Project D2:

Origin of complex non-axisymmetric structures in type 2 transition disks

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Check if all are part of the proposal. Links to other projects.

Requested positions: 1 Postdoc

Abstract:
Transition disks have recently been shown to display spectacular structures such as large scale spirals, blobs, tilts etc. These features indicate that highly dynamic processes are going on in these disks, allowing us to test our understanding of the physics of protoplanetary disks. This project aims to understand these structures in terms of dynamic models of disks.

1. State of the art and preliminary work

With the spectacular new capabilities of observatories in the millimeter wavelength range (ALMA) and at optical wavelengths (Subaru and VLT coronographic imagers, most recently: VLT-SPHERE), protoplanetary disks are found to be much more complex than previously thought. Until only a few years ago observations of protoplanetary disks were consistent with the idea of them being mostly axi-symmetric rotating structures around young stars.

Recent observations have now shown this picture to be false, in particular for transition disks. Many such disks, while remarkable in their own right due to their large inner holes (see project **D1**), are even more remarkable due to their often-present strong deviations from axisymmetry. At millimeter wavelengths, spatially resolved with ALMA, all transition disks show a strong dust emission ring just beyond the inner hole. Several of them, in particular the sources HD 142527 and Oph IRS 48, show this ring to be strongly lopsided: one side being clearly much brighter than the other side (Casassus et al. 2013; van der Marel et al. 2013). These appear to be vortices created by the Rossby wave instability (Regály et al. 2012). This raises the exciting possibility that these are *dust-trapping vortices*, predicted to play an important role in planet formation (Barge & Sommeria 1995; Klahr & Henning 1997).

At optical and near infrared wavelengths many of these sources show another remarkable and unexpected feature: grand design spiral waves (e.g. the sources HD 135344b, MWC 758, HD 100453). While $m = 1$ spiral waves were expected as a result of newborn planets embedded in these disks, the spirals observed in many Type 2 transition disks are symmetric $m = 2$ modes, making them look like the galaxy M51. The origin of these spirals is still hotly debated and planetary/stellar companions (Dong et al. 2016) and gravitational instabilities (Tomida et al. 2016) are often suggested to be at their origin, as is residual infall into the disk (Lesur et al. 2015). Recently an even more unorthodox and intriguing scenario was proposed: The bright ring of scattered light (the illuminated inner rim of the outer disk as seen with the Subaru and VLT telescopes) of HD 142527 has two conspicuous dark spots on almost opposite sides. Marino et al. (2015) were able to show with 3-D radiative transfer modeling that these dark spots are most likely the shadows cast by an inclined small inner disk. If this scenario is confirmed, HD 142527 (and possibly HD 100453 and other transition disks) is an "inclined disk inside a disk" (a warped disk). According to Montesinos et al. (2016) these two shadows on opposite sides of the bright rim may even be the origin of the $m = 2$ spiral waves, caused by the brief loss of pressure in these shadows. This is an intriguing possibility, as it would indicate that Type 2 transition disks may be related to warped disks, and perhaps be the origin of the misalignment effects seen in many exoplanetary systems with the Rossiter-Mclaughlin effect.

But how can the inner disk have a different rotation axis as the outer one? Is this a result of an inclined planet or brown dwarf orbiting inside the gap? For HD142527 a companion star is known to exist, but it is at the current epoch still rather close to the main star compared to the size of the cavity, so it is not directly clear that this companion is responsible for the large cavity. Or is this due to late accretion of different angular momentum molecular cloud material? Thies et al. (2011) suggest this scenario to explain misaligned exoplanetary systems. It might also explain misaligned outer disks. Or could the Kozai-mechanism caused by a companion at large radii cause this?

These enigmatic non-axisymmetries in Type 2 TDs offer a unique opportunity to test our understanding of the physical processes occurring in these disks. The features appear to be highly organized, not random. This suggests that a strong and well-defined physical mechanism is at work. If we identify this mechanism (or these mechanisms), we do not only solve the mystery of these non-axisymmetric features, but also get a better understanding of the dominant physical processes at work in these disks. It is hoped that this may allow us to get a better understanding of the process of planet formation. For instance, several attempts have been made to explain the spiral structures by embedded planets (Muto et al. 2012; Benisty et al. 2015; Pohl et al. 2015), though it turns out that planetary spiral features are usually single-armed ($m = 1$) instead of the double-armed ($m = 2$) spirals often seen. Also the giant central cavity of Type 2 TDs were investigated in the context of gap-opening planets, though it turns out that this is not easy and requires at least multiple planets to work (Zhu et al. 2011). The bright dust rings with often lopsided geometry seen in Type 2 TDs strongly suggest dust trapping at work. These rings are consistent with the radial dust trapping suggested by Whipple (1972), and the lopsidedness appears to be a result of dust trapping in a huge vortex (Barge & Sommeria 1995; Klahr & Henning 1997; Birnstiel et al. 2013; Ataiee et al. 2013; Zhu & Stone 2014; Baruteau & Zhu 2016). What is the origin of these dust traps remains unsolved. Regály et al. (2012) suggest that this is a result of a change in viscosity in the disk at the outer edge of the “dead zone”. They find not only a strong ring-shaped pressure bump forming (which can trap dust), but they see this ring also periodically becoming lopsided by forming a giant anti-cyclonic vortex. The formation of such vortices was first reported by Lovelace et al. (1999), and it seems that with Type 2 TDs we now see evidence for their existence. Given that dust tends to get trapped in these vortices, an exciting question is whether these vortices are the birthplaces of new planets.

The goal of this proposal is to attemp to understand the non-axisymmetric features in Type 2 TDs from the perspective of gas dynamics. Particular emphasis will be put on “non-standard” dynamics such as out-of-plane companions, secondary infall and shadow-driven dynamics. Ultimately we wish to find out if Type 2 TDs are oddballs or not, and if they teach us something about the formation of planets or are too exotic to do so.

1.1 Preliminary work

As a preparation for this project we have conducted several small preliminary investigations in the context of Bachelor projects. We are also involved in several collaborations involving VLT-SPHERE scattered light images of Type 2 TDs as well as ALMA observations.

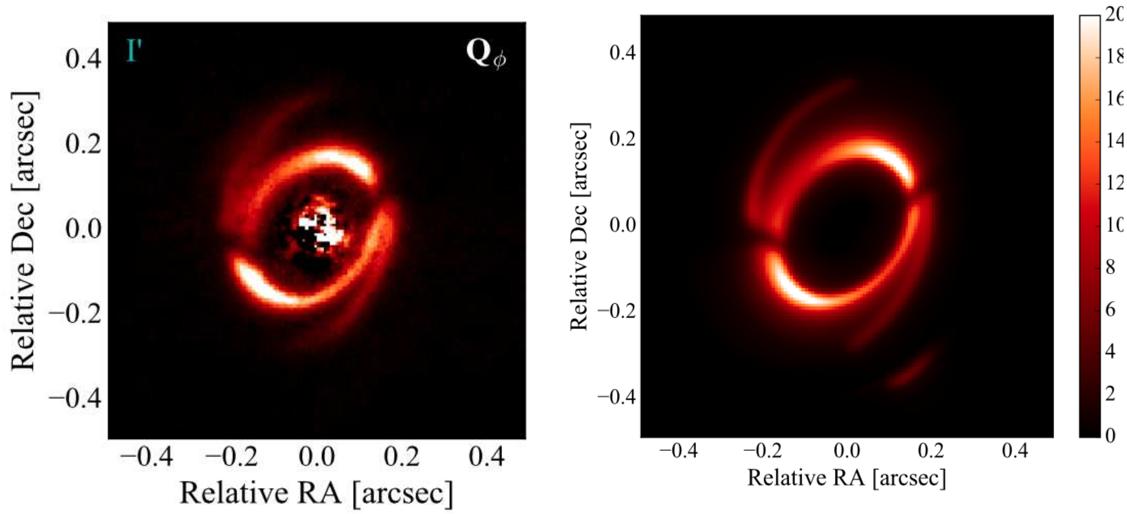

Figure 1: Polarized scattered light observations of the Type 2 TD HD100453. **Left:** Actual observations with VLT-SPHERE in the I' band. **Right:** Synthetic model image made with the MCMax Monte Carlo code. From: Benisty et al. (2016).

