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An inversion method for cometary atmospheres

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ABSTRACT

Remote observation of cometary atmospheres produces a measurement of the cometary emissions integrated along the line of sight. This integration is the so-called Abel transform of the local emission rate. The observation is generally interpreted under the hypothesis of spherical symmetry of the coma. Under that hypothesis, the Abel transform can be inverted. We derive a numerical inversion method adapted to cometary atmospheres using both analytical results and least squares fitting techniques. This method, derived under the usual hypothesis of spherical symmetry, allows us to retrieve the radial distribution of the emission rate of any unabsorbed emission, which is the fundamental, physically meaningful quantity governing the observation. A Tikhonov regularization technique is also applied to reduce the possibly deleterious effects of the noise present in the observation and to warrant that the problem remains well posed. Standard error propagation techniques are included in order to estimate the uncertainties affecting the retrieved emission rate. Several theoretical tests of the inversion techniques are carried out to show its validity and robustness. In particular, we show that the Abel inversion of real data is only weakly sensitive to an offset applied to the input flux, which implies that the method, applied to the study of a cometary atmosphere, is only weakly dependent on uncertainties on the sky background which has to be subtracted from the raw observations of the coma. We apply the method to observations of three different comets observed using the TRAPPIST telescope: 103P/ Hartley 2, F6/ Lemmon and A1/ Siding Spring. We show that the method retrieves realistic emission rates, and that characteristic lengths and production rates can be derived from the emission rate for both CN and C_2 molecules. We show that the retrieved characteristic lengths can differ from those obtained from a direct least squares fitting over the observed flux of radiation, and that discrepancies can be reconciled for by correcting this flux by an offset (to which the inverse Abel transform is nearly not sensitive). The A1/Siding Spring observations were obtained very shortly after the comet produced an outburst, and we show that the emission rate derived from the observed flux of CN emission at 387 nm and from the C_2 emission at 514.1 nm both present an easily-identifiable shoulder that corresponds to the separation between pre- and post-outburst gas. As a general result, we show that diagnosing properties and features of the coma using the emission rate is easier than directly using the observed flux, because the Abel transform produces a smoothing that blurs the signatures left by features present in the coma. We also determine the parameters of a Haser model fitting the inverted data and fitting the line-of-sight integrated observation, for which we provide the exact analytical expression of the line-of-sight integration of the Haser model.

1. Introduction

Comets are relatively small size bodies formed at the early stages of the Solar System evolution some 4.6 billions of years ago. They are often considered as potential tracers of conditions prevailing at that time (Ehrenfreund and Charnley, 2000). They mainly consist of an icy water nucleus with other constituents such as carbon monoxide (CO), carbon dioxide (CO_2), and dust. When these bodies escape their reservoirs, mainly the Oort cloud and the Kuiper belt, and approach the Sun, they slowly warm up under the effect of solar radiation and their ices start to sublimate, releasing water vapor, CO, CO_2, dust and other minor species. This process produces a large, highly rarefied, expanding atmosphere: the coma, surrounding the icy nucleus.

The coma is exposed to the Sun radiation and in particular to the ultraviolet solar flux, which is capable to trigger photochemical processes such as dissociation and ionization of the gaseous

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material. Many previous studies focused on the complex photochemistry of the coma from a theoretical and observational standpoint. Among others, Bhardwaj and Raghuram (2012) developed a photochemical model of the coma of comet C/1996 B2 (Hyakutake) to analyze the metastable oxygen O(^{1}D) and O(^{1}S) populations and emissions accounting for photo dissociation and electron impact dissociation of H_2O, OH, CO and CO_2, as well as the dissociative recombination of ions H_2O^+, OH^+, CO^+ and ${CO_2}^+$ and direct electron impact on oxygen atoms. Loss mechanisms of metastable oxygen were the radiative decay, quenching and reaction with H_2O, CO and CO_2. The densities of the major species of the coma (H_2O, CO, CO_2 and OH) were given by a Haser model (Biver et al., 1999). Bhardwaj and Raghuram (2012) conducted an analysis aimed at matching the observed and computed ratio of the 557.7 nm green emission of O(^{1}S) to the 630.0 and 636.4 nm red emissions of O(^{1}D), from which they derived the CO_2 abundance and several photochemical parameters. Raghuram and Bhardwaj (2012) also applied the same model with adapted parameters to comet C/1995 Hale Bopp. Bisikalo et al. (2015) developed a model of the photochemistry of O(^{1}D) and O(^{1}S) using a Monte Carlo method to solve the Boltzmann equation to retrieve the energy distribution of these species across the expanding coma. They showed that the exothermic nature of the photochemical mechanisms producing metastable oxygen yields a strongly non-thermal distribution of their kinetic energy, which in turn produces a strongly non-Gaussian emission line profile.

