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 modality of disc dispersal 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 comprehensive radiation-hydrodynamical calculations of irradiated discs, coupled to photoionisation, chemistry and radiative transfer calculations for a large parameter space, covering stars of different masses and X-ray properties. This will constitute the backbone for the work carried out in several sub-projects of this proposal (e.g. 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 several 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 to date is considered to be photoevaporation by radiation from the central star (e.g., Clarke et al. 2001), because, when combined with viscous theory for the accreting disc, matches many of the observational timescale constraints. As described in more details below, in this model the disc is dispersed because the mass loss rate due to a photoevaporative wind eventually exceeds the mass accretion rate through disc, allowing the disc to quickly be eroded from the inside-out.

Recent work suggests that magnetohydrodynamic (MHD) effects may also drive disc winds (Bai & Stone 2013, e.g.,) 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. Some preliminary estimates suggest that MHD winds may be comparable to photoevaporative winds in their strength, and that non-ideal MHD effects may also dominate over magneto-rotational-instability (**?**, MRI,) in the transport of angular momentum (i.e. accretion) through the disc. While these models are still in their infancy and the mass loss and accretion rates from MHD winds are at present highly uncertain, they still raise important questions about the validity of the majority of disc models which rely on α prescriptions. However a number of important uncertainties need to be resolved before the relevance of non-ideal MHD effects to disc evolution can be assessed. These include 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) Another key ingredient is the level of ionisation in the atmosphere of discs, which determines the nature of the gas coupling to the 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, where the underlying physics is better understood and the observations can be used to constrain a number of important parameters, thus reducing the degrees of freedom involved.

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), 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 going through the transition disc pahse, before disappearing completely. (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. The 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 much 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 and the migration 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).