1.1.1 VLT-SPHERE observations of Type 2 TDs

Th. Henning, one of the collaborators on this project, is involved in VLT-SPHERE scattered light image observations of Type 2 TDs. A particularly spectacular example, where the PI was also involved in, is the very recent image of the Type 2 TD HD 100453 (Benisty et al. 2016). This is a Transition Disk with an inner disk spanning out to 1 AU, and an outer disk spanning between 20 AU and 45 AU. It features a prominent $m = 2$ spiral pattern originating from a bright ring that features two bright arcs (presumably due to the scattering phase function) and two dark spots (presumably due to the shadowing caused by an inclined inner disk, as in HD 142527 (Marino et al. 2015)). The observed polarized intensity and the synthetic model image are shown in Fig. 1. The synthetic image was made with the MCMax radiative transfer code, and the setup involved in tilted inner disk that produced the shadow features on the ring, and parameterized spiral features.

1.1.2 ALMA observations of Type 2 TDs

Dr. Akimasa Kataoka has been a postdoc at the ITA since April 2015 on his own JSPS-Fellowship grant. During this period he successfully applied for substantial ALMA time to observe the Type 2 TD source HD 142527 using the newly available polarization mode. The observations we obtained have turned out to be quite spectacular (Fig. 2). The strongly lopsided arc-shaped dust emission was already well known since (Casassus et al. 2013). But the shape of the polarized light image contains a huge amount of additional information. Please note that it is not the purpose of this project to investigate how to use this new technique of polarized thermal emission at millimeter wavelengths. This is the topic of another – completely separate – DFG proposal that was submitted in the summer of 2016 (DFG DU 414/17-1). Here we merely show the kind of objects we study and the type of observations we are involved in, which will (in addition to published data from other groups) serve as observational evidence for the complex disk geometries seen in Type 2 TDs.

The PI has also been involved in an ALMA observational study of the source IRS 48 from the team of Ewine van Dishoeck, where an even stronger lopsided dust emission was found (van der Marel et al. 2013).

The PI and collaborators on this project are continuing involvement (and leading) of such observa-

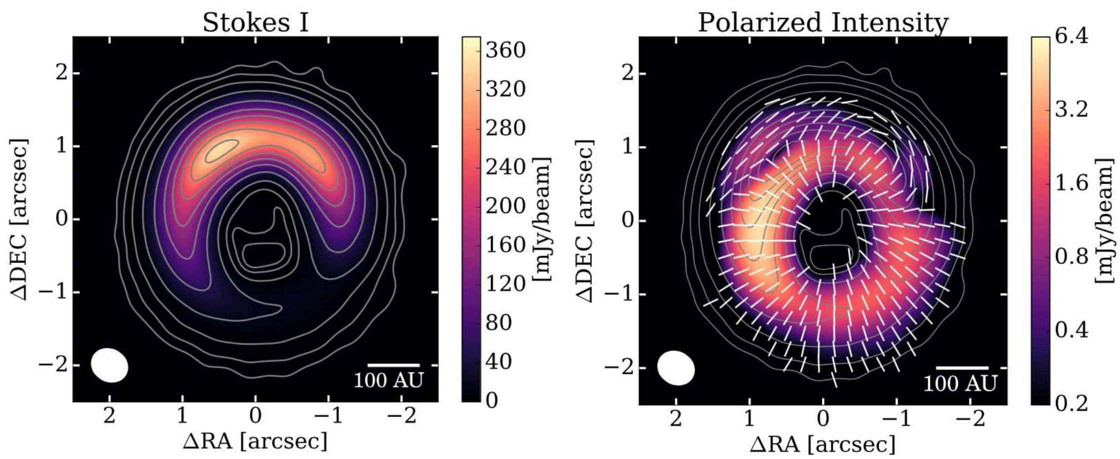

Figure 2: ALMA Observations of the Type 2 TD HD 142527. **Left:** The continuum (Stokes I component) at 850 μm showing the well known arc-shaped structure believed to be dust trapped in a Rossby-vortex. **Right:** The polarized intensity with the polarized direction overlayed. From: Kataoka et al. (2016).

tional campaigns.

1.1.3 Preliminary models of out-of-plane companion-disk interaction

Out-of-plane planet disk interaction models have been made by Bitsch & Kley (2011) and Bitsch et al. (2013) using a fully 3-D radiation hydrodynamics grid-based code. The focus here was on intermediate mass planets inducing moderate disk warps, and the aim was to understand inclination damping and migration. Other work include Xiang-Gruess & Papaloizou (2013) who employ a Smooth Particle Hydrodynamics code to study the effect of such an inclined companion on the disk structure, and back on the planet. Also here the planet mass was intermediate and the induced warps were moderate.

For the present purpose we need to go to more extreme cases: higher inclinations, higher planet masses, and focusing on the change of the appearance of the disk shape to be able to compare this with observed Type 2 TDs.

As a preliminary test case for such modelling, we performed a set of simple models using the Smooth Particle Hydrodynamics code Gadget-2. We set up an initially smooth planar disk, but add a low mass companion on an inclined circular orbit. The orbit crosses the disk twice each orbital period. The results of one such model is shown in Fig. 3. As time passes by, this process opens up a strong gap in the disk. The gravitational torque of the planet on the inner and outer disk, however, cause both to precess. The inner disk precesses faster than the outer disk. As a result, the inner and outer disks become tilted with respect to each other (they are no longer co-planar). The “warp” can be seen in all three panels of Fig. 3, but the tilt between inner and outer disk is only seen in the middle panel, which is a snapshot at 50000 years. This model was initially set up by Dr. Daniel Harsono and further developed and applied by Matthew Herbst during his Bachelor thesis project. These results show that for a brief period the inclined companion can lead to tilted inner/outer disks, but eventually the outer disk aligns with the plane of the planetary orbit, and the inner disk disappears by viscous accretion. This viscous accretion appears to be strongly boosted by excessive numerical viscosity due to too few SPH particles. This excessive viscous accretion also appears to be the cause of the very bright outer disk ring. This is presumably not realistic, so this simulation can merely serve as a proof-of-concept. Much higher resolution models have to be made, with more careful testing of the viscosity of the model.

