Project B1:

The radiation-hydrodynamics of photoevaporative winds with chemistry

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Requested positions: 1 Postdoc

Abstract:
Type 1 Transition discs (TDs) are most likely discs in an advanced stage of dispersal (see introduction to the Research Unit). The dispersal mechanism of discs has been shown to be of fundamental importance to planet formation, yet the responsible mechanism is still largely unconstrained. Photoevaporation from the central star is currently a promising avenue to investigate, but the models developed to date do not yet have enough predictive power for a piecewise comparison with the observations. In this project we aim at building the most up-to-date radiation-hydrodynamical calculations of irradiated discs, coupled to photoionisation, chemistry and radiative transfer calculations. This will constitute the backbone for the work carried out in several sub-projects of this proposal (B2, C2), which together aim at performing quantitative spectroscopy of disc winds. Comparison with existing and upcoming observations will allow us to constrain the mass loss rates and the launching regions of the wind and thus pin down the underlying driving disc dispersal mechanism. The models developed in this project will also the able to tackle important outstanding questions about the formation and evolution of Type I TDs, as discussed in more detail below.

1. State of the art and preliminary work

1.1 Scientific Background

Understanding disc dispersal is a key piece in the puzzle of planet formation. Type 1 TDs, which are considered to be objects caught in the act of dispersal provide a tight constraints on the underlaying dispersal mechanism. For example, their (low) frequency, in relation to the global disc population in a given cluster, implies dispersal timescales of order 10% of the global disc timescale, and their evolution on the colour-colour plane (e.g. K-[8] versus K-[24]) points to an inside-out mode of dispersal (e.g., Ercolano et al. 2011; Koepferl et al. 2013; Ercolano et al. 2015).

The most successful of the various disc dispersal mechanisms proposed because it matches many of the observational constraints, is photoevaporation by radiation from the central star (e.g., Clarke et al. 2001). As described in more details below, in this model the disc is dispersed because the mass loss rate due to photoevaporation eventually exceeds the mass accretion rate through disc, the wind can quickly destroy the disc, eroding from the inside-out.

Recent work suggests that magnetohydrodynamic (MHD) turbulence may also drive disc winds (e.g., Bai & Stone 2013) which may lead to disc dispersal and at the same time remove angular momentum from the system, thus allowing the inward flow of material, i.e. accretion. What is certain, however, is that if MHD winds are indeed as vigorous as some authors claim, they would change the way we understand disc evolution and dispersal, raising questions about models that rely on alpha-type discs. However, these models are still in their infancy and the mass loss and accretion rates from MHD winds are at present highly uncertain. Some of the main sources of uncertainty include the strong dependence of the wind and accretion rates on the completely unknown magnetic flux distribution through the disc and, most importantly, magnetic flux evolution as a function of surface density of the disc (e.g. discussion in Armitage et al. 2013) **Check if reference is the right one** Another key ingredient is the level of ionisation in the atmosphere of discs, which determines the nature of the gas coupling to this unknown magnetic field. While details of the magnetic field structure and evolution are difficult to determine at present, the joint efforts of sub-projects B1, B2 and C2 can deliver the most detailed case-specific assessment to date of the ionisation structure in disc atmospheres. This is indeed one of the aims, which is described in project B2 (PIs Caselli & Ercolano).

In this project we focus solely on photoevaporative winds. In the following two sections the state-of-the art for photoevaporation models, to which the PI and collaborators have made significant contributions, will be discussed.

1.1.1 Photoevaporation models

All models of photoevaporation show that radiation from the central star heats the disc atmosphere, where a thermal wind is established. The wind is centrifugally launched from the location where the thermal energy of the heated gas exceeds the local gravitational binding energy. Disc dispersal then sets in as a consequence of the wind when the mass loss rate exceeds the accretion rates in the disc. According to viscous theory, young discs accrete at a vigorous rate, which naturally decreases as time goes by (e.g., Hartmann 2008), **Check if this is the right reference** until, after a few million years, accretion rates fall to values smaller than the wind rates, allowing photoevaporation to take over the further evolution of the disc. Once the dispersal sets in the disc is then quickly eroded from the inside out (see e.g., Alexander et al. 2014; Armitage 2011, for recent reviews of this process).

While the community now agrees on this broad brush picture, quantitatively speaking, the dispersal mechanism is still largely unconstrained. There is currently a hot debate in the literature as to what type of radiation may be the main driver of the wind: Extreme-, Far-UV or X-ray. This is a fundamental question as the mass-loss-rates implied by the different models can differ by orders of magnitudes. Mass loss rates determine the timescales of dispersal for given initial disc conditions. The wind profile, i.e. the region of the disc that is most affected by photoevaporation, is also very different in each scenario (e.g. Alexander et al. 2014; Armitage 2011). Figure 1 shows the mass loss profile for the X-ray+EUV (Owen et al. 2010), EUV-only (Font et al. 2004) and FUV (Gorti et al. 2009) profiles. The X-ray profile is more extended than the EUV profile, which predicts mass loss only from a vary narrow range of disc radii. The FUV model is again very different, showing mass loss from the outer regions of the disc, hence predicting in some cases an outside-in mode of dispersal. These differences have important implications for the planet formation process. For example, the total mass loss rates in the disc sets the timescales for the formation of gas giants, and together with the wind profiles it sculpts the disc density distributions, profoundly affecting the evolution of all planetary systems, by putting a stop to migration via the formation of gaps in the gas. As an example, we have shown that the photoevaporation profile strongly influences the final semi-major axis distribution of exo-planets (Ercolano & Rosotti 2015).

