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TITAN: A TRANSFER-PHOTOIONISATION CODE FOR HOT, THICK MEDIA

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Abstract. The photoionization code TITAN, developed by our team, is well suited for the study of both optically thick and thin ionized media. It treats all relevant physical processes from each level and all induced processes, computing the gas structure in thermal and ionization equilibria. It gives as output the ionization, density, and temperature structures, as well as the reflected, emitted outward, and absorbed spectra. Its advantages over other photoionization codes are the exact transfer of both the lines and the continuum, using the Accelerated Lambda Iteration method, and the possibility of treating the ionized gas in total (gas+radiation) pressure. Models in pressure equilibrium present temperature discontinuities which, however difficult to tackle, can be adressed with TITAN. The most recent version of our code allows to choose between the hot and the cold stable solutions in the multi-branch regime of the S-curve, and then to compute a fully consistent photoionisation model with the chosen solution. For the first time, it is thus possible to compare the true stable solution models with the approximate solution model, used so far. We have studied the thermal instabilities in thick stratified X-ray illuminated media and compared the behavior of both kind of models. Our studies may be applied to media in any pressure equilibrium conditions, like constant gas pressure, constant total pressure, or hydrostatic pressure equilibrium.

1 The photoionization code TITAN: past, present and future

TITAN is a non-LTE, photoionization-transfer code developed at Paris Observatory (see, for instance, Dumont et al. 2000, 2002; Collin et al. 2004); it is aimed at studying dense, warm (temperature $\sim 10^4$–10^7 K), and optically thick media (Thomson thickness $\sim$ 0.1–100), although it can also be applied to thin media (Thomson thickness $\sim$ 0.01–0.1). It assumes a 1D plane-parallel geometry, with a slab of gas illuminated on one side (eventually on the two sides) by an irradiating X-ray source. TITAN computes the gas structure in ionization and thermal equilibrium, including all relevand processes: photoionization, radiative and di-electronic recombination, ionization by high-energy photons, fluorescence, radiative and collisional excitation/de-excitation, etc. The energy balance is ensured locally with a precision of 0.01%, and globally with a precision of 1%. In adition to the density, pressure, temperature and ionization structures, in provides the outward, transmitted and reflected spectra. The atomic data include ions and atoms of H, He, C, N, O, Ne, Mg, Si, S, and Fe; for the time being, they omit features like the Unresolved Transition Array (UTA) and the inner shell transitions (except the iron K lines), but these will be added in a forthcoming update of the atomic data.

Until 2002, the code used a 2-stream approximation for the line transfer; the Accelerated Lambda Iteration (ALI) method was applied to the continuum, only. Both the incident continuum and the outward flux were treated isotropically. Already then, the TITAN code allowed for the modeling of gas in constant density or constant pressure — either gas pressure, or total (gas + radiation) pressure. Applications of these early stages of the code included, for instance, the modeling of the accretion disk structure in Active Galactic Nuclei (AGN) (Madej & Różańska 2000; Różańska et al. 2002).

From 2002 to 2006 the code suffered some improvements; in particular, we replaced the 2-stream approximation treatment of the lines by the ALI method; line and continuum fluxes were thus treated in a consistent and precise way. This is a major improvement over other photoionization codes such as Cloudy (Ferland et al. 1998), XSTAR (e.g. Kallman & Bautista 2001), or ION (Netzer 1993, 1996) which use, at least for the lines, an integral formalism called the "escape probability approximation". Furthermore, ALI enables a multi-direction

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utilisation of the code, allowing for any illumination angle (including the normal direction) and any direction of the outward and reflected emission. A turbulent component was added to the total pressure computation. In what concerns the atomic data, these have been improved with additional lines of Fe and O. This fully operational version of the code has recently been used to study the soft X-ray spectra of AGN (Chevallier et al. 2006) and applied to model real data, as the Warm Absorber in NGC 3783 with a single medium in total pressure equilibrium (Gonçalves et al. 2006), or the spectra of bright ultraluminous X-ray sources (Gonçalves & Soria 2006).

Most recently, we have developped and implemented a new algorithm into the TITAN code, allowing to address the thermal instabilities observable in photoionized gas in thermal equilibrium. In TITAN's previous computational scheme, the thermal energy balance equation was solved for a given density at a given depth (that of the previous iteration); this method provided a unique solution for the temperature. The model corresponding to this scheme is called "intermediate" model. In the new version of TITAN, the energy balance equation is solved for a given total pressure, assumed to be constant along the slab. In some regions of the cloud, this computational scheme leads to two stable solutions, described by two separate models. In one of the models, the "hot" solution is systematically chosen for all layers, while in the other model the "cold" solution is systematically preferred. These models are called "hot" and "cold" models, respectively. This new algorithm was applied to the study of optically thick, stratified media, in total pressure equilibrium; we have chosen to work with a few models encompassing the range of conditions valid for the Warm Absorber in AGN. Our studies can be applied to media in any pressure equilibrium conditions, e.g., constant gas pressure, constant total pressure, or hydrostatic pressure equilibrium.

