Charge exchange processes that make comets radiate
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6 Astrophysical Implications

6.1 Introduction

Comets were observed throughout the whole human history. Their beautiful appearance always attracted the people’s attention. They are also interesting from a physical point of view. Many of the processes examined in our research play an important role in cometary atmospheres. Therefore we performed some model calculations partly in order to show our data’s significance.

First of all let’s start with answering the question: What is a comet and what are the main physical processes involved? One could consider a comet as a dirty snowball. More precise it is a celestial object which has a long, far reaching orbit around the Sun and it contains lots of water ice and frozen molecules beside other solid constituents: dust and rocks. One can only observe a comet with bare eyes when it approaches the Sun within several Sun-Earth distances. Then the Sun’s radiation heats up the comet and the ice starts to sublimate. The sublimated gases expand into space without obstacle, for the comet’s gravitational force is very weak. It cannot sustain an atmosphere as in the case of big planets. That is why the gas molecules can travel far away from the comet. About 10 million km distance from the core the gas density is still significantly higher than the interplanetary background density. The quickly expanding gases carry dust particles with them. The dust particles reflect the sunshine. The reflected sunshine can be observed from the Earth and the observation shows a hazy “coma” around the solid core. The radiation pressure then pushes away the dust particles so they form a “tail” at the anti-sunward side. The particles’ original Keplerian orbit is only little modified by the radiation pressure, so the tail points not exactly in the anti-sunward direction but it bends towards the inverse of the comet’s velocity vector.

The Sun emits not only photons but also charged particles and they form the so-called “solar wind”. The major constituents are protons and electrons but one can find other ionic species as
well. The second most abundant ion is $\text{He}^{2+}$ and additionally there are some heavier species: C, O, N, Ne and Mg in different charge states. These ions interact with the cometary molecules. The molecules become excited or ionized and the ionized molecules are swept away by the solar wind forming an ionic tail pointing basically towards the anti-sunward direction. This tail can be very bright due to radiative de-excitation processes and often can be observed by bare eye too as a second tail next to the dust tail.

A surprising fact about comets is their X-ray emission. It was discovered by the ROSAT satellite\(^2\), and the observed intensity was far beyond the most optimistic estimates. This puzzled the scientists since comets are very cold objects and therefore hot plasma processes cannot be used as an explanation. The observations give us some clues about the X-rays’ origin. The emission comes from a crescent-shaped region on the sunward side indicating that the radiation is related to the sun. According to one explanation the radiation is due to absorbed and reemitted X-rays coming from the Sun. If the molecular cloud was thick enough that the radiation coming from the sun could not penetrate into the central region of the comet a crescent-shaped emission profile could be expected. Another explanation is that the collisions between solar wind ions and cometary molecules result in X-ray emission due to charge-exchange processes. The ions emit several spectral lines as the electrons captured into highly excited states are cascading down to lower lying states. The shape of the emission profile can be explained by the ions’ neutralization as they pass through the dense regions. The neutralized and de-excited ions do not contribute to the X-ray emission so the central and anti-sunward regions remain dark in X-ray. The magnitudes of known charge-exchange cross sections combined with the measured cometary gas production rates satisfactorily match to this model. Recently observed line emission in cometary X-ray spectra also supports the idea of the charge-exchange origin of the cometary X-rays. So today this is believed to be the most likely source\(^3\).

We therefore are interested in the interactions of the most abundant ions in the cometary atmospheres, protons, $\text{He}^+$ and $\text{He}^{2+}$ ions. Their distance dependent fluxes have been calculated using charge exchange cross sections. The measurements of
Giotto spacecraft at its close flyby to comet Halley in 1986 provide us a comparison for our models. The processes that define the fluxes are quite complex. In the following we present a simple model, which includes the most relevant basic processes. The cometary photon emission in the VUV resulting from the spectral lines of helium has also been simulated using our line emission cross sections (see chapter 4 and 5). We compared the results with recent VUV and X-ray observations of comet Hyakutake and Hale-Bopp.

6.2 Comet – solar wind interaction model

6.2.1 Basic processes

In our model it is assumed that the solar wind ions can pass through the cometary atmosphere without changing their velocity. The ions move along straight trajectories parallel to the comet – Sun axis. As they proceed their charge state changes due to collisions with cometary molecules. A He$^{2+}$ ion can capture one or two electrons simultaneously forming a singly charged ion or neutral atom. The singly charged helium can undergo a second collision and capture another electron. In a dense atmosphere eventually all ions become neutralized by single or double step processes.