While the importance of the final stages of disc evolution to understand planet formation and explain the diversity of exoplanets is largely recognised, a quantitative model describing this phase is still lacking. The reason for that is that all current models are incomplete. Some models focus on hydrodynamics and assume isothermal gas (e.g. the EUV-only model of Font et al. 2004) others focus on chemistry but do not perform hydrodynamical calculations (e.g. the FUV model of Gorti et al. 2009). None of the existing models take into account dust evolution in the underlying disc and entrainment of grains in the wind. Together with a PhD student I co-supervised at the Institute of Astronomy in Cambridge, I performed the only existing radiation hydrodynamic calculations of X-ray + EUV driven

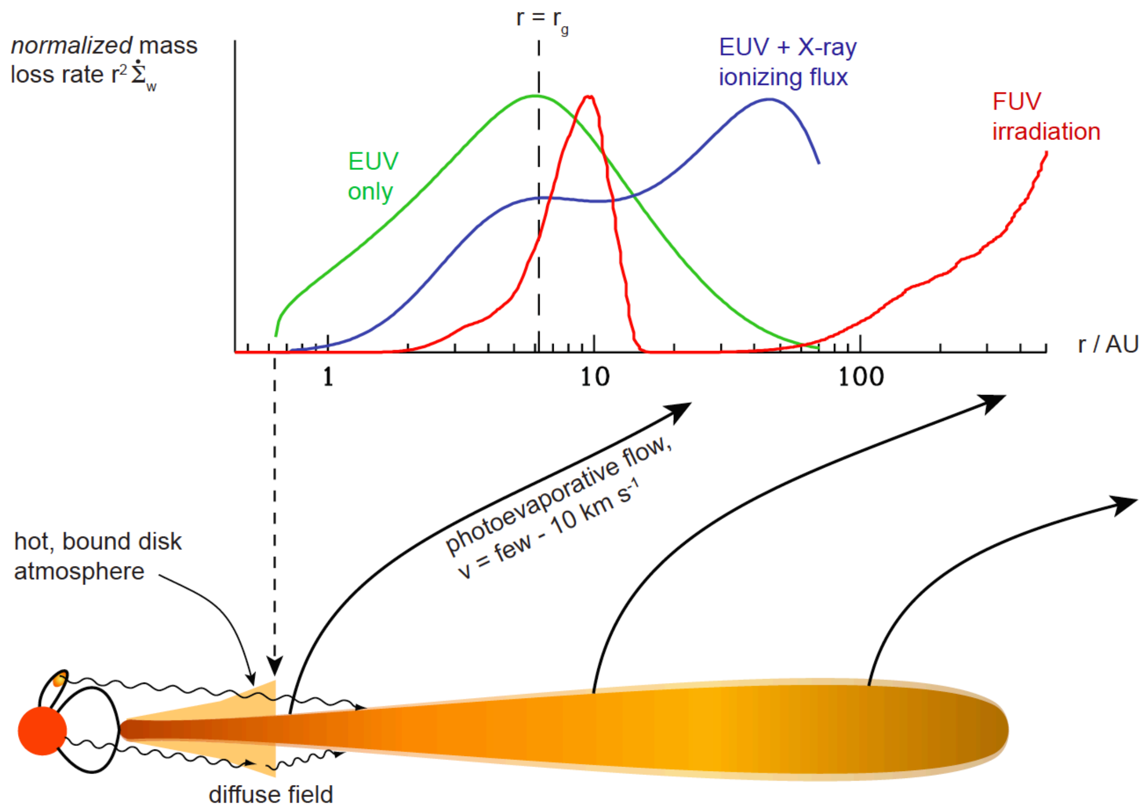

Figure 1: From Armitage (2011). Different photoevaporation profiles corresponding to the EUV-only model of Alexander et al. (2006a,b), the EUV+X-ray of Owen et al. (2010) and FUV model estimates of Gorti et al. (2009). The profiles have been normalised, where the total mass loss rates can differ by over two orders of magnitude.

winds to date (Owen et al. 2010, 2011, 2012), using realistic gas temperatures obtained from X-ray photoionisation calculations (Ercolano et al. 2008a, 2009). This led to a fundamental re-think to the whole problem, as previous isothermal calculations had yielded much lower mass loss rates (by two orders of magnitude). However, our models, which still represents the state-of-the-art, also have important limitations, since, most importantly, they do not include chemistry and ignore the dust phase. Furthermore the resolution at which the simulations were performed is insufficient to study lines with emission regions extending close to the disc inner edge. These limitations make the application of current models to observations impossible.

As well as the uncertainties on mass loss rates and wind profiles, which directly affect planet formation, there are also a number of open questions regarding photoevaporation and the formation of the observed TDs. A recent review by Owen (2016) provides a discussion of the current successes and problems of theoretical models in explaining the origin and evolution of TDs. Here we will just list a few issues that we think should have priority in the development of a quantitative theory which can be used to interpret observations.

1. The observations of TDs have yet to reveal objects with large holes that do not accrete. Photoevaporation, however, predicts a significant population, unless the final removal is dominated by a process called "thermal sweeping" (Owen et al. 2012). The efficiency of "thermal sweeping" has however recently been called into question (Haworth et al. 2016).