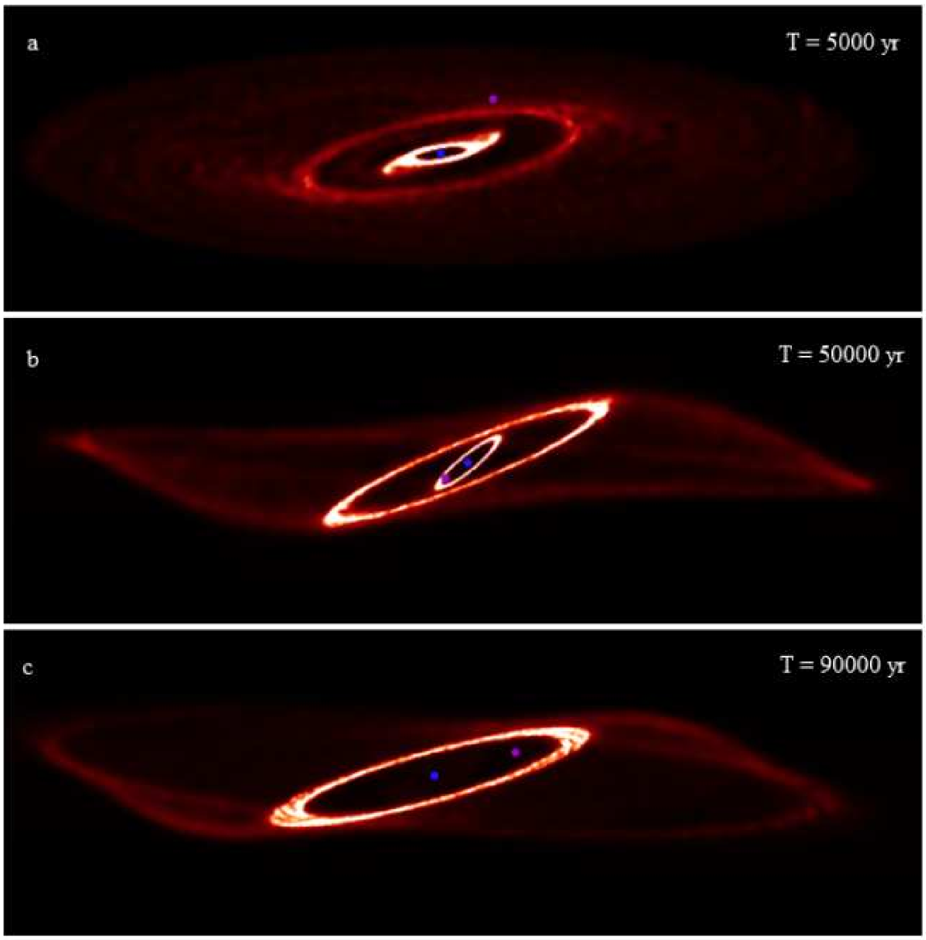

Figure 3: Time snapshots of the shape of a circumstellar disk disrupted by an inclined planetary companion passing through the disk twice each orbit. The star is blue, the planet is purple. The gas SPH particles are shown in shades of red (low column density) and yellow (high column density). The star has a solar mass. The planet orbital inclination is 33 degrees, the semi-major axis 40 AU, the mass 0.01 $M_{\odot}$. The disk is initially 200 AU in radius and has a mass of 0.01 $M_{\odot}$. The surface density is shown as a projection with respect to a camera. The angle of the camera is not the same in each snapshot, but chosen such that the warp in the disk is better seen. From: Bachelor Thesis by Matthew Herbst, Heidelberg University, 2016.

1.1.4 Preliminary models of secondary disk formation

As a proof of concept for the secondary accretion of material from a low mass molecular cloudlet we performed a simple set of grid-based numerical hydrodynamic models. The model setup is a rectangular grid of $256 \times 256 \times 64$ cells covering $10 \times 10 \times 2.5$ kAU (one kAU = 1000 AU). The initial cloud setup is a simple Gaussian shaped spherical cloud:

$$\rho(\mathbf{r}) = \rho_0 + (\rho_1 - \rho_0) \exp\left(-\frac{|\mathbf{r}-\mathbf{r}_{\rm cl}|^2}{2D_{\rm cl}^2}\right) \tag{1}$$

where ρ_0 is the background density, ρ_1 is the initial peak density at the cloud center, $\mathbf{r}_{\rm cl}$ is the initial location of the cloud and $D_{\rm cl}$ is the cloud initial size. The temperature is kept constant at all times and locations, such that the sound speed is 1 km/s. The gas velocity at all locations in the grid is initially the same everywhere, but will of course change due to the gravitational pull of the star and the hydrodynamics of the gas. The star is kept at a fixed location $\mathbf{r}_*$ at the center of the box, and the cloud motion has a non-zero impact parameter b with respect to the star. The gravitational potential of that star was smoothed, but only very mildly so:

$$\Phi(\mathbf{r}) = -\frac{GM_*}{(|\mathbf{r}-\mathbf{r}_*|^8 + r_{\rm smooth}^8)^{1/8}} \tag{2}$$

The 8th power was chosen to minimize the effect of smoothing on the solution, essentially limiting the smoothing only to the few cells around the star. We used a 3-D Riemann-solver hydrodynamics code (developed by the PI many years ago for the purpose of a lecture on numerical hydrodynamics, but not public). The main parameters of the model are the size of the cloud $D_{\rm cl}$, the initial position of the cloud $\mathbf{r}_{\rm cl}$, the Mach number of the velocity $\mathcal{M}$ and the impact parameter b. Using this setup and code, a series of models were made in the context of the Bachelor thesis of Manuel Kramer during the summer of 2016. One such model is shown in Fig. 4. This result shows that such a secondary cloud accretion tends to produce disks with strong one-armed spiral structure at large scales. Which shape is seen depends not only on the parameters, but also on the timing of the snapshot. The geometries can vary a lot. The ones seen in Fig. 4 are reminiscent of some geometries seen at large scales around several Type 2 TDs. We also made synthetic scattered light images that can be directly compared to data. An example is shown in Fig. 5. This image bears resemblance to the arc-shaped envelope around the disk of the Transition Disk star AB Aurigae as imaged by Grady et al. (1999).

1.2 Project-related publications

Birnstiel, T., **Dullemond, C.P.** & Brauer, F., *Gas and dust evolution in protoplanetary disks*, 2010, A&A 513, 79. In this paper we present the basic code for the evolution of the disk and the dust. The disk evolution is followed using the time-dependent viscous disk equations, the dust part follows the dust coagulation, fragmentation, settling and radial drift of the dust.

Ataiee, S., **Dullemond, C.P.**, **Kley, W.**, Regaly, Z., & Meheut, H. *Planet-vortex interaction: How a vortex can shepherd a planetary embryo*, 2014, A&A, 572, A61. This paper is an example of our work on how a planet is interacting with a non-axisymmetric transition disk featuring a huge vortex.

Ataiee, S., Pinilla, P., Zsom, A., **Dullemond, C.P.**, Dominik, C., & Ghanbari, J., *Asymmetric transition disks: Vorticity or eccentricity?*, 2013, A&A, 553, L3. This paper shows our work on how a massive planet can make the disk asymmetric (lopsided) in two independent ways: by making the disk eccentric or by creating a vortex. We show how to distinguish observationally between these two scenarios. It is an example of how we make a link between modeling and observations.

Müller, T.W.A., & **Kley, W.**, *Modelling accretion in transitional disks*, 2013, A&A, 560, 40. This paper shows our experience with modeling the dynamics of transition disks. In this paper the gas flow through the planet-induced gap is studied, which is very relevant for the type 2 TDs which usually still have substantial accretion onto the star and have inner disks.

D. Thun, R. Kuiper, F. Schmidt, **W. Kley**, *Dynamical friction for supersonic motion in a homogeneous gaseous medium*, 2016, A&A, 589, A10. Since we will be dealing with extremely inclined companions interacting with the disk in part of this project, the experience gained in this paper will be used.

