Merged Ionization/Dissociation Fronts in Planetary Nebulae

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MERGED IONIZATION/DISSOCIATION FRONTS IN PLANETARY NEBULAE

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ABSTRACT

The hydrogen ionization and dissociation front around an ultraviolet radiation source should merge when the ratio of ionizing photon flux to gas density is sufficiently low and the spectrum is sufficiently hard. This regime is particularly relevant to the molecular knots that are commonly found in evolved planetary nebulae, such as the Helix Nebula, where traditional models of photodissociation regions have proved unable to explain the high observed luminosity in H$_2$ lines. In this paper we present results for the structure and steady state dynamics of such advection-dominated merged fronts, calculated using the Cloudy plasma/molecular physics code. We find that the principal destruction processes for H$_2$ are photoionization by extreme ultraviolet radiation and charge-exchange reactions with protons, both of which form H$_3^+$, which rapidly combines with free electrons to undergo dissociative recombination. Advection moves the dissociation front to lower column densities than in the static case, which vastly increases the heating in the partially molecular gas due to photoionization of He$^+$, H$_3^+$, and H$^0$. This causes a significant fraction of the incident bolometric flux to be reradiated as thermally excited infrared H$_2$ lines, with the lower excitation pure rotational lines arising in 1000 K gas and higher excitation H$_2$ lines arising in 2000 K gas, as is required to explain the H$_2$ spectrum of the Helix cometary knots.

Subject headings: hydrodynamics — molecular processes — planetary nebulae: individual (NGC 7293)

1. INTRODUCTION

The ultraviolet photons from hot stars, such as main-sequence OB stars or the central stars of planetary nebulae (CSPN), will dissociate and ionize the surrounding circumstellar and interstellar gas. In the classical picture (e.g., Hollenbach & Tielens 1997), the extreme ultraviolet (EUV) photons with energies $h\nu > 13.6$ eV photoionize the hydrogen gas, forming an H II region bounded by a relatively sharp ionization front (IF), while the far-ultraviolet (FUV) photons with energies $6$ eV $< h\nu < 13.6$ eV penetrate the IF to form a neutral photo-dissociation region (PDR) that surrounds the H II region. The dissociation of H$_2$ in such a PDR is dominated by a two-step radiative process (Stecher & Williams 1967; Abgrall et al. 2000), in which absorption of an FUV photon leaves the H$_2$ molecule in an electronically excited state, from which it has a certain probability ($\approx 10\%$) of decaying to the vibrational continuum of the ground electronic state.

However, as shown by Bertoldi & Draine (1996), a classical extended PDR cannot exist if the FUV flux is sufficiently weak compared with the EUV flux at the IF; rather, the IF and dissociation front (DF) should merge. Bertoldi & Draine considered the case of H II regions around OB stars and found that this regime was most relevant for cases in which the dust optical depth through the ionized gas is low, which corresponds to a low-ionization parameter (the ionization parameter is a dimensionless number equal to the ratio of the number density of ionizing photons to the number density of hydrogen nuclei). To date, no models have been calculated of the structure and emission properties of such fronts, which are also expected to show strong deviations from static chemical and ionization equilibrium.

In this paper, we calculate in detail the internal dynamics and chemistry of merged ionization/dissociation fronts (IF/DFs), concentrating on the particular case of compact photo-evaporating molecular knots in evolved planetary nebulae (PNe) such as those seen in the Helix Nebula (Young et al. 1999; Meixner et al. 2005; Hora et al. 2006; O'Dell et al. 2007, hereafter OHF07). The stellar spectrum from the hot central star of a PN is harder than that from an OB star, leading to an EUV luminosity that is much greater than the FUV luminosity. In addition, the ionization parameter of the knots is much lower than is typically seen in H II regions, resulting in very little attenuation of the EUV flux by recombinations in the ionized gas. Both of these factors place the knots firmly in the merged IF/DF regime. The most comprehensive existing theoretical study of PDRs in planetary nebulae is that of Natta & Hollenbach (1998), who present detailed modeling of the time-dependent evolution of an expanding circumstellar shell as the luminosity and spectrum of the CSPN evolves, finding that soft X-rays can be important in exciting the molecular gas at late times. However, OHF07 showed that this is not the case in the Helix, since it is only in the EUV band that the CSPN luminosity is sufficient to excite the knot PDRs. Natta & Hollenbach used an analytic treatment of the H II region, which is assumed to have absorbed all the EUV radiation, and were thus unable to model the case of a merged IF/DF.