2. The role played by FUV heating in the removal of the outer disc is unclear, due to the lack of hydrodynamical calculations that include this channel. FUV heating may provide a solution to the previous item, at least in some cases.

3. Current estimates of the TD populations predicted by the X-ray model are based on extrapolations of the results with stellar mass and stellar emission properties. The validity of these extrapolations has yet to be proved.

1.1.1.1 Contribution of this team to the current state-of-the-art

The first photoevaporation models to be developed were based on EUV irradiation only. This was mainly due to the need of simplifying the hydrodynamics by assuming the gas is isothermal. An EUV heated gas, where hydrogen is almost fully ionised, is indeed roughly isothermal ($\sim 10^4$K), while the temperatures of a quasi-neutral X-ray heated gas generally vary from a few hundred to a few thousand Kelvin. Here the hydrogen gas is in a quasi-neutral state of ionisation, with the exact ionisation level influencing the efficiency of the X-ray heating. While the EUV-photoionisation process occurs of via the removal of a single valence electron, X-rays generally remove an inner-shell electron. The ejected supra-thermal electron produces then secondary ionisations. A further complication is that multiple electrons may be ejected as a consequence of inner shell ionisations, linking together non-adjacent ionisation levels.

The host of microphysics regulating X-ray ionisation and heating is self-consistently included in the three-dimensional photoionisation code MOCASSIN (Ercolano et al. 2003, 2005, 2008b) and has been applied to the X-ray photoionisation and photoevaporation process of protoplanetary discs (Ercolano et al. 2008a, 2009; Ercolano & Owen 2010, 2016; Owen et al. 2010, 2011, 2012)

In Ercolano et al. (2008a, 2009) the relevance of the photoevaporation process to the dispersal of discs was proven for the first time. Indeed the mass loss rates calculated were approximately two order of magnitude larger than those previously obtained by the EUV-only model, able to compete with observed accretion rates from T-Tauri stars. These early results were based on hydrostatic calculations, which were later improved by our 2D radiation-hydrodynamic calculations (Owen et al. 2010, 2011, 2012), which still represent the state-of-the-art in this field. This work also provided detailed mass-loss radial profiles that have been used by us and others to study the photoevaporation process in combination with planet formation in 1D and 2D (e.g., Rosotti et al. 2013, 2015).

We explored several possibilities to test and refine our models against observations. In Ercolano & Owen (2010, 2016) and in Schisano et al. (2010) we produced synthetic line profiles of forbidden transitions of heavy metals observed in the optical and in the mid-infrared. We came to the conclusion, however that the strong temperature dependance of these lines makes them unsuitable for use as wind diagnostics.

In Ercolano & Clarke (2010) we explored the metallicity dependance of the mass loss rates, hoping for hints from disc statistics in several regions. While available data support our predictions (Yasui et al. 2009, 2010), these observations are challenging and have remained sparse. The importance of the effects we noted in this work for planet formation has however been widely recognised (e.g., Lopez 2016).

In Owen et al. (2013) we tested the models using predictions in the radio. We were able to show in that work that our observations of the famous transition disc around GM Aur were consistent with our models, but could not really distinguish between a EUV-only or an X-ray driven scenario. This line of work was however used again by Pascucci et al. (2014) to show that the EUV flux impinging on protoplanetary discs is generally low, hence arguing against a EUV-only model for dispersal.

The work described here has provided the basis for many theoretical and observational investigations, which cannot all be described here. We will only finally mention our most recent application where we were able to use our model to argue that the inner-most gap imaged with ALMA by Andrews et al. (2016) in the disc around TW Hya, is likely photoevaporative in origin (Ercolano et al. 2017).

1.2 Preliminary work

The determination of gas temperatures in a photoionised gas, in a photodissociation region (PDR) or in an X-ray dissociated region (XDR) is computationally expensive. It requires, first of all performing a radiative transfer (RT) calculation in order to determine the radiation field at each point of the region. Then matrices of thermal and ionisation balance and/or rate equations have to be solved. The RT and the balance/rate equation are often coupled through the temperature-dependent gas opacities, and one needs to iterate to obtain a solution. There is a host of microphysics that needs to be taken into account, last but not least the thermal coupling of the gas and the dust phase. Even a extremely simplified version of the above has large computational costs if it needs to be performed at every time-step of a hydrodynamical calculation.

In such cases it is convenient to look for parameterisations of the gas temperature in terms of quantities that are easy to determine in the hydrodynamics code (e.g. gas properties and/or column density). Indeed using such a temperature paremeterisation, determined via detailed X-ray photoevaporation models using the MOCASSIN code (Ercolano et al. 2008a, 2009) we have performed the only existing radiation hydrodynamic calculations of X-ray + EUV driven photoevaporative winds to date (Owen et al. 2010, 2011, 2012), as was described in the previous section. The models were run with a version of the ZEUS2D code which was modified by us to include a temperature scheme derived from the detailed X-ray and EUV photoionisation calculations of protoplanetary discs of Ercolano et al. (2008a, 2009). In that work it was shown that, within the penetration depth of $\sim$1keV X-rays ($\sim 10^{22} cm^{-2}$), the temperature of a parcel of gas with hydrogen number density, n_H, at distance r from the central star, could be roughly approximated by a function of the ionisation parameter, defined as $L_X/(r^2 n_H)$, whereL_X is the stellar X-ray luminosity. The error on the temperature was found to be small for high ionisation parameter values, but it becomes systematically larger at the low end.