The comet cores mainly emit water molecules. A smaller but significant amount of carbon monoxide molecules is also present but the fractions of other molecular species are negligible. For simplicity we regard the atmosphere to have a uniform constitution of an effective molecule with effective cross sections. The gas emission is supposed to be isotropic, therefore the molecular density changes inversely squared as a function of the distance from the comet core:

$$\rho_m = \frac{Q}{4\pi r^2 v_{gas}},$$ (6.1)

where $Q$ is the number of molecules emitted per second and $v_{gas}$ is the expansion velocity of the gases.
6.2.2 The populations of the different charge states of ionic helium in a comet atmosphere

Initially all the helium ions in the solar wind are doubly charged. Their flux is decreased by two processes: single- and double- electron capture. The decrease is proportional to the local gas density and the corresponding cross sections. We can write a differential equation for the flux of He$^{2+}$ in analogy to light absorption in a medium:

$$\frac{d\Phi_{\text{III}}(z)}{dz} = -\sigma_{21} \rho_m(z) \Phi_{\text{III}}(z) - \sigma_{20} \rho_m(z) \Phi_{\text{III}}(z), \quad (6.2)$$

where $\Phi_{\text{III}}(z)$ is the flux of HeIII (He$^{2+}$), $\rho_m(z)$ is the number density of the cometary molecules, $\sigma_{21}$ and $\sigma_{20}$ are the total one- and two-electron capture cross sections of HeIII. (6.2) describes the flux changes along the ion trajectories, which are parallel to the comet – Sun axis. The position along this axis is denoted by $z$ in such a way that the comet is at 0 position and the Sun is far away on the negative side. The gas distribution that the ions “see” as they pass through the cometary atmosphere depends on the impact parameter ($b$) with respect to the comet center (see Figure 6.1). Therefore, for each impact parameter another differential equation with another $\rho_m(z)$ has to be solved.

Figure 6.1: Overview of the cometary model. A neutral atmosphere is created around the nucleus by sublimation of the “cometary ice”. The solar wind ions enter into the atmosphere and collide with the molecules.
The general solution of (6.2) is:

\[ \Phi_{\text{III}} (z) = \Phi_0 e^{-\int^z (\sigma_{21} + \sigma_{20}) \rho_m (z') dz'} . \] (6.3)

Single-electron capture by He\textsuperscript{III} creates a He\textsuperscript{II} population. The developing He\textsuperscript{II} population is described by the following differential equation:

\[ \frac{d\Phi_{\text{II}} (z)}{dz} = \sigma_{21} \rho_m (z) \Phi_{\text{III}} (z) - \sigma_{10} \rho_m (z) \Phi_{\text{II}} (z) , \] (6.4)

where the first term on the right hand side describes the creation of He\textsuperscript{+} ions and the second term describes their destruction by neutralization via one-electron capture. Since the ionization cross sections are orders of magnitude lower than charge exchange cross sections at the relevant energies the ionization processes are neglected. The solution, using (6.3) and the condition that initially there are no He\textsuperscript{+} ions, is:

\[ \Phi_{\text{II}} (z) = \Phi_0 \sigma_{21} \left( 1 - e^{-\int^z (\sigma_{21} + \sigma_{20} - \sigma_{10}) \rho_m (z') dz'} \right) \frac{\int^z \sigma_{10} \rho_m (z') dz'}{\sigma_{21} + \sigma_{20} - \sigma_{10}} e^{-\int^z \sigma_{10} \rho_m (z') dz'} . \] (6.5)