2 Thermal instabilities in thin and thick media

First, let us introduce the subject of thermal instabilities in thin and thick media, and address the main differences observed in each case. It is well known that a photoionized gas in thermal equilibrium can display a thermal instability (e.g. Krolik et al. 1981). The phenomenon manifests itself in the S-shape of the net cooling function, or, which is equivalent, through the curve giving the temperature versus the radiation-to-gas-pressure ratio. Such an S-shape curve allows for the co-existence of gas at different temperatures and densities for the same pressure ratio. For a given value of the radiation-to-gas-pressure ratio, the gas can then be in 3 states of thermal equilibrium. One of these states is thermally unstable; the two others (a "hot" and a "cold" solution) are stable. Such thermal instabilities are, for instance, at the origin of the two-phase model for the interstellar medium (Field et al. 1969) and the two-phase medium interpretation of the Broad Line Region in AGN (Krolik et al. 1981). Since Krolik et al., many studies have been devoted to the S-shape curve, but always in the optically thin case. Thanks to the most recent developments of the TITAN code, it is now possible to address, for the first time, the thermal instabilities in the case of optically thick[1] media such as the Warm Absorber (WA) in type 1 AGN, the X-ray line-emitting gas in type 2 AGN, or irradiated accretion discs in AGN and X-ray binaries.

In optically thin media, the radiation pressure keeps a constant value, and the energy balance equation solution depends on the gas pressure only. When the gas pressure is small compared to the radiation pressure, there is a unique, stable, "hot" solution, where both the heating and the cooling are dominated by Compton processes. As the gas pressure increases, atomic processes become important, and multiple solutions arise. The harder the spectrum, the more extended is the region encompassed by the multiple solutions. Then, above a given gas pressure, again a unique, but this time "cold" solution, arises.

The thermal instability problem in thick media is very different from what happens in thin media, this for mainly two reasons. First, the spectral distribution of the mean intensity J_ν at the illuminated surface of the medium is different from the incident spectrum, as it equally contains a "returning" radiation component emitted by the slab of gas itself. Figure 1 shows the spectral distribution of the mean continuum intensity at the slab surface for three models with different values of the column density, $N_{\rm H}$. All the models were computed under total pressure equilibrium, null turbulent velocity, and cosmic abundances; the hydrogen numerical density at the illuminated surface was 10^7 cm^{-3}. The thermal and ionization structures are mainly determined by the

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[1] Note that by "optically thick", we here mean media optically thick to the photoionization continuum; this is the case for gas irradiated by a continuum that gets absorbed at one or more ionization edges, being therefore altered when passing through the medium. In a weakly ionized medium, this can occur for a column density as small as 10^{18} cm^{-2}.

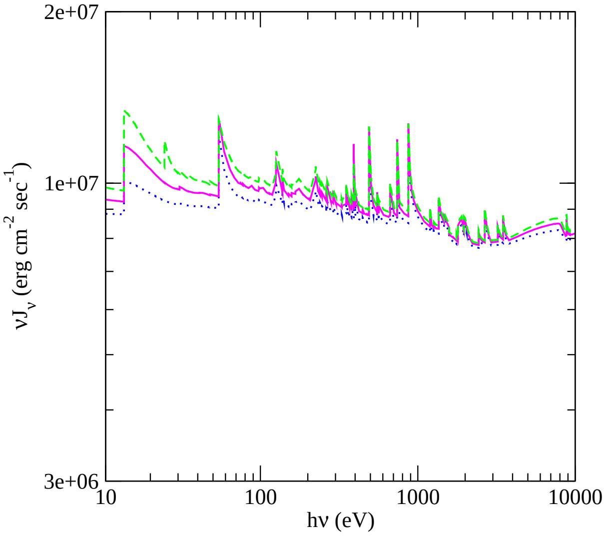

Fig. 1. Spectral distribution of the mean continuum intensity, computed at the illuminated surface of the slab, for three models with the same ionization parameter ($\xi = 1000$) and different column densities: $N_{\rm H} = 2\,10^{23}$ cm^{-2} (dotted line), $2.5\,10^{23}$ (filled line), and $3\,10^{23}$ (dashed line). For the sake of clarity, the spectral lines have been supressed from this figure, where only the continuum is shown; this displays important discontinuities, which increase with the slab thickness.