2. MODELS

In order to investigate the structure of advective IF/DFs in PNe, we have calculated steady state, plane-parallel slab models using the Cloudy plasma/molecular physics code (Ferland et al. 1998). Details of the computational scheme used to treat the steady state dynamics are given in Henney et al. (2005), and these methods have now been coupled to a hydrogen chemical network (Abel et al. 2005) and combined with the 1893-level model of H$_2$ described in Shaw et al. (2005).

In this initial study, we restrict ourselves to models with elemental abundances from Henry et al. (1999) that are illuminated by a blackbody source of luminosity $120 L_\odot$ and an effective temperature of 130,000 K, chosen to match the CSPN
of the Helix Nebula (Bohlin et al. 1982; adjusted for the trigono-
metric parallax of 217 pc [Harris et al. 2007]). We have also
calculated some models using a Rauch (2003) stellar atmo-
sphere with the same luminosity and effective temperature.

We vary three different model parameters so as to span the
range of physical and illumination conditions that are seen in PN
knots: distance from the CSPN, $D$; hydrogen nuclei density at the
illuminated face, $n_i$; and gas velocity at the illuminated face, $u_v$.
Table 1 summarizes the input parameters of our models.

The magnitude of advective effects in the models is, to first
order, dependent only on the dimensionless combination:
$\lambda_{ad} = n_i u_v 4\pi D^2/Q_H$, where $Q_H$ is the ionizing photon lumi-
nosity of the source. This advection parameter (Henney et al.
2005) is the ratio of particle flux to photon flux, which increases
with $u_v$ and decreases with ionization parameter. The appro-
appropriate value of the downstream flow velocity $u_v$ depends
sensitively on the boundary conditions at the illuminated face
and on the global geometry of the flow. In the case of a
photoevaporating knot with negligible confining pressure on
the ionized side, $u_v$ will be of order the ionized sound speed
($\sim 10$ km s$^{-1}$), and this is the case we concentrate on in this
paper. In the case of a more shell-like configuration of the
molecular gas, $u_v$ would tend to be lower.

3. PREDICTED MODEL STRUCTURE

Figure 1 shows the results from a typical advective model,
B06, while Figure 2 shows results from a static model, B00,
with exactly the same incident flux and density as B06. For
ease of discussion, we divide the model into three broad zones:
zone I is closest to the ionizing source and is largely ionized,
with a very low molecular fraction; zone II is the dissociation
front, in which the hydrogen is half-neutral and half-molecular
(for the advective models, this zone is subdivided into IIa and
IIb); and zone III is farthest from the ionizing source, where

---

### TABLE 1

<table>
<thead>
<tr>
<th>Model</th>
<th>$D$ (pc)</th>
<th>$u_v$ (km s$^{-1}$)</th>
<th>$n_i$ (cm$^{-3}$)</th>
<th>$Q_H$</th>
<th>$\lambda_{ad}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A10</td>
<td>0.137</td>
<td>10</td>
<td>3162</td>
<td>3.36 $\times 10^4$</td>
<td>0.94</td>
</tr>
<tr>
<td>A06</td>
<td>0.137</td>
<td>6</td>
<td>3162</td>
<td>3.36 $\times 10^4$</td>
<td>0.56</td>
</tr>
<tr>
<td>A03</td>
<td>0.137</td>
<td>3</td>
<td>3162</td>
<td>3.36 $\times 10^4$</td>
<td>0.28</td>
</tr>
<tr>
<td>A01</td>
<td>0.137</td>
<td>1</td>
<td>3162</td>
<td>3.36 $\times 10^4$</td>
<td>0.09</td>
</tr>
<tr>
<td>A00</td>
<td>0.137</td>
<td>0</td>
<td>3162</td>
<td>3.36 $\times 10^4$</td>
<td>0.00</td>
</tr>
<tr>
<td>AA10</td>
<td>0.137</td>
<td>10</td>
<td>1000</td>
<td>3.36 $\times 10^4$</td>
<td>0.30</td>
</tr>
<tr>
<td>B10</td>
<td>0.244</td>
<td>10</td>
<td>1000</td>
<td>1.06 $\times 10^4$</td>
<td>0.94</td>
</tr>
<tr>
<td>B06</td>
<td>0.244</td>
<td>6</td>
<td>1000</td>
<td>1.06 $\times 10^4$</td>
<td>0.57</td>
</tr>
<tr>
<td>B00</td>
<td>0.244</td>
<td>0</td>
<td>1000</td>
<td>1.06 $\times 10^4$</td>
<td>0.00</td>
</tr>
<tr>
<td>C10</td>
<td>0.433</td>
<td>10</td>
<td>316</td>
<td>3.36 $\times 10^4$</td>
<td>0.94</td>
</tr>
<tr>
<td>C06</td>
<td>0.433</td>
<td>6</td>
<td>316</td>
<td>3.36 $\times 10^4$</td>
<td>0.56</td>
</tr>
<tr>
<td>C00</td>
<td>0.433</td>
<td>0</td>
<td>316</td>
<td>3.36 $\times 10^4$</td>
<td>0.00</td>
</tr>
</tbody>
</table>