Bitsch, B., & **Kley, W.**, *Evolution of inclined planets in three-dimensional radiative discs*, 2011, A&A, 530, 41. This paper shows our experience with modeling out-of-plane 3-D planet-disk interaction. This paper focused mostly on how the disk damps the inclination of the planet, and focused on small inclinations and masses lower than about half a Jupiter mass. In this proposal we will shift our attention to more extreme cases, as suggested by the large observed disk tilts of up to 70 degrees, and focus on how the disk shape is changed as a result.

Kley, W., & Dirksen, G., *Disk eccentricity and embedded planets*, 2006, A&A, 447, 369. This was the original paper demonstrating how a massive planetary companion can make a disk eccentric.

N. van der Marel, E.F. van Dishoeck, S. Bruderer, T. Birnstiel, P. Pinilla, **C.P. Dullemond**, T.A. van Kempen, M. Schmalzl, J.M. Brown,

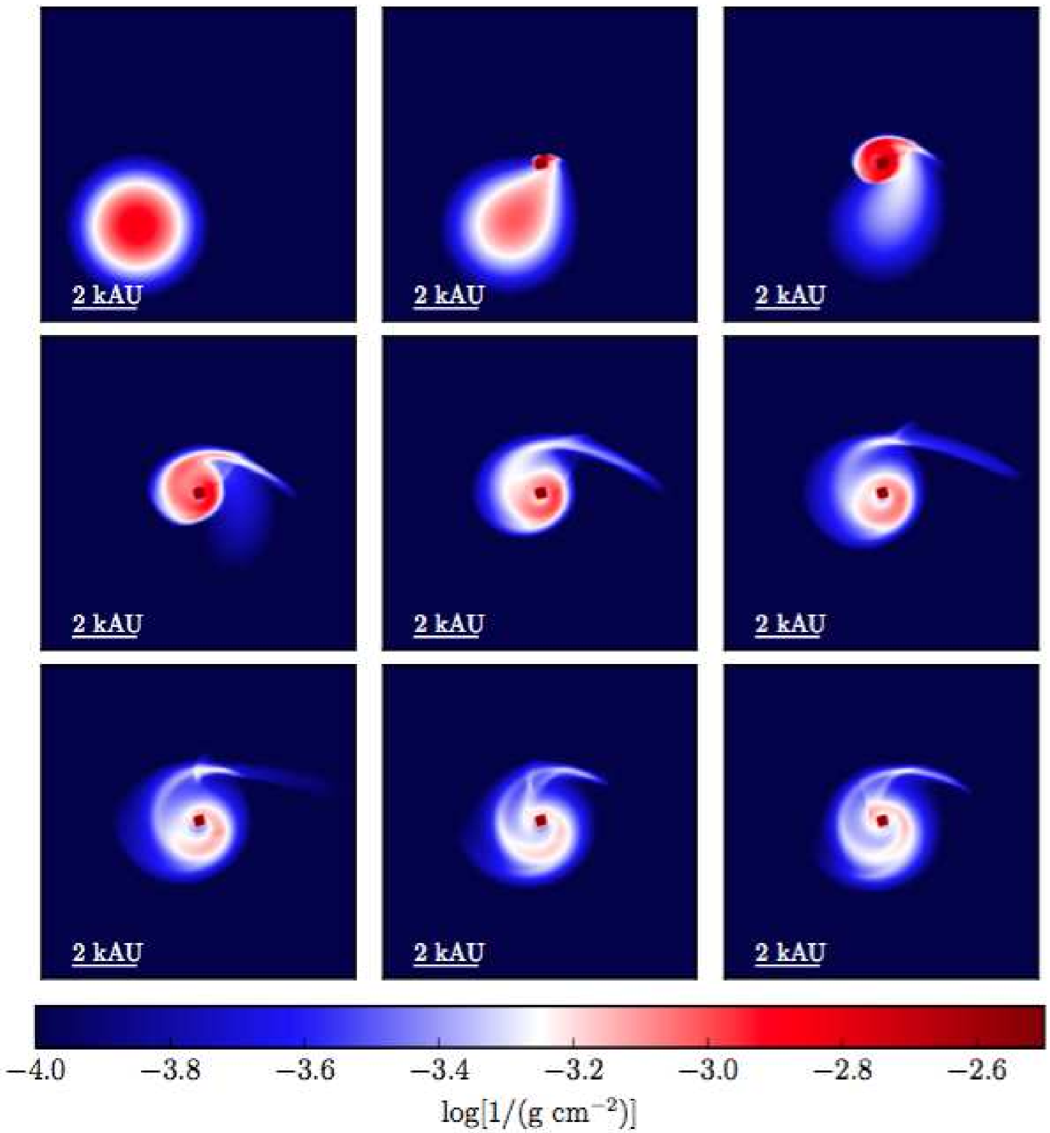

Figure 4: Time sequence of off-center accretion of a small low-mass spherical Gaussian molecular cloud by a star. The star is at the center, the cloud moves initially from left to right. The star is kept fixed, i.e. the cloud mass is small compared to the star mass. Time snapshots (**from left to right, top to bottom**) are with 4.8×10^3 years intervals. The color bar is surface density in g cm^{-2}. The star mass is 1.4 $M_{\odot}$, the Mach number of the cloud velocity with respect to the star. From: Bachelor Thesis by Manuel Kramer, Heidelberg University, 2016.

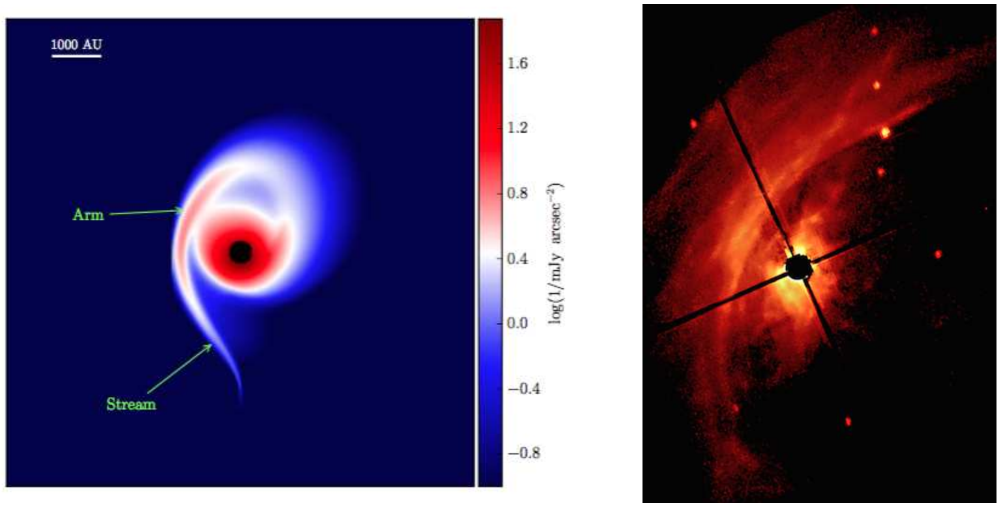

Figure 5: **Left:** Scattered light synthetic image computed for a snapshot of the simulations of an off-center accretion of a small low-mass spherical Gaussian molecular cloud by a star. The color bas unit is mJy/arcsec^2. From: Bachelor Thesis by Manuel Kramer, Heidelberg University, 2016. **Right:** Observed scattered light image of the arc-shaped envelope around the Type 2 TD star AB Aurigae by P. Kalas (Grady et al. 1999).