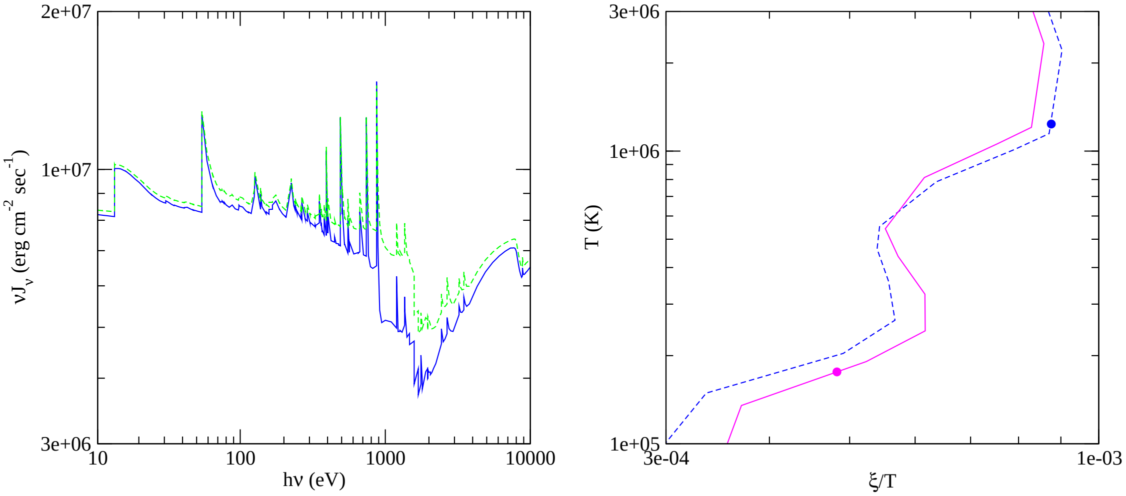

Fig. 2. Results for the $\xi = 1000$ and $N_{\rm H} = 2\,10^{23}$ cm^{-2} model. Left-hand panel: the spectral distribution of the mean continuum for two layers located at different depths in the gas slab: $1.66\,10^{17}$ cm (dashed line) and $1.90\,10^{17}$ cm (solid line). Right-hand panel: the S-curves giving the temperature T versus ξ/T for the same two layers (the same line-codes apply); the dots represent the equilibrium temperature found for each layer.

ionization parameter ξ and the shape of the incident continuum, here a power-law of photon index $\Gamma = 2$, covering the $10-10^5$ eV energy range. We observe that the spectrum at the irradiated surface contains strong discontinuities, whose amplitude increases with the slab thickness, as does the intensity of the whole spectrum. Second, the spectral distribution changes as the radiation progresses inside the medium; as a consequence, the shape of the S-curve also changes, and instead of traveling along a given S-curve as the radiation-to-gas pressure ratio decreases, the temperature follows successively different curves. This behaviour is illustrated in Fig. 2, which shows the spectral distribution of the mean continuum for two layers located at different depths in the gas slab, and the corresponding curves giving T versus ξ/T. We can see that the S-curves are different for the two represented layers and that the deeper layer displays a larger multi-branch region; this is due to its larger absorption trough.

3 Some results and observational implications

Our studies have shown that a thick, stratified medium, ionized by X-rays, behaves differently from a thin ionized medium. This happens for mainly two reasons: first, the spectral distribution of the mean intensity at the illuminated surface of the slab is different from the incident spectrum, as it equally contains a "returning" radiation component emitted by the slab itself; second, the spectral distribution changes as the radiation progresses inside the medium and, as a consequence, the shape of the S-curve also changes. These effects depend on the thickess of the medium and on its ionization.

This has observational implications in the emitted/absorbed spectra, ionization states, and variability. It is impossible to know what solution the plasma will adopt when attaining the multi-solutions regime: it can oscillate between the hot and cold solutions, it can fragment into hot and cold clumps which will coexist together, or it can take the form of a hot, dilute medium confining cold, denser clumps. In addition, the relative proportion of those phases could be varying with time. Nevertheless, one expects the emitted/absorbed spectrum to be intermediate between those resulting from pure cold and hot models.

When comparing the results obtained with models based on the pure hot/cold solutions, and the approximate, intermediate solution, we conclude that the hot/cold models represent two extreme results corresponding to a given gas composition and photoionizing flux, being compatible with the two stable solutions. The three (hot, cold, and intermediate) models differ not only in the layers where multiple solutions are possible, but all along the gas slab, this because the entire radiation field suffers modifications while crossing a thick medium.

The spectra emitted or absorbed by a given ionized medium, consisting of a mixture of gas in the hot and cold phases, should thus be intermediate between those resulting from the pure cold and hot models; therefore, the intermediate model provides a good description of such a mixed-phase medium. The differences between the emitted and absorbed spectra obtained with the stable solutions can therefore provide an indication for the maximum error bars associated to the spectra computed with the "intermediate" solution previously used by TITAN to circumvent the problem of thermal instabilities. The differences amount at most to 1–2% for the outward emitted spectrum, and to 20% for the absorption spectrum. The agreement is much better for the outward emission in the X-ray range. The lines have similar intensities in all the spectra.

An important point to take into account when choosing which computational method to apply, is that the full computation of the "hot" and "cold" models described here is extremely time-consuming; this is because the process is strongly unstable and requires thus more iterations than the isodensity scheme models. We have shown that it is reasonable to use the simpler, isodensity scheme to compute constant pressure models or hydrostatic equilibrium models. This procedure is less ad-hoc than to choose arbitrarily between one of the possible solutions resulting, in the end, in gas structures and emitted/absorbed spectra very close to what is expected from an ionized medium consisting in similar proportions of gas in the hot and cold phases.

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