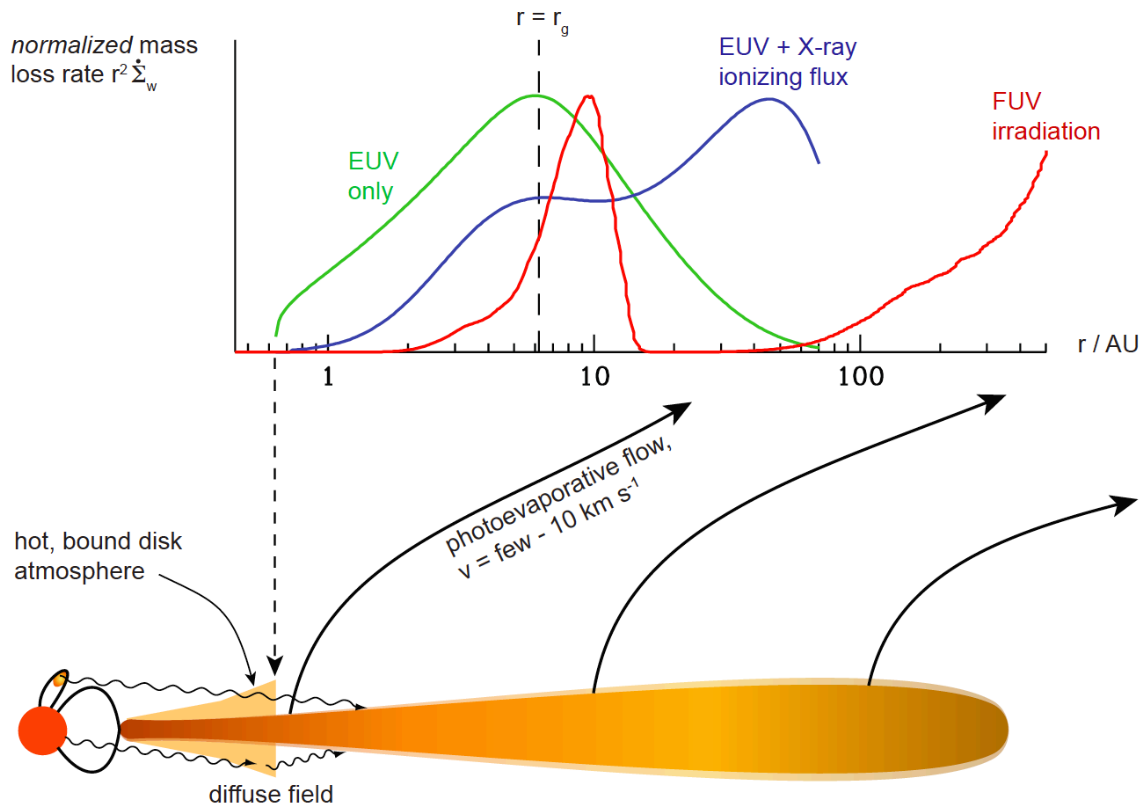

Figure 1: From Armitage (2011). Different photoevaporation profiles corresponding to the EUV-only model of Alexander et al. (2006a,b), the EUV+X-ray of Owen et al. (2010) and FUV model estimates of Gorti et al. (2009). The profiles have been normalised, where the total mass loss rates can differ by over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

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 somewhat 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 James Owen, a former 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 winds to date (Owen et al. 2010, 2011, 2012). For this calculation we used 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. The parameter space covered by these models is also rather small. 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 that a significant population of them should exist, 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). A detailed calculation of thermal sweeping is still lacking.
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 heating 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 developed were based on EUV irradiation only. This was mainly due to the need of simplifying the hydrodynamics by assuming the gas is isothermal (Alexander et al. 2006a,b). An EUV heated gas, where hydrogen is almost fully ionised, is indeed roughly isothermal ($\sim10^4$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 cannot directly be ionised by the X-ray so it 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 from a metal (e.g. C, N, O). The ejected supra-thermal electron produces then secondary ionisations (of mostly H and He). 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 in this section 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 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 use the MOCASSIN code to present a first estimate of the magnitude of the X-ray photoevaporation process in protoplanetary discs. We obtain mass loss rates that are significantly higher than previous estimates, showing the relevance of this process to the dispersal of discs. Before this work the importance of X-ray photoevaporation had not been recognised.

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, which confirm our previous conclusions that the X-ray photoevaporation process is a main player in the dispersal of discs. These calculations provide the starting conditions for the full hydrodynamical investigations to Owen et al. (2010).

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. For that we modified a standard hydrodynamics code (ZEUS-2D) to include the X-ray heating rates calculated in the previous papers (Ercolano et al. 2008, 2009). 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 those with massive outer discs and with residual gas in their inner holes, which provides 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. We suggest that the deserts and peaks seen in the distributions are a result of photoevaporation parking the giant planets at specific radii.

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, [OI] 6300 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 and suggest that a thermochemical model of the wind launching region is necessary.

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. We demonstrate how all current observational data fit the predictions of the model and provide new estimates for the timescales of dust-draining from the inner disc.

Keto E. and **Caselli P.** *The Different Structures of the Two Classes of Starless Cores*, 2008, ApJ 683, 238. We construct a reduced chemical network for oxygen chemistry (including water and carbon monoxyde), include it into a hydrodynamical code of the evolution of Bonnor-Ebert (BE) spheres and compare the results with observations. For the first time, we demonstrate that dense cloud cores contract as unstable quasi-equilibrium BE spheres, while the singular isothermal sphere and Larson-Penston solutions for dense core contraction do not reproduce the observed line profiles. This was only computationally possible because the number of reactions was reduced to the core. A similar approach will be used in B1 and B2.

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.

2.3.1 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).

2.3.2 Research Plan

2.3.2.1 Preparatory work

In this section we will describe preparatory work that is currently being carried out by Dr G. Picogna. Dr Picogna is employed in the group of Prof. Ercolano via an Excellent Initiative grant from the LMU, awarded to the PI to carry out preparatory work for this Research Unit proposal. The grant ends in November 2017.

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 an extremely simplified version of the above has large computational costs, if it needs to be performed at every time-step of a hydrodynamical calculation.