As the gas temperature enters the hydrodynamics via the square root dependance in the sound speed, the small error at high values of the ionisation parameter, typical for the regions where the bulk of the wind is driven from in primordial discs, is unlikely to produce large uncertainties in the mass loss rates. For more evolved objects, like transition discs in the phase of final dispersal, however, the ionisation parameter decreases dramatically as the cavity becomes larger. The evolution of transition discs depends thus sensitively on the temperature of the gas at low ionisation parameters,

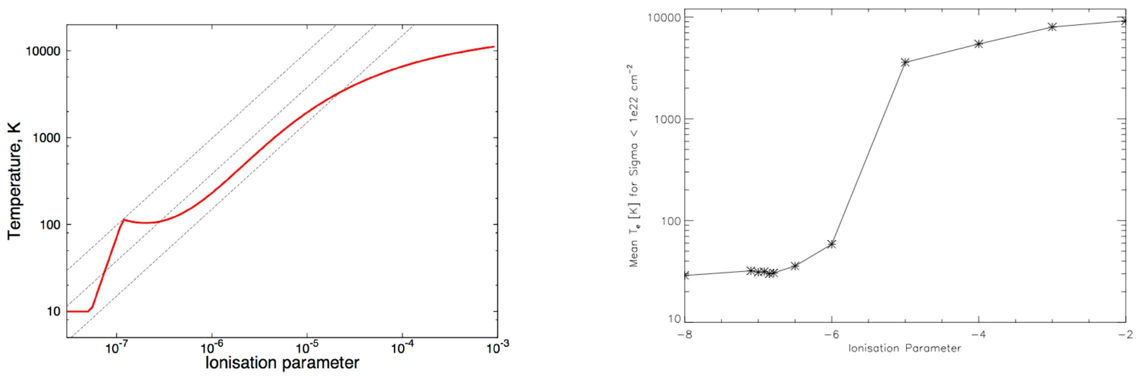

Figure 2: The electron temperature versus ionisation parameter relation in the calculations of Haworth et al. (2016), **left panel**, compared to our most recent calculations Ercolano, Picogna & Owen, (in preparation), **right panel**.

which is currently poorly represented by the parameterisation of Ercolano et al. (2008a, 2009). Note that the recent work of Haworth et al. (2016), described in the previous section, presents a form of the temperature ionisation parameter relation which is incorrect at low values of the ionisation parameter. The kink at ionisation parameters just above 10^{-7} (left panel of Figure 2) is an artefact of their implementation of the photoionisation models. We have recently performed new detailed photoionisation calculations and obtained the curve shown in the right panel of Figure 2 (Ercolano, Picogna & Owen, 2017, in preparation). Figure 2 shows the behaviour of the temperature parameterisation at low ionisation parameter and for different column densities. Our collaborators J. Owen and C. Clarke, have been informed of the problem and agree with our more recent calculations. Furthermore we have now found a more accurate scheme that allows us to reduce the error on the temperature by introducing column density as an additional parameter.

As well as the major shortcoming highlighted above, the Owen et al. (2010) calculations which were used to make predictions on the ionised phase of the wind spectra (Ercolano & Owen 2010, 2016), suffered from low spatial resolution, precluding us from being able to model the inner region of the bound disc, which may be relevant to interpret the broad wings of some of the wind-tracing emission lines presented in the recent work of Simon et al. (2016). Furthermore, a very limited parameter space was investigated, which included only two values for stellar mass, 3 values of X-ray luminosity for primordial discs and a single stellar mass and X-ray luminosity value for transition discs with 3 values for the cavity radius. This is nowhere near enough to draw any significant conclusions about trends in possible wind diagnostics.

In this project we aim at constructing new photoionisation models to remedy the shortcoming of the current models highlighted above. To that aim we have modified the hydrodynamical code PLUTO (Mignone et al. 2007, 2012) to include the effects of X-ray and EUV irradiation using the temperature-ionisation parameter from Ercolano et al. (2008a, 2009) also employed by Owen et al. (2010) for the ZEUS2D calculations. We have implemented the standard scheme in order to be able to compare our wind solutions to those available for a 0.7 and 0.1 $M_\odot$ central stars (Owen et al. 2010, 2011, 2012), for similar spatial resolution. This will ensure that we have implemented the algorithm correctly in PLUTO. This work is being carried out by Dr. Picogna, who is employed on a LMUExcellent grant awarded to the PI to carry out preparatory work for the Research Unit. The grant ends in November 2017.

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1.3 Project-related publications

Ercolano, B., Drake, J.; Raymond, J., Clarke, C. *X-Ray-Irradiated Protoplanetary Disk Atmospheres. I. Predicted Emission-Line Spectrum and Photoevaporation*, 2008, ApJ 688, 398. In this paper we present a first estimate of the magnitude of the X-ray photoevaporation process.

Ercolano, B., Clarke, C., Drake, J. *X-Ray Irradiated Protoplanetary Disk Atmospheres. II. Predictions from Models in Hydrostatic Equilibrium*, 2009, ApJ 699, 1639. We further develop our models to include the feedback of X-ray heating on the disc-structure in hydrostatic equilibrium, and obtain more accurate estimates of the photoevaporation rates.

Owen J., **Ercolano B.**, Clarke, C. *Radiation-hydrodynamic models of X-ray and EUV photoevaporating protoplanetary discs*, 2010, MNRAS, 401, 1415. We perform the first radiation-hydrodynamic calculations of an X-ray and EUV irradiated disc in 2D. The rates obtained here for the standard model still represent the state of the art and are widely used in the community.