G.J. Herczeg, G.S. Mathews, V. Geers, *A Major Asymmetric Dust Trap in a Transition Disk*, 2013, Science, 340, 1199. This was the first discovery paper of a dust trapping vortex, and still is the best example of such an object so far. The role of the PI was the interpretation of the discovered lopsided dust clump as evidence for a dust-trapping vortex.

M. Benisty, T. Stolker, A. Pohl, J. de Boer, G. Lesur, C. Dominik, **C.P. Dullemond**, M. Langlois, M. Min, K. Wagner, T. Henning, A. Juhász, P. Pinilla, S. Facchini, D. Apai, R. van Boekel, A. Garufi, C. Ginski, F. Ménard, C. Pinte, S.P. Quanz, A. Zurlo, A. Boccaletti, M. Bonnefoy, J-L. Beuzit, G. Chauvin, M. Cudel, S. Desidera, M. Feldt, C. Fontanive, R. Gratton, M. Kasper, A.M. Lagrange, H. LeCoroller, D. Mouillet, D. Mesa, E. Sissa, A. Vigan, J. Antichi, T. Buey, T. Fusco, D. Gisler, M. Llored, Y. Magnard, O. Moeller-Nilsson, J. Pragt, R. Roelfsema, J-F. Sauvage, F. Wildi, *Shadows and spirals in the protoplanetary disk HD 100453*, 2016, A&A in press. This is the paper presenting the spectacular scattered light image of HD 100453 with the ring, the two shadows and the two perfect spirals (the SPHERE image shown in Fig. 1). The PI is closely associated with several members of the SPHERE consortium who made this observation, and is co-author of this paper having contributed theoretical interpretations.

A. Kataoka, T. Tsukagoshi, M. Momose, H. Nagai, T. Muto, **C.P. Dullemond**, A. Pohl, M. Fukagawa, H. Shibai, T. Hanawa, K. Murakawa, *Submillimeter Polarization Observation of the Protoplanetary Disk around HD 142527*, 2016, ApJ, 831, L12. This paper shows the power of ALMA observations of lopsided disks.

2. Objectives and work programme

2.1 Anticipated total duration of the project

3 years.

2.2 Objectives

This project aims to study the *dynamics* of non-axisymmetric Type 2 TDs, with the goal of trying to learn from these spectacular "disk dynamics laboratories" of Nature. The origin of these strange structures, including single- and double-armed spirals, heavy gas+dust rings with lopsided asymmetry, inclined/warped inner/outer disk geometry, is not yet understood. We plan to carry out numerical hydrodynamic simulations to test a variety of possible explanations for these non-axisymmetric features.

Concretely, we intend to study:

1) The effect of one or more planetary and/or brown dwarf companions on the disk, in particular focussing on the effect of their eccentric and/or out-of-plane orbits on the disk. Could this open

up a large gap as observed? Could the out-of-plane orbit lead to precession of the inner disk with respect to the outer disk, and thus explain the inclined inner disk with respect to the outer disk?

2) Are the arc-shaped features in Type 2 TDs really a proof of there being an anticyclonic, dust-trapping vortex, or can disk eccentricity induced by a massive enough companion cause equally strong density contrast along the ring (see e.g. Kley & Dirksen 2006)? We have investigated this question in the past (Ataiee et al. 2013) and came to the conclusion that the contrasts along the ring were not strong enough to match the strong asymmetry seen in HD142527 and IRS 48 (at that time the only two ALMA-confirmed lopsided disks). However, Ragusa et al. (2017) calls this conclusion in question, at least for HD 142527. By assuming a particularly massive companion (i.e. a stellar companion) they appear to be able to create rather strongly lopsided rings with contrasts along the ring of up to a factor of 10, even without dust trapping. With the exception of IRS 48 they conclude that all other famous lopsided TDs (HD 142527, HD 135344b, SR 21, DorAr 44 and LkHα 330) can be explained by just disk eccentricity, without a dust-trapping vortex. A reinvestigation from our side is necessary to find out who is right, where we would use a grid-based method, as opposed to Ragusa et al. (2017), who use an SPH method.
3) Can the outer disks have originated from late-time infall of gas+dust from a passing low-mass molecular cloud filament? Could this explain the tilted/warped inner/outer disk geometry seen in several Type 2 TDs? What would the remnants of this cloud look like at large scales? Could this explain the arc-shaped large scale features seen arouns several Type 2 TDs?
4) What is the effect of photoevaporation on a tilted inner/outer disk configuration? The irradiation of the inner edge of the outer disk can take place without extinction by the inner disk, and so it would be expected to be extremely effective. How long would it take to destroy the outer disk by photoevaporation?
5) Is Rossby-wave instability really the main reason for the lopsided heavy rings seen in Type 2 TDs? If so, why are some sources *much* more lopsided than others? Could this be a time-sequence effect (the vortex becoming stronger and weaker periodically as seen in the simulations by Regály et al. (2012)), or must it be an intrintic effect?
6) What are the effects of shadowing in tilted/warped disks on the dynamics of the outer disk? Montesinos et al. (2016) suggest that the shadows cast by the tilted inner disk on the outer disk may trigger the spiral waves seen in the outer disk of HD 142527. This may also work for the source HD 100453, which also shows these conspicuous pair of dark spots along the ring on opposite sides of the star (see Fig. 1), and shows even more prominent spirals emanating from them. Our own experiments have found that this may not be so easy. We think that the puffing-up of the inner-edge of the outer disk due to the direct radiation may help, because the shadowing effect by the inclined inner disk would then be much stronger at this edge than beyond. It would thus perturb the disk at a single radius instead of throughout the outer disk, and might thus lead to stronger spirals than found in Montesinos et al. (2016). This is what we wish to investigate.

2.3 Work programme including proposed research methods

2.3.1 Tools for the proposed project

For this project we will require the following main tools:

1) **A 3-D hydrodynamics modeling code.** Depending on which of the above subquestions we wish to address, the requirements for the hydrodynamics code will be different.
    - For models of how an out-of-plane companion affects the dynamics of the disk, the classical grid-based codes may not be suitable. Fixed-grid codes, when applied to disks that are not aligned with the grid, tend to cause numerical precession and artificial alignment. These effects can easily dominate over the real precession and alignment effects, making the results very unreliable. Even if these numerical effects are kept small by using a large numerical resolution, due to the large number of orbits that have to be modeled, they can still become

problematic. Lagrangian hydrodynamics codes would be more suitable for this problem, in particular because this problem is dominated by orbital dynamics and gravitational torques. The simplest of this class of methods is the Smooth Particle Hydrodynamics (SPH) method. The Gadget-2 SPH code (Springel 2005) would be a suitable option. Perhaps even better would be the Arepo code (Springel 2010), since it has the orbital dynamics of an SPH code, but the hydrodynamics of a grid-based Riemann solver: it uses dynamic Voronoi cells comoving with the fluid to solve the finite volume problem. SPH codes are, however, a bit easier to handle, so we will start with that type of code, and switch to Arepo if the advantage to effort ratio turns out to be large enough.

- For the problem of external capture of a low-mass molecular cloud fragment, an SPH code will not really be suitable, because to reproduce the large scale geometry of the remnant of that cloud, a too large number of SPH "particles" is required (because even very low density remnants would scatter light and remain visible). An SPH code does not have the required dynamic range in density. For this we therefore resort to a Riemann Solver. We could use again Arepo, but since we wish to post-process the results with a scattered-light radiative transfer code, better and smoother images can be produced with a fixed grid. Which code we use will depend on the candidate for the position. But two popular publicly available Riemann codes that could be suitable are RAMSES (Teyssier 2002) and PLUTO (Mignone et al. 2007). The RAMSES code has a working moment-based radiative transfer module included for radiation-hydrodynamic modeling.
- For the study of the effects of shadowing by the inner inclined disk on the outer disk we may resort to the FARGO-3D code by Pablo Benítez-Llambay and Frederic Masset[1]. This code also has a working Flux-Limited Diffusion (FLD) radiative transfer module included for radiation-hydrodynamic modeling. We will use this code also for any other in-plane companion-disk interaction modeling.