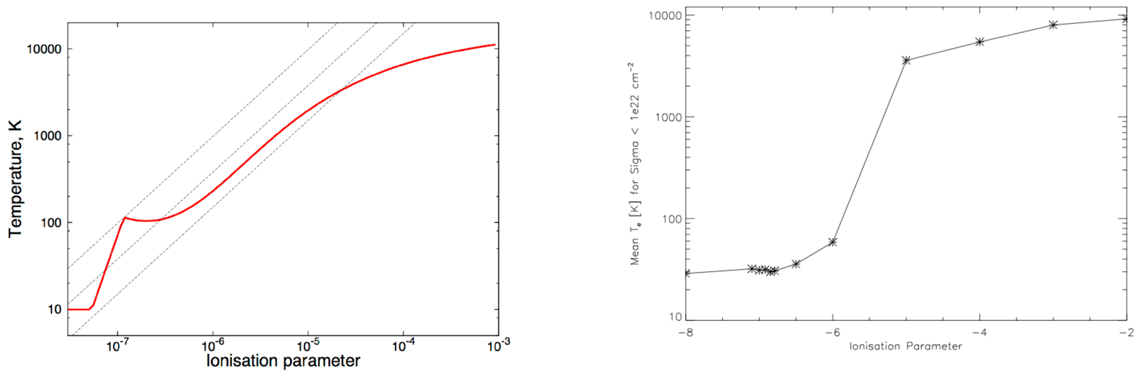

Figure 2: The electron temperature versus ionisation parameter relation in the calculations of Haworth et al. (2016), **left panel**, compared to our most recent calculations Ercolano, Picogna & Owen, (in preparation), **right panel**.

In such cases it is convenient to look for parameterisations of the gas temperature in terms of quantities that are easy to determine on the fly during the hydrodynamical run (e.g. gas properties and/or column density). Indeed the radiation-hydrodynamical calculations of X-ray + EUV driven photoevaporative winds of Owen et al. (2010, 2011, 2012), described in the previous section, were performed using such a temperature paremeterisation. The parameterisation was determined via detailed X-ray photoevaporation models using the MOCASSIN code (Ercolano et al. 2008a, 2009) The models were run with a version of the ZEUS2D code which was modified by us to include a temperature scheme based on the ionisation parameter at each cell in the calculation. This was based on our previous work (Ercolano et al. 2008a, 2009). where it was shown that, within the penetration depth of ~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, which is currently poorly represented by the parameterisation of Ercolano et al. (2008a, 2009). Note that the recent work of Haworth et al. (2016), 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 no kink in the temperature parameterisation at low ionisation parameter, which is important as the results of Haworth et al. (2016) are a consequence of this. 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