In Figure 6.2 the calculated ion fractions can be seen. (The ion densities and the fluxes are related by: \( n = \Phi / v \) with \( v \) the solar wind velocity, so for constant velocity, fluxes and densities are proportional to each other.) As a result of charge exchange, the fraction of the initially pure He\textsuperscript{III} population becomes smaller and smaller as the ions penetrate into the comet’s atmosphere. The He\textsuperscript{II} charge state is populated from He\textsuperscript{III} by charge exchange, and therefore its population increases initially as more and more ions from the He\textsuperscript{III} population take part in charge exchange events. With decreasing He\textsuperscript{III} population, the source for the He\textsuperscript{II} population is sooner or later exhausted, and the He\textsuperscript{II} population starts to decrease due to charge exchange neutralization. Finally both of the charge states vanish because all the ions become neutralized. The He\textsuperscript{II}/He\textsuperscript{III} ratio takes up a certain value, after passage through a high integral atmospheric...
density (i.e. \( \int_{-\infty}^{z'} \rho_m(z')dz' \)), which is dependent on the cross sections. From (6.3) and (6.5) we get:

\[
\frac{\Phi_{II}(z)}{\Phi_{III}(z)} = \sigma_{21} \left( e^{\frac{(\sigma_{21}+\sigma_{20}-\sigma_{10})}{\sigma_{21}+\sigma_{20}-\sigma_{10}} \int_{-\infty}^{z'} \rho_m(z')dz'} - 1 \right). \tag{6.6}
\]

If \((\sigma_{21}+\sigma_{20}-\sigma_{10})\) is positive the destruction of HeIII is faster than that of HeII. In this case the HeII dominates the ionic population in the end and the ratio becomes infinite. If \((\sigma_{21}+\sigma_{20}-\sigma_{10})\) is negative the ratio approaches a finite value: \(-\sigma_{21} / (\sigma_{21}+\sigma_{20}-\sigma_{10})\). In this case in the end a mixed population develops, in which the relative abundances are determined by the cross sections. Comparing the existing cross sectional data, \((\sigma_{21}+\sigma_{20}-\sigma_{10})\) is found to be positive at all relevant energies. The dominance of electron capture by HeIII over electron capture by HeII is particularly pronounced at high energies, but below 1 keV/amu the dominance is weak.

The trajectory of the Giotto satellite did not follow the comet sun axis but had an angle of 73° with it. The situation is depicted in Figure 6.3. To compare measurements and calculations the ion densities have to be calculated along the Giotto’ trajectory. Calculations have to be performed for the different solar wind trajectories that the Giotto crossed. The comparison between measurements and calculation can be seen in Figure 6.4. In the calculation the HeIII density is normalized to 0.2 cm\(^{-3}\) at infinity, which was measured by the Giotto probe 1.2×10\(^6\) km far from the core just outside of the bow shock. The general trends of the measurement and calculation are similar, but in some regions deviations are found. The increase of HeIII density between 5×10\(^5\) and 10\(^6\) km can not be understood by this simple model since charge exchange can only decrease the HeIII population. The measurements might be affected by solar wind fluctuations. However, in such a short period a factor of 8 increase of the solar wind density, which would explain this anomalous behaviour, is unlikely. It is more likely that this increase is due to piling of the ions. As the solar wind is
In Figure 6.4 the relative density of HeII compared to the total density of ionic helium (HeII+HeIII) can be seen. The HeII ions represent the “charge-exchanged” portion of the helium minus the neutral helium, which’s fraction was not measured. The measurements show that the conversion of HeIII into HeII happens faster than our model indicates. Up to the magnetic pile-up boundary (2×10⁵ km from the nucleus) the measurements and calculations are close to each other. Further downstream an abrupt increase of the fraction of HeII is observed strongly deviating from the calculations. One possible explanation is that the ions’ trajectories curl up in the stronger magnetic field thereby dramatically increasing the effective path length of the ions.
From our calculations and the measured cross section data it is expected that at shorter distances to the nucleus HeII dominates over HeIII and therefore HeII/(HeII+HeIII) becomes one. Those regions start below $10^4$ km from the nucleus and were not reached by Giotto spacecraft. Accordingly the measured ratio was always less than one.

### 6.2.3 Spectral line emission of comets

Recently, a lot of data becomes available about cometary X-ray and VUV emission as the number of satellite-based observations is increasing day by day. The VUV spectral lines of helium are prominently present in the observed spectra. With our line emission cross sections it is possible to predict the production rate of the different lines of helium in comets. Helium is a relatively simple atom with only three charge states, therefore it is relatively simple to follow its dynamics in the cometary atmospheres as we have seen in the previous section. We have
calculated photon emissions at 30.4 nm (HeII(2p→1s)) and 58.4 nm (HeI(1s2p→1s2)) for comet Hyakutake and Hale-Bopp and for comparison we used the EUVE observations by Krasnopolsky et al.\textsuperscript{12,13}.