In Heidelberg and Tübingen there is ample experience with all five codes mentioned here.

2) **A 3-D diagnostic radiative transfer code.** The radiative transfer modeles used in the hydrodynamics codes for radiation hydrodynamics are generally not suited for diagnostic radiative transfer: i.e. the computation of synthetic images and spectra. It is necessary to apply a separate 3-D radiative transfer code to post-process snapshots of the model. We have in-house software for this: the popular publicly available RADMC-3D code package (Dullemond 2012). This software allows us to compute scattered-light images based on Monte-Carlo simulations using the full Müller matrix phase function for randomly oriented dust particles. The code also self-consistently computes the dust temperatures in the disk, using the Bjorkman & Wood (2001) Monte-Carlo algorithm, and thus allows for self-consistent spectral energy distribution calculations. Finally, the code also allows for the computation of molecular line maps from the hydrodynamics model. The observations of molecular line maps are a way to infer the dynamics of these disks.

2.3.2 Work plan

The work plan consists of several sub-projects that aim to explain the non-axisymmetric features mentioned above. In each of these sub-projects we will not only do the (radiation-)hydrodynamic modeling, but also compare their predicted appearances (using RADMC-3D) with the copious VLT/SPHERE and ALMA observations of these objects. With ALMA, in addition to continuum data, we will use line data to constrain the dynamics. Access to these data will be in part through public data, and in part through collaboration with observational teams. The PI is member of several ALMA consortia, as well as external member of the SPHERE disk consortium.

1. **Companion inside the disk: The in-plane 2-D case**
   The first project will be a "simple" start up project. We will use the FARGO-3D code to model

[1] `http://fargo.in2p3.fr`

the effect of a single, massive companion, either on a circular or eccentric, but always in-plane, orbit on the circumstellar disk. At first we will do just 2-D (r, ϕ) models and revisit and reproduce older models that we have already done in the past (Kley & Dirksen 2006; Ataiee et al. 2013). We will then employ larger companion masses and see if we can reproduce the lopsidedness of a factor of 10 found by Ragusa et al. (2017). They use an SPH code. Such codes are known to be more numerically viscous than grid-based codes. It is known that a strong viscosity in the disk tends to drive eccentricity, so perhaps viscosity is also responsible for the formation of the strong arc-shaped overdensities. A verification with a grid-based code is therefore important to be able to make strong conclusions. A next application of these in-plane companion-disk interaction models will be to test if these models can explain the huge radial range of the gap. Many Type 2 TDs have inner disks of only about 1 AU radius and outer disks starting beyond many tens of AU (in the extreme case of HD 142527 the inner disk is about 10 AU in radius while the outer disk starts beyond 120 AU). Can a single companion cause this? And will there still be gas flowing through the gap? What is the effect of a possible orbital eccentricity of the companion on the disk? What kind of gap *shape* does the companion produce? In scattered light observations of the star HD 142527 (Rodigas et al. 2014) it is clearly seen that the outer edge of the gap is eccentric with respect to the position of the star (though that does not exclude the possibility of its arc-shaped ALMA continuum peak being due to dust trapping in a vortex), with the star being to the north of the center of the disk. Also this outer edge appears to be a bit ragged (also seen in an earlier image by Rameau et al. 2012). Can this eccentricity and these irregularities (deviations from a perfect keplerian ellipse) be understood in the context of a companion-disk interaction model? This sub-project will be done in close collaboration with the postdoc of project D1, as that project is specialized on planets in disks. Project D1 focuses on multi-planet systems being responsible for the cavity in Type 2 TDs because single planets have not been proven to be able to explain TDs. Here we focus on Brown Dwarf or M star companions, possibly on strongly eccentric orbits. Yet, technically there are several similarities, making a strong collaboration beneficial.

2. **Companion inside the disk: The in-plane 3-D case**
Next we will go more into detail in the comparison of our in-plane models with observations: we will employ the RADMC-3D code to make detailed scattered-light Monte Carlo calculations to predict what the scatted-light images should look like, and compare those to the observed scattered light observations in optical and near-infrared. At first we will use the 2-D models mentioned above, and turn them into 3-D by using a suitable vertical structure model. But eventually it will be necessary to go to full 3-D. Fortunately the FARGO-3D code is perfectly suitable for this kind of modelling. We can alternatively also apply the PLUTO code, using spherical coordinates, depending on which turns out to be more suitable. To obtain the correct scattered light images, the vertical structure of the disk is essential to get right. This is because a small increase of the vertical height of the surface of the disk (the $\tau \simeq 1$ location of the disk) may cause strong effects of shadowing, because of the grazing incidence of the stellar light onto the disk's surface. The problem is that in order to get the vertical structure right, we need to get the temperature right. This requires us to treat the heating and cooling of the disk correctly. Since we are mostly interested in the outer regions of the disk (may tens of AU) the internally produced viscous heating can be ignored. Instead, the disk is heated entirely due to the irradiation by the star. While at first we will employ simple estimates of the resulting temperature structure (e.g. simply assuming a power law with radius), we will eventually be forced to include radiative transfer and do a proper *radiation hydrodynamics* simulation. A two-phase procedure to do this correctly for irradiated disks and other circumstellar nebulae was described by us (Kuiper et al. 2010), and similar procedures have since been adopted by many other codes as well. The FARGO-3D code has this built in and we have our own module for the PLUTO code. We will then insert snapshots of these self-consistent 3-D models into the RADMC-3D code and compute scattered-light images to compare to observations. In doing this

we must use the full polarization mode of RADMC-3D, and we must use realistic dust models with properly calculated scattering matrices. This is because many of these scattered light observations in the optical and near-infrared employ *polarimetric differential imaging*, in order to better separate the scattered light from the disk from the point spread function of the star. Once we have these images we will study the shape of the outer edge of the gap, and also find out if spiral features can be seen, which may be similar to those found in the observations. This sub-project will be done in close collaboration with the postdoc of project D1, as that project is specialized on planets in disks, as well as on the radiation hydrodynamics of 3-D planet-disk models.

3. **Companion inside the disk: The out-of-plane case**
Since we know by now that many TDs are warped, it is entirely natural to investigate what happens to the disk if the star has a companion (planetary or stellar) that has orbital elements carrying it out of the plane of the disk. Could such a configuration cause the inner/outer disk to precess and explain the weird warped/tilted disk systems such as HD 142527 and HD 100453? To model this problem we will resort to another kind of hydrodynamics code. We will start with the SPH code Gadget-2, set up the problem starting from the simulations we did previously (see preliminary work) and improve those calculations in various ways. First, we will use many more particles, and compute our models on a computer cluster. We will carefully investigate the viscosity effects and how they scale (reduce) with increasing number of SPH particles. We will then move to the Arepo code, which uses the same underlying data infrastructure as Gadget-2, so that the switch to Arepo should be reasonably doable. We will investigate if this code has, for the same number of sampling points ("particles") a lower (and therefore more realistic) numerical viscosity. The first investigation of the results can be done by computing quantities such as tilt angle, disk eccentricity etc, which can be directly compared to the equivalent observed quantities. A more detailed comparison to the observations will again require radiative transfer. In principle we are then again faced with the problem of radiation hydrodynamics (see above). For this kind of highly complex geometries it might be not yet feasible to do this. In Gadget-2 this kind of radiative transfer (Flux-limited diffusion) is not yet built in. In Arepo such a method is implemented (Petkova & Springel 2011), but testing its feasibility for the kind of models discussed here might be too time-consuming. We might try, but we might also use a simple power law as a function of distance. However, for the scattered-light observations we again use RADMC-3D. The Arepo grid is, however, a Voronoi grid. This is not yet built in into RADMC-3D. We will therefore instead regrid a snapshot from Arepo on an oct-tree cartesian adaptive mesh before inserting this into RADMC-3D. In Project D1 mild inclinations of planetary mass companions are modelled, while here we focus on extreme inclinations of stellar mass companions. In the latter case the star, being too massive, is unlikely to be forced back into the plane of the disk; instead the disk is likely to be torqued by the companion.