Ercolano B., Owen J. *Theoretical spectra of photoevaporating protoplanetary discs: an atlas of atomic and low-ionization emission lines*, 2010, MNRAS 406,1553. We postprocess the models of Owen et al. (2010) and obtain synthetic observations of atomic and low-ionisation emission lines to be compared with the observations. We show that our models compare favourably with the observations available at the time.

Owen J., **Ercolano B.**, Clarke C. *Protoplanetary disc evolution and dispersal: the implications of X-ray photoevaporation*, 2011, MNRAS, 412, 13. We explore the role of X-ray photoevaporation in the evolution and dispersal of viscously evolving T Tauri discs. Our models confirm that X-rays play a dominant role in the evolution and dispersal of protoplanetary discs giving rise to the observed diverse population of transition discs, including some of those with massive outer discs, some of those with gas in their inner holes and some of those with detectable accretion signatures.

Owen J., Clarke & **Ercolano B.** *On the theory of disc photoevaporation* 2012, MNRAS, 422, 1880. We derive analytical scaling relations and derive estimates for the total mass-loss rates, as well as discussing the existence of similarity solutions for flows from primordial and transition discs. In this paper we catch a first glimpse at a new process for the clearing of the very last stages, which we name "thermal sweeping".

Ercolano B.,Rosotti G. *The link between disc dispersal by photoevaporation and the semimajor axis distribution of exoplanets*, 2015, MNRAS 450, 3008. We show here that details of the photoevaporation models (rates and profiles), strongly affect the planetary system configurations emerging from those discs.

Ercolano B., Owen J. *Blueshifted [O I] lines from protoplanetary discs: the smoking gun of X-ray photoevaporation*, 2016, MNRAS 460. 3472 We produce new synthetic observations of a particularly promising diagnostic, and demonstrate that the observations available at the time (before Simon et al. 2016) are consistent with the photoevaporation model. We show however that this line cannot be used to measure mass-loss-rates.

Ercolano B., Rosotti G., Picogna G., Testi L. *A photoevaporative gap in the closest planet-forming disc*, 2017, MNRAS 464L, 95 In this letter we show that the innermost gap in the disc around TW Hya, recently imaged by Andrews et al. (2016) with ALMA, is very likely due to X-ray photoevaporation.

Keto E. and **Caselli P.** *The Different Structures of the Two Classes of Starless Cores*, 2008, ApJ 683, 238. In this paper we developed an extremely simplified network which however we show to adequately describe CO-chemistry for the examples at hand. Similar techniques will be applied in this project.

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

The overarching aim of this project, in common with projects B2 (PI Caselli & Ercolano) and C2 (PI Ercolano), is to identify new wind tracers and use them to constrain mass loss rates and hence disc dispersal models, leading to the formation and evolution of Type 1 transition discs.

The new comprehensive radiation-hydrodynamics photoevaporation models developed in this project will enable a quantitative spectroscopic evaluation of new diagnostics of disc winds, via detailed astrochemical models developed together with project B2, using the dust model for the wind and atmosphere from project C2.

We will perform a comparison between TDs and primordial disc to provide important constraints on the wind architecture and the mechanism driving the dispersal. Type 1 TDs, are particularly interesting as the streamline architecture of their winds and the profiles of the lines that are produced in the wind differ from those of primordial discs. (e.g. Ercolano & Owen 2010, Ercolano & Pascucci, 2017, in preparation). Indeed the lines are expected to be broader and brighter for e.g. inner cavities of a few to 10 AUs.

The immediate objective of project B1 is to produce a new set of X-ray+UV photoevaporation models which goes well beyond the current state-of-the-art, described in the previous section.

The new models will constitute the backbone for the joint investigation to be carried out in projects B2 and C2, as well as allowing us to address the following important unsolved questions in the formation of Type 1 transition discs and their further evolution:

1. How fast do Type 1 TDs evolve/disappear after the inner disc has drained?

2. How does the formation & evolution of Type 1 TDs scale with stellar mass and stellar emission properties?
3. What is the role of FUV heating in the late evolution of Type 1 transition discs?

2.3 Work programme including proposed research methods

In this project we will construct a library of high resolution X-ray+EUV wind solutions for an extended grid of X-ray luminosities and stellar masses, covering all observed values. Our new calculations will make use of a new temperature scheme (Ercolano, Picogna & Owen, 2017, in preparation), derived from new more extensive X-ray + EUV photoionisation models. The new temperature scheme significantly reduces the error at low ionisation parameter values, allowing us to make solid predictions of the late evolution of transition discs.

Furthermore, our previous calculations (Owen et al. 2010, 2011, 2012), could only account for heating in the ionised phase of the wind, ignoring that the region beyond the layer heated by the soft X-ray ($< 1keV$) which could be heated by FUV radiation with typical PDR or XDR characteristics. While we show in Owen et al. (2012), that this should not affect the mass loss rates at around 1-10 AU, the effect of FUV heating at larger radii may be important. This is particularly relevant to the late evolution of transition discs, when the cavity becomes larger than approximately 30 AU. Indeed one of the problems with current photoevaporation models is the prediction of a large number of non-accreting transition disc with large holes (e.g., Owen 2016). In this project we will be able to test the suggestion that FUV heating may take over the late-stage evolution of transition discs, speeding up their final complete erosion.

