

So far, I have discussed what happens when vapour condenses into ice, but ignored the details of the opposite process: sublimation of ice into vapour. However, pebbles at the water ice line are composed of both ice and rock, meaning that even though the icy part sublimates, solids remain. Whether or not the remaining solid part is a mostly intact aggregate, or if it instead disrupts into smaller dust particles when the icy component sublimates is however not yet clear. Several theoretical studies have assumed disruption of the aggregates, with the underlying assumption that sublimation of the ice content is breaking the adhesion forces between dust grains inside the pebble. This might lead to pile-up of small silicate particles interior of the ice line, which can aid planetesimal formation (Saito & Sirono, 2011; Ida & Guillot, 2016). Schoonenberg & Ormel (2017) modelled both a scenario where pebbles disrupt, and a scenario in which they stay intact, and also found a larger pile-up of silicates when disruption of pebbles was assumed, than when they remained intact.

Since the outcome of sublimation matters for how we model particle growth around the ice line we need a better understanding of sublimation of icy aggregates. Aumatell & Wurm (2011) experimentally investigated the disruption of condensed ice crystals by sublimation and found that these fluffy aggregates disrupted when going through fast sublimation. However, as these experiments did not include dust grains it is difficult to draw any conclusions from this. In Paper III, we therefore set out to investigate the sublimation of pebbles consisting of

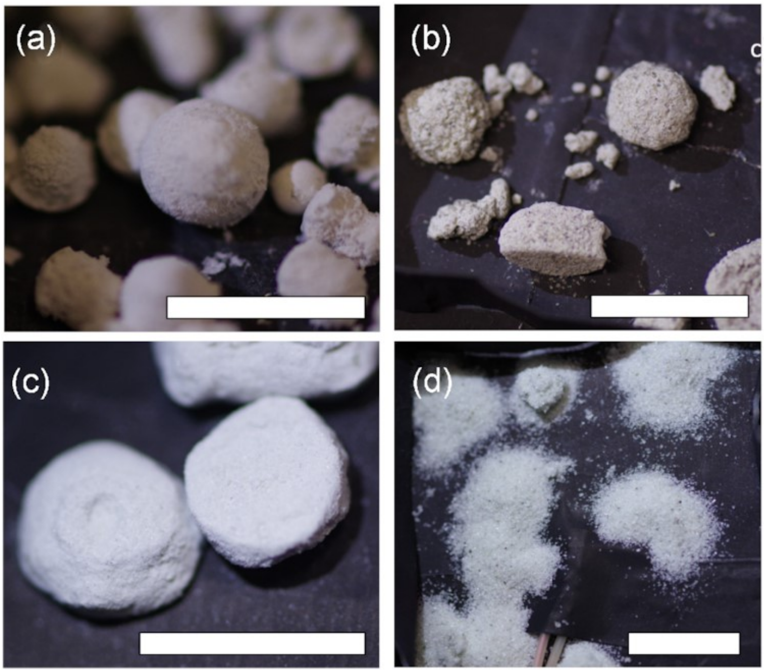

Figure 3.3: Different outcomes of the experiment: Pebbles can preserve their 3D shape or disrupt in piles of dust. (a) Preserved olivine pebble with high ice-content and small grain sizes. (b) Preserved pyroxene pebble with low ice content and medium-sized dust. (c) Preserved olivine pebble with low ice content and medium-sized dust. (d) Disrupted pyroxene pebble with low ice content and coarse dust. All scale bars are adjusted to be 1 cm. Figure from Paper III, reproduced with permission.

ice and different types of silicate dust.

To do this, we developed two different types of icy pebbles using different silicate dusts, and exposed them to low-temperature and low-pressure conditions in a vacuum chamber. We then studied the conditions for which pebbles are preserved through sublimation without disrupting, while increasing the temperature in the chamber. In contrast to previous studies, we found that pebbles can survive sublimation relatively intact. This is in agreement with recent ALMA observations of the protoplanetary disc of V883 Ori, where the observed spectral indices indicate that pebbles stay intact through sublimation (Houge et al., 2024). Our results also showed that the composition of the pebbles matter for their survival chances. Pebbles with a high ice content (50% in mass) survive sublimation better than low-ice-pebbles (15%). Finally, the sizes of the dust particles that make up the pebbles matter as well, with aggregates consisting of dust particles smaller than 50 μm having a better chance of surviving sublimation intact than aggregates of larger dust particles.

3.6 Condensation growth after accretion outbursts

In most works of dust growth around ice lines, a static ice line position is assumed, since the overall radial shifting of the ice line is slow compared to particle growth time scales. However, young stars are also thought to undergo frequent accretion outbursts, such as FU Orionis outbursts, that heats a substantial part of the disc, leading to much more dramatic ice line shifts. These outbursts have cooling time scales of the order of $100 - 1000$ yr and affect large parts of the disc, moving the ice line outwards several to tens of astronomical units. This effectively resets the particle distribution as the ice sublimates all the way out to the outburst ice line. This has been observed through ALMA observations of dust emission in the case of the outbursting protoplanetary disc V8883 Ori, where the ice line was found to have been shifted outwards to 42 au (Cieza et al., 2016).

As the ice line moves back inwards on the cooling time scale particle growth can again resume by nucleation and subsequent deposition of vapour, and through collisions. Collisional growth, with the assumption of instantaneous redistribution of vapour on particles, after an outburst have been modelled by Houge & Krijt (2023), who found that a fragmentation-coagulation equilibrium is restored after a few thousand years at the original ice line location. In Paper IV, we took the opposite approach of isolating the mechanisms of nucleation and deposition, in order to understand how these vapour-dependent mechanisms would impact the particle distribution after an outburst.