4. **Tilted disks: The effect of Photoevaporation**
The UV and X-ray photons from the star may photoevaporate the disk (see projects B1 and B2). It is known from model calculations that, once the stellar radiation can impinge directly onto the inner edge of the disk, the photoevaporative destruction can accelerate dramatically (coined "thermal sweeping" by Owen et al. 2012). In normal disks without warping this requires the entire inner disk to vanish. Once it is vanished, the sweeping begins and the outer disk quickly vanishes too. With the tilted Type 2 TDs, however, we have an interesting new situation: due to the tilt of the inner disk, the stellar photons can reach the inner edge of the outer disk unobstructed (barring two small shadows where the two disk planes intersect). The question is therefore: should we expect these outer disks to be subject to thermal sweeping, and if so, how rapidly would this destroy the outer disk? And is this time scale consistent with the statistics of known tilted TDs? We will take the tilted disk models of the previous subproject and pick a time snapshot. We will then subject this to a radiative transfer calculation of UV and X-ray photons. We will collaborate with Prof. Barbara Ercolano, and use her MOCASSIN code for

this (Ercolano et al. 2003, 2005, 2008b). This will then give an estimate of the typical volume of heated gas in this outer disk edge, and with this we will *estimate* what the evaporation rate will be, using the same approach as in Ercolano et al. (2008a, 2009). We will not model this evaporation directly, because the geometry is full 3-D and this is presumably too numerically expensive. However, we might, in addition, make a 2-D (r, z) axisymmetric model of the outer disk without inner disk (i.e. ignoring the two shadow spots by the inner disk) and do a run similar to the 2-D models of Owen et al. (2012) to see what the time scale will be. This sub-project will benefit strongly from a collaboration with the postdoc of project B1, since he/she will work with hydrodynamic models of photoevaporative winds. In particular the 2-D axisymmetric approximation model can presumably be set up quite easily by the postdoc of project B1.

5. **Exploring the possibility of shadow-induced spirals**
Montesinos et al. (2016) suggest that the two shadow spots cast by the tilted inner disk in HD 142527 and HD 100453 could cause the gas of the disk that passes through these shadows to briefly lose pressure and start collapsing. Once the gas re-emerges from the shadow, the pressure is restored and the collapse is halted. This may lead to oscillations in the inner rim of the disk (see also Benisty et al. 2016) that may trigger the formation of an $m = 2$ spiral pattern. One problem encountered by Montesinos et al. (2016) is that this mechanism, taken at face value, is too weak to produce substantial contrast in the spirals. To enhance the spirals, they assumed that the disk is near to gravitational instability, so that the shadowed-triggered spirals will self-amplify. In this project we would like to test another possibility: since the inner rim of the outer disk is strongly illuminated by the central star, its pressure scale height is slightly enhanced with respect to the disk behind it. This means that the disk behind it is primarily heated by indirect infrared radiation diffusing through the disk, and the disk is thereby a bit cooler and less vertically extended than the rim. Any shadowing effects will thus affect the inner rim of the outer disk much more strongly than the disk behind it. This may lead (in contrast to the model of Montesinos et al. (2016)) to a radially restricted perturbation (restricted to the irradiated rim only), which can then propagate outward hydrodynamically. This would, for fixed shadows, lead to *leading* spiral wave patterns. We intend to investigate the feasibility of this scenario using FARGO-3D with radiation-hydrodynamics.

6. **Secondary infall of a low-mass molecular cloudlet**
Next we will explore the idea that the tilted disk geometry seen in HD 142527 and HD 100453 could be as a result of late infall of fresh envelope material with a different angular momentum axis than the earlier primordial collapsing cloud from which the star has formed (the scenario by Thies et al. 2011, but now applied to disks). We will employ the PLUTO or RAMSES code in cartesian coordinates and set up a model of the kind we already started in the preliminary work (see above). We will improve on these models in several ways. First we will perform models with much higher resolution. Second we will start the cloud much farther from the star. This all requires modeling on a substantial computer cluster. In our initial models we will ignore the inner disk and focus only on the formation of the outer disk from the capture of the cloudlet. To test whether the geometries we find are not too strongly affected by the gridding, we will repeat some models with the same setup, but randomly rotated with respect to the grid. The resulting outcome should ideally become the same (apart from being rotated). We will compute the scattered light images using RADMC-3D and compare these images with observed images of these disks in the optical and near-infrared, particularly focusing on the large scale structure, what people tend to call the “envelope”. We may also compute images at other wavelengths, as well as molecular line maps, and compare with what is present in the literature. For instance, for AB Aurigae the envelope structure (see Fig. 5) has been studied in quite some detail at many wavelengths, including molecular lines (Semenov et al. 2005), and with our new geometry we can do a better analysis, including the predictions for the doppler shifts. Finally, we will zoom further in and include the inclined inner disk. Given that the grid-based codes tend to lead to numerical alignment of disks, and given that the inner disk will have to perform many more

rotational periods than the outer disk for the same time span, we will adjust the system such that the inner disk is aligned with the grid, while the outer disk is not.

7. **Revisit the Rossby-wave instability**
Finally, if we still have time, we will (in strong collaboration with D1) revisit the the Rossby-wave instability origin of the observed vortices, comparing the different scenarios of inner hole formation against each other (planets, massive companion, inclined companion, photoevaporation): do they all predict these vortices? And are vortices and spirals predicted simultaneously or mutually exclusively? The relation to dust-trapping makes a connection to project **C1** natural. Project D1 aims, among other things, to follow the dust kinetics and dust trapping in TDs. This fits well into the topic of non-axisymmetric TDs, as some of them display lopsided dust emission believed to be due to a huge dust-trapping vortex. This sub-project will thus be either lead by the postdoc of D1 or by the postdoc of this project.

We are aware that this is an ambitious set of projects. It is likely that some of these projects will have to be carried over to the second funding period of the Research Unit.

TIME PLAN?

2.4 Data handling

The model data we produce will be made immediately available online, once the corresponding paper is accepted.

2.5 Other information

2.6 Information on scientific and financial involvement of international cooperation partners

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We request 1 Postdoc E13 position for three years, to be based in Heidelberg.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Theoretical numerical research can only be done when sufficient and appropriate computational facilities are available. While production runs will be done on supercomputer facilities, a substantial part of the work in this project is code development. Testing these codes on realistic problems requires a workstation – which is beyond the standard base equipment (*Grundausstattung*). We therefore request one workstation-grade desktop computer for 4000 Euro.

4.1.2.2 Travel Expenses

Participation at at least one conference per year, or similar is anticipated for the postdoc. In addition to travel funds for conferences for the PIs, regular mutual working visits at Heidelberg/Tübingen/München are planned.