2.4 Research Tools

For this project we will need the following tools:

1. A hydrodynamical code modified to include the effects of X-ray + EUV irradiation as we did in Owen et al. (2010). For that we use the Pluto code, for which extensive expertise exists in our team.
2. An efficient astrochemistry package to include a reduced chemical network into PLUTO. For that we will use KROME (Grassi et al. 2014) and link it with PLUTO.
3. An efficient radiative transfer algorithm to model the region just beyond the X-ray dominated region. We can use initially the implementation of radiative transfer and stellar irradiation for the PLUTO code (Kolb et al. 2013), developed by the group of Kley (PI of project D2). If insufficient the PI also has experience in the development of hybrid algorithms (Owen et al. 2014).

2.5 Research Plan

A grid of significantly improved new photoevaporation models including an accurate temperature scheme which includes X-ray, EUV and FUV heating will be developed in this project, by means of radiation-hydrodynamic calculations.

2.5.1 Months 1-12

In the preparatory work described in the previous section we have implemented the standard temperature scheme from Ercolano et al. (2008a, 2009) into PLUTO and have benchmarked the results against the work of Owen et al. (2010). In the first 12 months of the Research Unit we will then proceed with the implementation of the new, more accurate temperature scheme described in the previous Section (Ercolano, Picogna & Owen, 2017, in preparation). We will compare the resulting wind rates and profiles for the primordial and transition disc case. While we do not foresee large changes in the rates for primordial discs, as described in the previous section the evolution of transition discs will be most likely affected.

The new models will have much higher spatial resolution extending much closer into the star, in order to allow tracking profile components which may be emitted from the inner bound atmosphere of the disc.

This first set of models for $\sim$solar mass stars at a typical X-ray luminosity ($\sim 10^{30}$erg/sec) will be then passed on to projects C2 and B2 for the dust and detailed chemistry calculations.

2.5.2 Months 13-24

The parameter space of the calculations will be then significantly extended for the mass of the central star and its X-ray luminosity. Furthermore models of transitions discs at several stages of evolution, as tracked by the radius of their inner cavity, will be performed.

With the new models we will also be able to investigate how the process scales with stellar mass and stellar emission properties. This will allow us to check the theoretical relations for X-ray photoevaporation predicted by means of semi-analytical models and ab-initio arguments by Owen et al. (2012). While these relations are being widely used in the literature, they have until now never been tested. This will allow us to construct accurate population synthesis calculations to match the demographics of Type 1 TDs with those obtained with our models.

2.5.3 Months 25-36

At this point a robust and well tested reduced chemical network should be available from project B2 (PI Caselli, Ercolano). We will now couple our modified version of the PLUTO code to the KROME package to solve the chemistry using the reduced network from B2 and obtain the temperatures of the gas on the fly in the regions beyond the X-ray dominated regions. For that we will receive help from our collaborator Dr. Grassi, who is the main developer of the KROME code. Dr. Picogna has already attended the KROME school this year (`http://kromepackage.org/bootcamp/`) and a simple feasibility test has shown that this is a realistic task. As an example, KROME is already implemented in a number of hydrodynamics codes (e.g. RAMSES, ENZO, FLASH, GASOLINE, GIZMO). A number of publications performed with these codes are listed on the KROME webpage (`http://www.kromepackage.org/`).

A streamlined form of radiative transfer will be needed in PLUTO at this point, meaning that these calculations will probably be expensive to run. This is likely necessary to estimate the value of the FUV field reaching different regions of the disc atmosphere, where the optical depth are not high enough to justify the use of a (grey) flux limited diffusion method. Implementation of an efficient radiative transfer algorithm in PLUTO will be carried out together with the PI who has experience in the development of hybrid algorythms (e.g., Owen et al. 2014). **Kees to Barbara: In the original text it said Owen, Clarke & Ercolano 2014, but I could only find Owen, Ercolano & Clarke 2014. Check.** A simple RT scheme is already available for PLUTO (Kolb et al. 2013), which was developed in the group of our Prof. Kley (PI from project D1). Hence there is a substantial body of experience within our Research Unit team to successfully perform this task.

Note that we do not plan to run a full parameter space grid including the effects of the FUV heating. Our simulations will be limited to a selected number of cases aimed at specifically testing how strongly, and for what initial conditions, FUV heating may affect the evolution of the outer regions of discs, in particular of those in transition.

2.5.4 Future Outlook

A natural further step of this work is to perform a small set of 3D simulations to explore the effects of asymmetries in the inner disc and/or the presence of giant planets in the disc. We expect to see dramatic effects in the photoevaporation profile and in the wind architecture, which may lead to the formation of large hole TDs. This avenue has never been explored before and, while these models come at severe computational costs, they are likely to provide us with important insights on the structure and origin of TDs.

2.6 Data handling

A library of the hydrodynamical solutions in steady state (gas density and velocity) will be shared initially amongst the Research Unit members only and will be made available online on the public partition of the Research Unit server at the end of the first funding period.