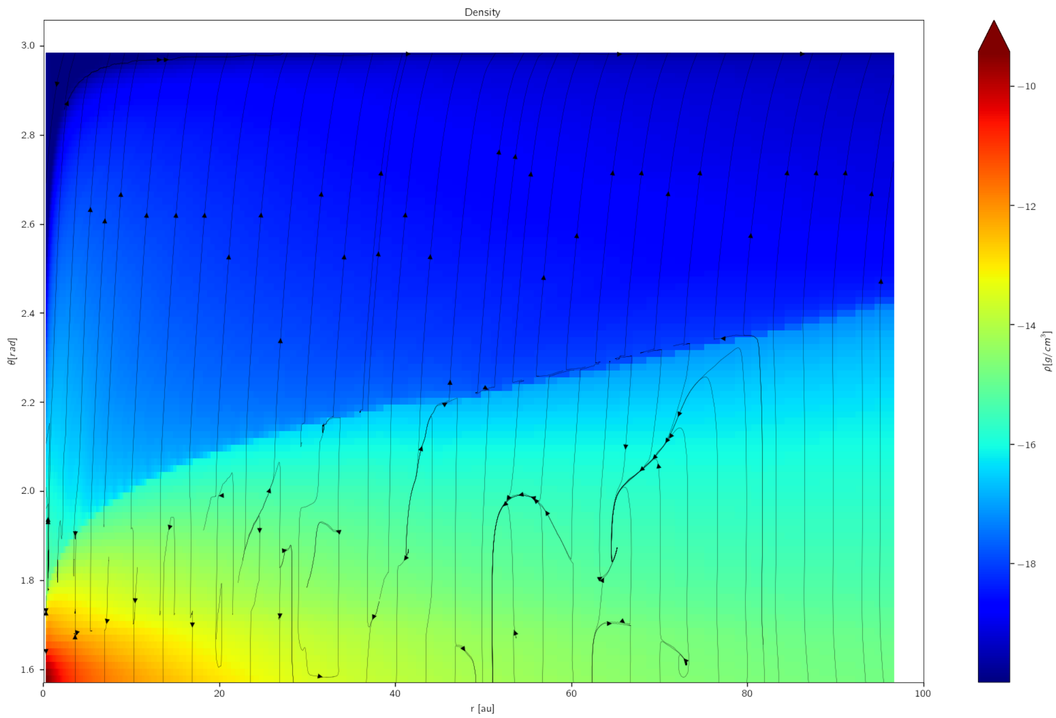

Figure 3: Column density map of our PLUTO simulation of the standard model from Owen et al. (2010), i.e. a 0.7 $M_\odot$ star with X-ray luminosity of $2{\times}10^{30}\,erg/sec$. The figure is in polar coordinate, where the colour scale indicates column density and the overlain black lines are the streamlines tracing the outflow.

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.

Figure**??** shows a snapshot from our most recent simulation with our modified version of PLUTO aiming at reproducing the standard model of Owen et al. (2010). This is for 0.7 $M_\odot$ star with X-ray

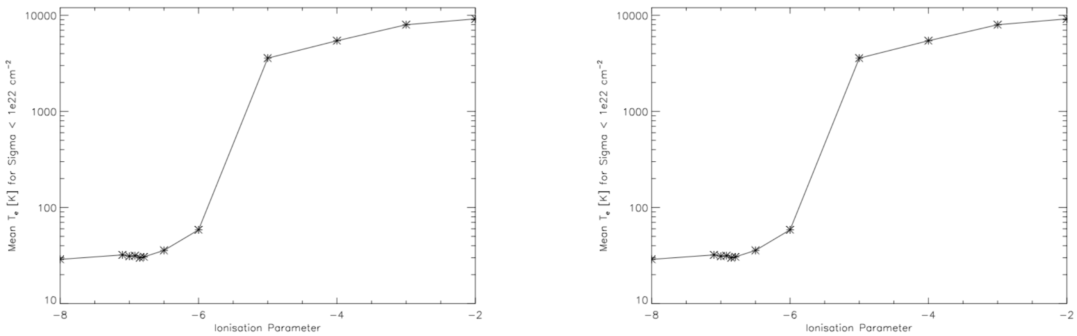

Figure 4: Left panel: The wind profile for our PLUTO calculation of the standard model by Owen et al. (2010). The plot shows the surface density wind rate multiplied by the square of the radius (i.e. it can be compared directly to the profiles shown in Figure 1 of this proposal. Right: The cumulative mass-loss-rate as a function of disc radius. The integrated value (to 100 AU) of the mass loss rate is approximately $1.2\times10^{-8} M_{\odot}/yr$.

luminosity of $2\times10^{30} erg/sec$. For further details on the simulation set-up we refer to Owen et al. (2010). The figure shows column densities in a quarter of the disc in polar coordinates. Overplotted black lines are streamlines showing the outflowing gas. In order to test that our implementation of the temperature scheme works correctly we have used the same parameterisation used by Owen et al. (2010). We match the global mass-loss-rate to within 15% (we obtain a value of $1.2\times10^{-8} M_{\odot}/yr$ (see right panel of Figure **??** and we show in the left panel of Figure **??** that we can reproduce the approximate wind profile. The plot shows the surface density wind rate multiplied by the square of the radius (i.e. it can be compared directly to the profiles shown in Figure 1 of this proposal.

2.3.3 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 presented by Owen et al. (2010). 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.