	Year 1	Year 2	Year 3	Sum
Conferences Postdoc	1500	1500	1500	4500
Conferences PIs	2000	2000	2000	6000
Working visits Heidelberg/TübingenMünchen	3000	3000	3000	9000
	6500	6500	6500	**19500**

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

This project strongly ties to observations of Type 2 TDs in scattered light (with VLT-SPHERE), thermal millimeter dust emission (with ALMA) and gas lines (with ALMA). We collaborate internally with Prof. Ewine van Dishoeck (on the ALMA data) and Prof. Thomas Henning (on the scattered light data). Over the last few years we have also strongly collaborated (and published several common papers) with Dr. Myriam Benisty and Prof. Carsten Dominik, both strongly involved in the VLT-SPHERE project. Recently we have started also a collaboration with Prof. Misato Fukagawa, who is strongly involved in both ALMA observations and Subaru scattered light images of transition disks. Early access to new data from these projects is very advantageous for our project, since it would allow us to tune our models to data about a year before the data become public, giving us a head-start over competitors. We will also continue our strong collaboration with Dr. Akimasa Kataoka, who will be moving to Tokyo in April 2017. For travel to/form Dr. Kataoka we will not ask funding here, because that travel will be funded through the Humboldt Foundation.

	Visit 1	Visit 2	Sum
Prof. Misato Fukagawa (Nagoya University)	2000	2000	4000
Dr. Myriam Benisty (Grenoble)	1000	1000	2000
Prof. Carsten Dominik (Amsterdam)	1000	1000	2000
	4000	4000	**8000**

4.1.2.4 Other Costs

4.1.2.5 Project-related publication expenses

Given the strong international competition in this field, it might now and then be necessary to publish in the Astrophysical Journal (ApJ), which takes page charges typically of the order of 1000 US dollar. Assuming two such papers, and sharing the page charge cost 50/50 between institute and project, we request for 1000 Euro additional funding for covering this.

5. Project requirements

5.1 Employment status information

Prof. Dr. Dullemond, Cornelis Petrus. W3 Professor (permanent) at Univertiät Heidelberg.
Prof. Dr. Kley, Wilhelm. W3 Professor (permanent) at Univertiät Tübingen.

5.2 First-time proposal data

5.3 Composition of the project group

[Text]

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

A key to the success of this project will be the comparison of the models to observations of Type 2 TDs. Access to the latest VLT-SPHERE images in scattered light is guaranteed through collaboration with the group of Thomas Henning. Access to the latest ALMA data is guaranteed through the groups of Leonardo Testi (see also project A1) and Ewine van Dishoeck. Direct collaboration with the PhD students from project A1 is forseen to help with the comparison of our models with these ALMA data. The postdoc of B2 will be working a lot with 3-D diagnostic radiative transfer modeling, so a collaboration on the technical side can be helpful here as well. This collaboration will also provide chemistry input for the abundances of molecules that can be traced with ALMA to determine the kinetics of the disks.

A strong collaboration within this Forschergruppe will be carried out with the postdoc of project D1. Projects D1 and D2 have several methods in common, in particular both employing 2-D and 3-D (radiation-)hydrodynamics of protoplanetary disks. On the technical side both postdocs are envisioned to collaborate closely. The first two sub-projects of D2 are also topically somewhat overlapping with project D1: focussing on planet-disk interaction as an explanation for Type 2 TDs. The differences are: in D2 we focus on *single massive* companions, presumably low mass stars rather than planets, while project D1 focuses more on multiple planet-mass companions. Secondly, D2 focuses on finding the origin of strong deviations from circular symmetry, in part by making the companion's orbit strongly eccentric. Finally, D2 aims at explaining the extremely tilted inner disks of several Type 2 TDs, which is not a goal of D1.

A connection to project B1 will be established when we intend to apply the photoevaporation models of B1 to the case of an outer disk photoionized/evaporated by the star, as a result of free irradiation due to the inclined inner disk.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

External collaboration with M. Benisty (Grenoble/Santiago) and C. Dominik (Amsterdam) is envisioned for the task of comparison to observational data with ALMA and SPHERE. In addition, collaboration with M. Fukagawa (Nagoya, Japan) and A. Kataoka (NAOJ, Japan) and other Japanese colleagues involved in studies of transition disks, is envisioned. The PI has established strong scientific links with these groups, in particular recently in the study of Type 2 TDs with ALMA, both from a modeling perspective and from ALMA observations.

We will also strengthen ties to Dr. Pablo Benítez-Llambay (currently at Copenhagen) who is the lead author of the FARGO-3D public code.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

Close collaboration is in boldface. The rest is due to large common consortia.

S. Andrews (CfA, Harvard), E. van Dishoeck (MPE Garching, Uni Leiden), C. Dominik (UvA, Amsterdam), A. Natta (DIAS, Dublin), L. Testi (ESO, Garching), J. Carpenter (Caltech, Pasadena), **C. Chandler (NRAO, Socorro),** A. Isella (Rice Uni, Houston), L. Ricci (Caltech, Pasadena), N. Calvet (Uni Michigan), S. Corder (ALMA), J. Greaves (Uni St. Andrews), **N. Turner (JPL, Pasadena),** A. Uribe (Coll. Charlston), **Z. Regaly (Konkoly Obs, Budapest), A. Juhasz (Cambridge), R. Klessen (Uni-Heidelberg), R. Kuiper (Uni Tübingen), C. Brinch (University of Copenhagen), M. Benisty (Uni Grenoble), P. Pinilla (Tucson), C. Mordasini (Uni Bern),** G. Guidi (ESO), **M. Tazzari (ESO), L. Perez (MPIfR, Bonn),** H. Linz (MPIA), A. Sargent (Caltech, Pasadena), L. Mundy (University of Maryland), S. Storm (University of Maryland), J. Lazio (JPL, Caltech), W. Kwon (Korea Astronomy and Space Science Institute), **B. Ercolano (Uni München), T. Muto (Kogakuin University),** M. Momose(Ibaraki University), **T. Tsukagoshi (Ibaraki University),** L. Klarmann (Uni Amsterdam), **H. Klahr (MPIA, Heidelberg), S. Ataiee (Uni Bern),** S. Paardekooper (Queen Mary University of London), M. Fukagawa (NAOJ Japan), H. Shibai (Osaka University), T. Hanawa (Chiba University), K. Murakawa (Osaka Sangyo University), **J. Ramsey (Uni Kopenhagen), J. Drazkowska (Uni Zürich)**

5.5 Scientific equipment

The project requires a considerable amount of CPU-time. For production runs we will rely on outside resources.

We have special access to computing resources supplied within the State of Baden-Württemberg (Baden-Württemberg High Performance Computing - Coordinated Compute Cluster Competence Centers: bwHPC-c5). A part of this initiative is the new BinAC-system[2] that has just gone online at the University of Tübingen and is dedicated to Astrophysics and Computer Science only, and is accessible for researchers from Heidelberg. BinAC offers over 236 CPU nodes with dual Intel Xeon E5-2630v4 each. Additional resources are available with bwHPC-c5 at the ForHLR-cluster at the Steinbuch Centre for Computing (SCC) in Karlsruhe. If further resources will be required we will apply for additional computer time at the high performance computing center HLRS, located in Stuttgart, and at other centers in Germany.

[2]see `http://www.bwhpc-c5.de/wiki/index.php/Category:BwForCluster_BinAC` for a detailed description of the hardware.