2.7 Other information

Not Relevant

2.8 Information on scientific and financial involvement of international cooperation partners

Not Relevant

3. Bibliography

Alexander, R., Pascucci, I., Andrews, S., Armitage, P., & Cieza, L. 2014, Protostars and Planets VI, 475
Alexander, R. D., Clarke, C. J., & Pringle, J. E. 2006a, MNRAS, 369, 216
Alexander, R. D., Clarke, C. J., & Pringle, J. E. 2006b, MNRAS, 369, 229
Andrews, S. M., Wilner, D. J., Zhu, Z., et al. 2016, ApJ, 820, L40
Armitage, P. J. 2011, ARA&A, 49, 195
Armitage, P. J., Simon, J. B., & Martin, R. G. 2013, ApJ, 778, L14
Bai, X.-N. & Stone, J. M. 2013, ApJ, 769, 76
Clarke, C. J., Gendrin, A., & Sotomayor, M. 2001, MNRAS, 328, 485
Ercolano, B., Barlow, M. J., & Storey, P. J. 2005, MNRAS, 362, 1038
Ercolano, B., Barlow, M. J., Storey, P. J., & Liu, X.-W. 2003, MNRAS, 340, 1136
Ercolano, B. & Clarke, C. J. 2010, MNRAS, 402, 2735
Ercolano, B., Clarke, C. J., & Drake, J. J. 2009, ApJ, 699, 1639
Ercolano, B., Clarke, C. J., & Hall, A. C. 2011, MNRAS, 410, 671
Ercolano, B., Drake, J. J., Raymond, J. C., & Clarke, C. C. 2008a, ApJ, 688, 398
Ercolano, B., Koepferl, C., Owen, J., & Robitaille, T. 2015, MNRAS, 452, 3689
Ercolano, B. & Owen, J. E. 2010, MNRAS, 406, 1553
Ercolano, B. & Owen, J. E. 2016, MNRAS, 460, 3472
Ercolano, B. & Rosotti, G. 2015, MNRAS, 450, 3008
Ercolano, B., Rosotti, G. P., Picogna, G., & Testi, L. 2017, MNRAS, 464, L95

Ercolano, B., Young, P. R., Drake, J. J., & Raymond, J. C. 2008b, ApJS, 175, 534
Font, A. S., McCarthy, I. G., Johnstone, D., & Ballantyne, D. R. 2004, ApJ, 607, 890
Gorti, U., Dullemond, C. P., & Hollenbach, D. 2009, ApJ, 705, 1237
Grassi, T., Bovino, S., Schleicher, D. R. G., et al. 2014, MNRAS, 439, 2386
Hartmann, L. 2008, Accretion Processes in Star Formation
Haworth, T. J., Clarke, C. J., & Owen, J. E. 2016, MNRAS, 457, 1905
Koepferl, C. M., Ercolano, B., Dale, J., et al. 2013, MNRAS, 428, 3327
Kolb, S. M., Stute, M., Kley, W., & Mignone, A. 2013, A&A, 559, A80
Lopez, E. D. 2016, ArXiv e-prints
Mignone, A., Bodo, G., Massaglia, S., et al. 2007, ApJS, 170, 228
Mignone, A., Flock, M., Stute, M., Kolb, S. M., & Muscianisi, G. 2012, A&A, 545, A152
Owen, J. E. 2016, PASA, 33, e005
Owen, J. E., Clarke, C. J., & Ercolano, B. 2012, MNRAS, 422, 1880
Owen, J. E., Ercolano, B., & Clarke, C. J. 2011, MNRAS, 412, 13
Owen, J. E., Ercolano, B., & Clarke, C. J. 2014, in Astrophysics and Space Science Proceedings, Vol. 36, The Labyrinth of Star Formation, ed. D. Stamatellos, S. Goodwin, & D. Ward-Thompson, 127
Owen, J. E., Ercolano, B., Clarke, C. J., & Alexander, R. D. 2010, MNRAS, 401, 1415
Owen, J. E., Scaife, A. M. M., & Ercolano, B. 2013, MNRAS, 434, 3378
Pascucci, I., Ricci, L., Gorti, U., et al. 2014, ApJ, 795, 1
Rosotti, G. P., Ercolano, B., & Owen, J. E. 2015, MNRAS, 454, 2173
Rosotti, G. P., Ercolano, B., Owen, J. E., & Armitage, P. J. 2013, MNRAS, 430, 1392
Schisano, E., Ercolano, B., & Güdel, M. 2010, MNRAS, 401, 1636
Simon, M. N., Pascucci, I., Edwards, S., et al. 2016, ApJ, 831, 169
Yasui, C., Kobayashi, N., Tokunaga, A. T., Saito, M., & Tokoku, C. 2009, in American Institute of Physics Conference Series, Vol. 1158, American Institute of Physics Conference Series, ed. T. Usuda, M. Tamura, & M. Ishii, 171–172
Yasui, C., Kobayashi, N., Tokunaga, A. T., Saito, M., & Tokoku, C. 2010, ApJ, 723, L113

4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We require funding for one Postdoc to work at the LMU in the group of Prof. Ercolano. In case of an award Dr Picogna has agreed to take on the post. Dr Picogna is currently employed in the group of the PI and is performing preparatory work for the project. Dr Picogna's expertise in astrophysical fluid dynamics and his familiarity with the subject is of great advantage for the achievement of the aims of this project. Dr Picogna's contract ends in November 2017,

4.1.2 Direct Project Costs

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

Will be provided by the host institution

4.1.2.2 Travel Expenses

Total: 9900 € Justification : Each year one national trip (meeting of Astronomical Society, national meetings) and one international trip (conference, visit collaborators). During the course of the PhD 2

one week long visits to our main international collaborator, Dr J. Owen (currently at Princeton University, will move to Imperial College London in 2017).
Cost estimate:

- National trip: 5 overnight stays, train/airfare, conference fee; 1000 € (3000 over 3 years).
- International trip: 6 overnight stays, airfare, conference fee; 1500 € (4500 over 3 years).
- Visit to/from J. Owen: airfare, 6 overnight stay 1200 € (2400 for 2 visits)

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

Not Relevant

4.1.2.4 Other Costs

None

4.1.2.5 Project-related publication expenses

We request 770 €/year (total 2250 €) for publication expenses.