In particular we will test the late evolution of transition discs to estimate whether there is a radius for the inner cavity at which photoevaporation stalls. In that case one would expect to be able to observe a population of transition discs with large cavity and no accretion signature (relic discs), which to date remains elusive. A solution to this problem, form the theoretical stand-point, would be the triggering of a fast final clearing phase, as the proposed final thermal sweeping (Owen et al. 2011). Our models will be able to test this hypothesis in detail for the first time, as previous works have all been limited by the uncertainties in the temperature parameterisation of the X-rays at low ionisation parameters (e.g. Haworth et al 2016). We will then create synthetic population to check the occurrence of relic discs and compare it with the limits shown by current observational surveys.

Furthermore, the new models will have much higher spatial resolution extending much closer into the star, in order to allow tracking the profile components of emission line which may be produced from the inner bound atmosphere of the disc (see discussion in Ercolano & Owen 2016 and in the Introductory section of this proposal).

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.

2.3.4 Months 13-24

Once our machinery is complete and well-tested we will be able to switch to production-mode and extend significantly the parameter space of the calculations. Specifically, we will vary the mass of the central star and its X-ray luminosity as well as the accretion properties of the disc. Furthermore models of transitions discs at several stages of evolution, as tracked by the radius of their inner cavity, will be performed.

As new models become available and we populate the parameter space, we will make the grids available immediately to projects C2 and B2 for the dust and detailed chemistry calculations. At this stage we will already start to regularly check our model predictions against observations, with the help of experts from projects A1 and A2.

The new models will also allow us to investigate how the photoevaporation process scales with stellar mass and stellar emission properties. We will test the theoretical relations for X-ray photoevaporation predicted by means of semi-analytical models and ab-initio arguments by Owen et al. (2012). These relations are already being widely used in the literature and they are a crucial ingredient for population synthesis models of planet formation, where photoevaporation is included in the disc evolution and affects the timescales and location for the formation of giant planets, as well as their successive migration.

The larger parameter space will also allow us to improve on our initial calculations to construct more accurate synthetical populations of evolved discs to match the observed demographics of Type 1 TDs. Note that project A1 will keep an up-to-date record of the transition disc demographics throughout the duration of the Research Unit.

2.3.5 Months 25-36

The role of FUV heating in supporting or competing with the X-rays in the removal of the disc is still uncertain. As we discussed in the previous sections, the work of Gorti, Dullemond & Hollenbach (2009), based on 1+1D thermochemical calculations in hydrostatic equilibrium, suggest that a vigorous thermal wind may be driven as a result of FUV-heating. For some disc parameters (in particular in the presence of PAHs), the FUV is shown to reach mass-loss-rates comparable to those driven by X-rays. An hydrodynamical calculation of an FUV driven wind is however still lacking and it is urgently needed in order to assess the importance of this process, in particular at large disc radii, which is relevant to the problem of disc relics, amongst other things.

At this stage of the Research Unit 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 however necessary in order 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). 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.

2.3.6 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.

In particular in the second funding period of the Research Unit, the results from sub-projects D1 and D2 will be available to us, and the natural further step will be to combine photoevaporation to planet-disc interaction calculations.

2.4 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.

2.5 Other information

Not Relevant

2.6 Information on scientific and financial involvement of international cooperation partners

Not Relevant

3. Bibliography

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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

Paola Caselli, Director of MPE and of the Centre of Astrochemical Studies at the MPE (permanent). Prof. Caselli will provide guidance in treating the heating and cooling channels due to chemistry at the base of the flow into our hydynamics calculations.

Dr. Wing-Fi Thi, postdoc (current contract ends in 2009), works in the CAS group of Prof. Caselli and is an expert in chemical models of protoplanetary discs.

Dr Alexei Ivlev, researcher (permanent), works in the CAS group of Prof. Caselli and is an expert in grain charging and X-ray transport.

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 & Prof. Ercolano) 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 & Prof. Ercolano) for the reduced network and on project A2 (PI Prof. Preibisch) for observational input. Specifically project A2 (Prof. Preibisch) can provide insights on the emission properties of the irradiating stars. We already have made used extensively of the results coming from the group of Prof. Preibisch in terms of realistic X-ray luminosity functions for the construction of population synthesis of discs and of the individual X-ray spectra, when considering the ionisation and heating of individual sources.

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 leads 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).