The radial distribution of cometary constituents is often described using a Haser model (Haser, 1957). This model is used for its simplicity and its ability to describe a spherically symmetric expanding coma. It relies on flux conservation and includes the effect of photochemical production and loss of any species in an ad hoc manner, instead of solving for the detailed photochemistry. Simple flux conservation produces a radial profile that varies as $1/r^2$, with r the radial distance:

$$n = \frac{Q}{4\pi r^2 \ v} \tag{1}$$

with n the density of the species considered (H_2O, for example), Q the rate at which the comet's nucleus releases that species, and v the radial outflow speed of the emitting particles. The concentration of a species that gets destroyed by photochemical processes decays exponentially with time, with a life time τ_p. This life time depends on solar activity, heliocentric distance, etc. and translates into a characteristic length L_p in the expanding coma, so that the density profile becomes:

$$n_p = \frac{Q_p}{4\pi r^2 \ v_p} e^{-\frac{r}{L_p}} \tag{2}$$

Here, the subscript p stands for "parent", as we are considering molecules outgassed by the comet's nucleus that decompose and produce "daughter" species, and which will be denoted by subscript d. The production rate of the daughter species is determined by the loss rate of their parent molecules. Daughter species can in turn be destroyed by photochemical processes, with a characteristic length L_d. Their density profile in the expanding atmosphere is then given by

$$n_d = \frac{Q_p}{4\pi r^2 \ v_d} \frac{L_d}{L_d - L_p} \left(e^{-\frac{r}{L_d}} - e^{-\frac{r}{L_p}} \right). \tag{3}$$

The model could even be further complexified to derive the density profile of grand-daughter species. Expression (1) is however not integrable over R^3 (accounting for the Jacobian of spherical coordinates) as $r \to \infty$, which clearly shows Eq. (1) does not suffice. The Haser model also assumes the characteristic length does not vary across the coma and that there exist only one production and one loss mechanism of the daughter species, which is not warrantied. As the daughter molecules are produced isotropically in a frame of reference moving with the expanding gas, there is no reason to assume that the expansion velocity of the different species can largely differ, and a single expansion velocity is generally used. However, the Haser model neglects molecular diffusion that can influence the density distribution. Integration of expressions (2) and (3) (multiplied by the appropriate Jacobian) over R^3 can be easily carried out analytically, giving $Q_p \ L_d/v_d$ for the total content of daughter species particles of the coma. Models of the coma, either idealized using the Haser approximation or based upon a mechanistic representation such as those of Bhardwaj and Raghuram (2012), Bisikalo et al. (2015), Combi (1996), Rubin et al. (2011), Weiler (2007, 2012), Combi and Fink (1997) and others have to be compared against observational data. However, the local densities, which are the natural outputs of the models, cannot be directly observed remotely, as we discuss in the next section. Moreover, comets are dynamic objects, and time variations of the activity translate to radial gradients in the density that are not accounted for by steady-state models, whatever their degree of sophistication. This is particularly significant when a comet produces an outburst.

Here, we present a method to retrieve the local emission rate from remote sensing observations of cometary atmospheres. Remote sensing of cometary emission provides only a line-of-sight integration of the emission rate, also called its Abel transform. We develop a method that inverts the Abel transform in the special case of cometary atmospheres. Section 2 presents the mathematical developments on which the inverse Abel transform relies. The result of this inversion must not be confused with a model of the coma. It is rather a direct processing of the observational data. Fundamentally, the result of the inverse Abel transform of the data contains essentially the same information as the initial line-of-sight integrated radial profile. In Section 3, we present results from numerical tests that were done to validate the inversion method and highlight its benefits. In Section 4, we present the results from applications of our inverse Abel transform method for three comets. These results are compared with Haser model fits to the data. Particular attention will be given to an outburst case. In Section 5 we discuss the reach of the results obtained with the inverse Abel transform. We conclude with a short summary of our results in Section 6. Appendix A provides additional analytical results that allow for a further refinement of the inversion method. These results do not appear to offer a crucial improvement in the case of cometary atmospheres but they could nevertheless prove useful for planetary atmospheres. Finally, Appendix B gives the results needed to perform the exact analytical computation of the Abel transform of a cometocentric profile described using a Haser model, which is a result that can be used for any study dedicated to the analysis of observations of comets under the Haser hypothesis.

2. The ABEL transform inversion

A distant observer looking at the coma of a comet has no direct access to the density profile of the constituents. Excited species relax by emitting photons and the observation sums up the emission rates along a full line of sight according to the geometry described in Fig. 1. If we denote by $n(r)$ the density of an excited atom or molecule (for example) and by A_{ul} the Einstein transition parameter for spontaneous emission of this excited particle by a transition from upper state u to lower state l, the emission rate at that radius is given by $f(r) = A_{ul} \ n(r)$. In principle, the local density can thus be immediately obtained, if the local emission rate profile is known. When molecular bands are observed and their spectral structure remains unresolved (which is generally the case), the characterization of the excited molecule density based on the emission rate may require a more sophisticated