4.1.3 Instrumentation

None

4.1.3.1 Equipment exceeding EUR 10,000

None

4.1.3.2 Major Instrumentation exceeding EUR 100,000

None

5. Project requirements

5.1 Employment status information

Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München (permanent)

5.2 First-time proposal data

Not Relevant

5.3 Composition of the project group

?????

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

This project will provide the radiation-hydrodynamic models of the wind which are needed by project B2 (PI: Prof. Caselli) for the chemical calculations and by project C2 (PI: Ercolano) for the dust entrainment. Project BI depends on input from project B2 (PI: Prof. Caselli) for the reduced network and on project A2 for observations. Specifically project A2 can provide insights on the emission properties of the irradiating stars.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

Dr. James Owen (Princeton) will be heavily involved in the project. Dr. Owen developed the original phoionisation models during his PhD project at the Institute of Astronomy in Cambridge, which was co-supervised by Prof. Ercolano. It is envisioned that Dr. Owen will pay regular visit to our group to help with the development of the new models.

Dr. Tommaso Grassi (STARplan Copenhagen, Denmark) is an expert of chemistry and the microphysics of the ISM coupled with hydrodynamical simulations of (e.g.) star-forming regions. He lead the development of the KROME package (http://www.kromepackage.org/) .

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

Maite Bertran (INAF-Osservatorio Astrofisico di Arcetri), Aaron Boley (University of British Columbia), Sandra Brünken (University of Cologne), Stephanie Cazaux (University of Groningen), Cecilia Ceccarelli (Univ. Grenoble Alpes), Francesco Fontani (INAF-Osservatorio Astrofisico di Arcetri), Thomas Hartquist (University of Leeds), Izaskun Jimenez-Serra (Queen Mary University London), Eric Keto (Harvard-Smithsonian Center for Astrophysics), Marco Spaans (University of Groningen), Jonathan Tan (University of Florida), Stephan Schlemmer (University of Cologne), Charlotte Vastel (Université de Tulouse), Malcolm Walmsley (INAF-Osservatorio Astrofisico di Arcetri); F. Niederhofer (STSci, USA); M. Hilker (ESO, Garching); N. Bastian (U. Liverpool, UK); M. Guarcello (U. Palermo, Italy); M. Tazzari (U. Cambridge, UK); A. Natta (Florence, Italy); R. Alexander (U. Leicester); D. Hubber (LMU); J. Dale (U. Hertfordshire, UK); C. Koepferl (LMU); I. Bonnell (U. St. Andrews, UK); A. McLeod (ESO, Garching); D. Boneberg (U. Cambridge, UK); R. Parker (U. Liverpool, UK); R. Wesson (UCL, London, UK); M. Barlow (UCL, London, UK); A. Glassgold (u. Berkeley, USA); C. Manara (ESA, Noordwjik, Netherlands); A. Danekhar (CfA, Harward, USA); Q. Parker (Sidney, Australia); S. Casassus (U. de Chile, Santiago, Chile); I. Pascucci (U. Arizona, USA); A. Bevan (UCL, London, UK).

5.5 Scientific equipment

The group of Prof. Ercolano has two own computer clusters comprising

- 2 CPU Intel Xeon X5650 (Westmere, beginning 2010, 2.66 GHz) 6 cores each 12 cores total (24 virtual) 74 GB ram.
- 4 CPU Intel Xeon E7-4850 (Ivy Bridge, beginning 2014, 2.30 GHz) 12 cores each 48 cores total (96 virtual) 660 GB ram.

Further computational power is provided through the C2PAP facility of the Excellence Cluster to which the group has guaranteed time. This comprises 126 nodes, each node with 2 CPU Intel Xeon E5-2680 (Sandy Bridge, beginning 2012, 2.7 GHz) 8 cores each 16 cores total (32 virtual) 64 GB ram.

Note that while the future of the Excellence Cluster Universe is uncertain, the C2PAP facilities will be in any case supported by the LMU.

The CAS group of Prof. Caselli has also its own cluster: an HPC cluster comprising of 25 nodes with 20 cores and 128 GB memory each; 4 nodes with 20 cores and 256 GB memory each (Infiniband, 50 TB storage, Login-Node, Batch-System; 2 Compute nodes, i.e. 2 nodes with 20 cores and 512 GB (10 TB storage).

The HPC facilities at the Leibniz Rechenzentrum (LRZ) are also available to us. These include iDataPlex HPC System HYDRA with Intel Ivy Bridge processors (3500 nodes with 20 cores at 2.8 GHz each).

Furthermore the CAS centre led by Prof. Caselli has available computer facilities for visiting scientists and students. CAS has its own cluster: an HPC cluster comprising of 25 nodes with 20 cores and 128 GB memory each; 4 nodes with 20 cores and 256 GB memory each (Infiniband, 50 TB storage, Login-Node, Batch-System; 2 Compute nodes, i.e. 2 nodes with 20 cores and 512 GB (10 TB storage).