The emission at 30.4 nm is the result of single electron capture by He\textsuperscript{2+}. The strength of the photon emission for a certain point of the comet’s atmosphere is given by the following:

\[ S_{30.4\text{nm}}(r) = \sigma_{2p \rightarrow 1s} \rho_m(r) \Phi_{\text{III}}(r). \]  

(6.7) gives us the number of photons emitted around \( r \) per unit volume and time, the so-called source function. \( \sigma_{2p \rightarrow 1s} \) is the line emission cross section for the 30.4 nm HeII(2p→1s) transition resulting from single-electron capture by He\textsuperscript{2+}. We used the CO data (see chapter 4 HeII(2p→1s) transition), which are assumably close to the effective cross section for the cometary gas mixture. The flux of He\textsuperscript{III} (\( \Phi_{\text{III}}(r) \)) is based on the previous calculation (see Eq. (6.3)), in which only the \( z \) dependency is given, but the result can be easily generalized to the 3D case. Since the trajectories are parallel with respect to the \( z \)-axis the \( x \) and \( y \) dimensions enter as constant parameters into the calculation via the density \( \rho_m(r) = \rho_m(x,y,z) \). So we only have to do the \( \rho_m(z') \rightarrow \rho_m(x,y,z') \) replacement in (6.3). The source function for 58.4 nm can be obtained in a similar manner. A photon at 58.4 nm is emitted subsequently after a He\textsuperscript{2+} ion captures two electrons into the HeI (1s2p) \( ^1 \text{P} \) state. Those He\textsuperscript{2+} ions that capture only one electron, forming He\textsuperscript{+} ions, can capture subsequently another electron and thus they can contribute to the emission at 58.4 nm too. Therefore we need the line emission cross sections for He\textsuperscript{+} ions too (presented in chapter 5). The source function for 58.4 nm is given by:

\[ S_{58.4\text{nm}}(r) = \sigma_{\text{dec1s2p} \rightarrow 1s^2} \rho_m(r) \Phi_{\text{III}}(r) + \sigma_{\text{sec1s2p} \rightarrow 1s^2} \rho_m(r) \Phi_{\text{II}}(r). \]  

(6.8)

The abbreviations \( \text{sec} \) and \( \text{dec} \) denote single- and double-electron capture respectively. Integrating the source functions over space the overall photon emission can be obtained. For the observations usually some apertures are used which limit the space from where
photons are collected. The angle of observation usually does not coincide with the comet-Sun axis. This has also an influence on the observed area. In the calculations we have taken this into account and the source functions were integrated over a cylindrical volume with a radius equal to the observation’s aperture, which was centered at the comet’s nucleus, and the cylinder axis was matched to the line of observation. The absolute photon intensities are primarily determined by the gas production rate and the Sun-comet distance. These were measured at the time of the observation, and the measured values have been used for the calculations. The solar wind’s He$^{2+}$ density was assumed to be $0.2 \text{ cm}^{-3}$ at 1 astronomic unit (A.U.) for both comets. It changes inversely squared as a function of the distance from the sun. This was also taken into consideration. The observational details and the measured luminosities are summarized in Table 6.1.

<table>
<thead>
<tr>
<th>Comet</th>
<th>Q(s$^{-1}$)</th>
<th>D(A.U.)</th>
<th>$r_{ap}$ (km)</th>
<th>$\alpha$</th>
<th>Luminosity (photon/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>30.4 nm</td>
</tr>
<tr>
<td>Hale-Bopp</td>
<td>$6 \times 10^{29}$</td>
<td>3.07</td>
<td>$2.5 \times 10^5$</td>
<td>19°</td>
<td>$\leq 7 \times 10^{25}$</td>
</tr>
<tr>
<td>Hyakutake</td>
<td>$2 \times 10^{29}$</td>
<td>1.07</td>
<td>$1 \times 10^5$</td>
<td>50°</td>
<td>$7.3 \times 10^{24}$</td>
</tr>
</tbody>
</table>

Table 6.1: Observational details and measured luminosities of comets$^{12,13}$. Q is the gas production rate, D is the heliocentric distance, $r_{ap}$ is the radius of the observational aperture, $\alpha$ is the angle of observation with respect to the Sun-comet axis.