We modelled a disc with two different cooling times $t_{\rm cool} = 100$ yr and $t_{\rm cool} = 1000$ yr, corresponding to typical time scales for FU Orionis outbursts. These cooling time scales are short enough that the dynamics of dust and vapour are not very important, however long enough for nucleation to be a rare event that allows only a subset of particles to grow.

We found that the cooling time scale does matter for the resulting particle sizes. Fast cooling results in high super-saturation levels at the ice line, which leads to high nucleation rates and therefore limited condensation growth since the main ice budget is spent in the nucleation. This means that the resulting particle sizes

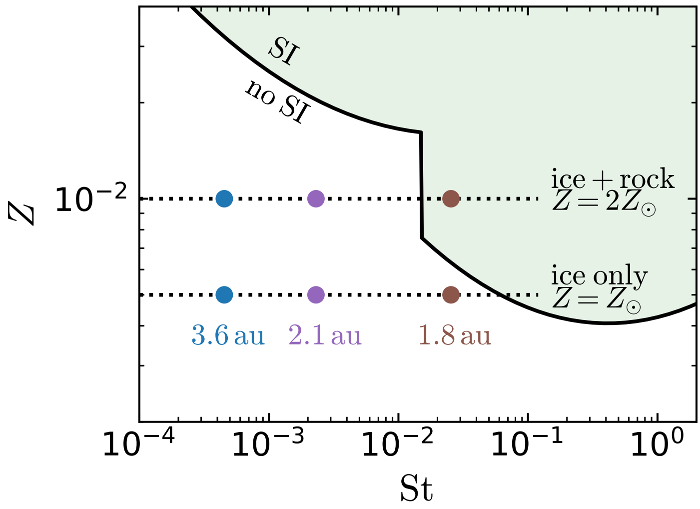

Figure 3.4: Threshold for particle clumping via the streaming instability for different particle stopping times and metallicities, from Li & Youdin (2021). The green area in the upper right part denotes the parameter space where clumping via streaming instability is possible. The filled coloured circles is data from Paper IV for different disc locations with a cooling time of tcool = 100 yr. The lower row corresponds to a solar metallicity disc where the interacting solids are made of ice, whereas the upper row is either a high-metallicity disc or a disc with solar metallicity where both ice and rock contributes to clumping.

are smaller. Slow cooling of on the other hand, leads to rare ice nucleation and efficient growth of ice-nucleated particles by subsequent deposition.

However, the main result from Paper IV was that the redistribution of vapour after an outburst indeed can lead to growth of large pebble-sized icy particles within only a few years, with sizes of several centimetres, for both time scales that we modelled. Interestingly, the resulting Stokes numbers of $\mathrm{St} = 0.01 - 0.02$ are high enough to trigger streaming instabilities in a disc with solar metallicity and low turbulence, when both ice and rocky material contributes to the clumping.

3.7 Conclusions

In conclusion, the work done in this thesis demonstrates that condensation at the water ice line is a robust growth mechanism for dust-sized to pebble-sized particles. We have explored this mechanism in both quiescent discs, and in discs cooling down after accretion outbursts, and find in both cases that particle growth to pebble-sizes is possible. Our experimental results indicate that icy pebbles can survive sublimation relatively intact, as opposed to disintegrating upon passing the ice line. We have also showed that nucleation is important to take into account, as it allows icy particles to grow to larger sizes, while the rocky dust present in the disc stays small. Although we have not fully investigated how condensation growth impacts the dust-to-gas ratio at the ice line, our results indicate that the resulting local metallicity in combination with large resulting pebble sizes could be high enough to trigger the streaming instability and lead to growth to planetesimals. The ice line thus seems to be a promising location for growth towards planets to be initiated.

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Part II

Scientific Publications

Author contributions

In this section, I give a summary of my contribution to each of the papers included in this thesis.

Paper I

Ice condensation as a planet formation mechanism
K. Ros and A. Johansen
Astronomy & Astrophysics, Volume 552, 2013

The original idea for this paper was proposed by Anders Johansen (AJ), and subsequently developed by me and AJ together. I wrote the original code, conducted and analysed the computer simulations, produced the plots for the study, and wrote the final paper.

Paper II

Effect of nucleation on icy pebble growth in protoplanetary discs
K. Ros, A. Johansen, I. Riipinen, and D. Schlesinger
Astronomy & Astrophysics, Volume 629, 2019

The original idea for this paper was developed by me and AJ. Ilona Riipinen and Daniel Schlesinger (DS) provided valuable and participated in discussions related ice nucleation and classical nucleation theory from a non-astronomy perspective. The code is mainly written by AJ, with smaller contributions from me. I ran and analysed the computer simulations, produced the plots and wrote the main part of the paper, while AJ and DS led the writing of the appendices.

Paper III

The fate of icy pebbles undergoing sublimation in protoplanetary discs
S. Spadaccia, H. L. Capelo, A. Pommerol, P. Schuetz, Y. Alibert, **K. Ros**, and N. Thomas
Monthly Notices of the Royal Astronomical Society, Volume 509, 2022

The collaboration for this paper originated from a research visit in 2019 to the group of Holly L. Capelo at Bern University, which includes the first author of this paper, Stefano Spadaccia. My contribution to the paper primarily involves providing insights into sublimation calculations relevant for protoplanetary discs in the discussion section. Additionally, I contributed to general discussions and provided comments on the manuscript.

Paper IV

Fast formation of large ice pebbles after FU Orionis outbursts
K. Ros and A. Johansen
Submitted to Astronomy & Astrophysics, under review

The original idea for this paper was developed by me and AJ. AJ wrote the code and ran the computer simulations, and the plots are produced by me and AJ. I analysed the computer simulations and wrote the final paper.

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