For comet Hale-Bopp the emission line at 58.4 nm has been detected. The emission line at 30.4 nm was too faint to be detected. For the luminosity therefore only a $2\sigma$ upper limit could be given. For comet Hyakutake the situation is vice versa, here a $1\sigma$ upper limit is given for the 58.4 nm line. We compare our calculations with the observations in Figure 6.6. The solar wind velocities were unknown at the time of the observations and therefore we used various values for the calculations. Typical solar wind velocities are in the range of 200-400 km/s for slow solar wind and 1000 km/s for fast solar wind. Neither of the observations fit perfectly to the calculations. For comet Hale-Bopp the measured values are approximately an order of
magnitude higher than the calculated ones while for Hyakutake they are an order of magnitude lower. The solar wind density can easily vary an order of magnitude on a daily basis. Since it was not known at the time of the observations and the luminosities are strongly dependent on it, there are rather large uncertainties in the calculations. On the other hand this implies that the luminosities can be used to determine solar wind densities.

Figure 6.6: Calculated and measured luminosities for comet Hale-Bopp and Hyakutake. The calculations were performed for several solar wind velocities, Hale-Bopp (●), Hyakutake (○).

The intensity ratio between the two lines is largely independent on the solar wind density, but it is very much dependent on the solar wind velocity. It is therefore expedient to compare the measured and calculated intensity ratios and deduce the solar wind velocities (see Figure 6.7).
Figure 6.7: Calculated intensity ratios of the 30.4 nm and 58.4 nm line emissions of comets as the function of solar wind velocity. The results almost coincide for comet Hale-Bopp and Hyakutake. The measured ratios (0.58, 7.3) indicate that the solar wind velocities were about 220 and 500 km/s in the case of Hale-Bopp and Hyakutake respectively.

The 30.4 nm /58.4 nm line intensity ratio shows a very steep velocity dependence. The results are almost identical for Hale-Bopp and Hyakutake, even though the cometary parameters are quite different for the two cases. This indicates that the intensity ratio is primarily defined by the solar wind velocity. Using for comet Hale-Bopp the given upper limit for luminosity at 30.4 nm (see Table 6.1), we determine a maximal intensity ratio of 0.58. From this we can conclude an upper limit of 220 km/s for the solar wind velocity, which is a typical value for slow solar winds. For comet Hyakutake a lower limit of 500 km/s can be obtained from the data presented in Table 6.1. This is close to the upper limit for slow solar wind.
6.3 Conclusions

As it is obvious from our model, cometary VUV emission can be interpreted as the result of charge-exchange between solar wind ions and cometary molecules. First we have calculated the densities of the different charge states of helium. We have compared the results with the measurements on comet Halley. The general behavior has been found to be similar, but in some regions deviations occur. The relative abundance of He\(^+\) ions compared to He\(^{2+}\) is increasing towards the nucleus due to charge-exchange. Up to the magnetic pile-up boundary the calculated relative abundances agree well with the measured ones. Based on the calculated densities the photon emission for the HeII\((2p\rightarrow1s)\) and HeI\((1s2p\rightarrow1s^2)\) lines have been calculated for different solar wind velocities. The observed luminosities for comet Hale-Bopp and Hyakutake differ by about an order of magnitude from the calculated ones. These deviations can be due to fluctuations in the solar wind density. In the calculations the relative intensity of the two lines appears to be independent of the cometary and solar wind parameters except for the solar wind velocity. This indicates that the HeII\((2p\rightarrow1s)\)/ HeI\((1s2p\rightarrow1s^2)\) line intensity ratio can be used for solar wind velocimetry. The solar wind velocities determined on the basis of the observed line intensity ratios for comet Hale-Bopp and Hyakutake, are typical for slow solar wind. The obtained results may improve by adding to the model some extra features, which would lead to too lengthy discussions, as the cometary gas composition, the solar wind deceleration by pick up ions, and the deviations from straight-line trajectories.

References:

decelerated during its interaction with the cometary atmosphere the decelerated ions accumulate increasing the ion density locally.

Figure 6.2: The calculated relative densities of the different charge states of helium (black line: HeIII, grey line: HeII) on the comet – Sun axis. The parameters are fitted to those of comet Halley by the time of observation of Giotto spacecraft. \( Q = 7 \times 10^{29} \) mol/s, gas expansion velocity: 1 km/s, solar wind velocity: 250 km/s

Figure 6.3: The Giotto’s path in the atmosphere of comet Halley.