Note.—Stellar parameters: $L = 120$, $L_{\odot}$, $T_{\text{eff}} = 130,000$ K.

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hydrogen is fully molecular. Table 2 shows typical physical
conditions in each zone for the advective models.

The differences between the advective and static models are
stark: in the advective model, the DF occurs at the very low
column density of $10^{18}$ cm$^{-2}$ from the illuminated face and
strongly overlaps with the ionization front, whereas in the static
model the DF occurs much deeper, at $2 \times 10^{19}$ cm$^{-2}$, in a region
where the ionization fraction is <0.01. Zone II is much warmer
in the advective model (2000 K in zone IIa, 1000 K in zone
IIb) than in the static model (500 K) and, as a result, H$_2$
line emission is more than an order of magnitude brighter.

The rates of formation and destruction of H$_2$ for model B06
are shown in Figure 3, where it can be seen that the destruction
rate (bottom panel) has a narrow peak at the leading edge of
zone IIa, due to collisional processes with protons and electrons,
together with a broader peak covering zones IIa and IIb, due to
photoionization by hard EUV photons. The principal reaction
channel for the H$_2^+$ ions formed by these processes is dissociative
recombination with free electrons (e.g., McCandliss et al. 2007),
with only $\sim 10\%$ reacting with H$^+$ to re-form H$_2$. Other H$_2$
formation mechanisms have even smaller rates (top panel),
with the result that, once they have been destroyed, most H$_2$
molecules never re-form during the $\sim 300$ yr that they remain in the DF.

The heating and cooling rates for model B06 are shown in
Figure 4. In zone I, as is typical for low-excitation H II regions,
the heating is dominated by H$^+$ photoelectric heating, while the
cooling is due to H lines and optical metal lines such as [N II]
$\lambda$6584. In zone IIa, H$^+$ photoelectric heating still dominates the
heating, whereas in zone IIb, photoelectric heating of He$^+$ and
H$_2$ increasingly take over. In all of zone II the cooling is over-
whelmingly dominated by H$_2$ line emission. In zone III, the
heating rate is much lower than in the other zones and is due

---

### TABLE 2

<table>
<thead>
<tr>
<th>Zone</th>
<th>Column Density (cm$^{-2}$)</th>
<th>$T$ (K)</th>
<th>$u$ (km s$^{-1}$)</th>
<th>$n_i/n_e$</th>
<th>$f_{H_2}$</th>
<th>$n/\lambda_n$</th>
<th>Heat</th>
<th>Cool</th>
</tr>
</thead>
<tbody>
<tr>
<td>I ...</td>
<td>$\leq 10^{18}$</td>
<td>10$^4$</td>
<td>5</td>
<td>0.6</td>
<td>$10^{-4}$</td>
<td>$H^+$ p.e.</td>
<td>Metal, H$^+$ lines</td>
<td></td>
</tr>
<tr>
<td>IIa</td>
<td>$1 \times 10^{19}$–$4 \times 10^{19}$</td>
<td>1000</td>
<td>0.5</td>
<td>0.1</td>
<td>0.3</td>
<td>$H^+$, He$^+$, p.e.</td>
<td>H$_2$ lines</td>
<td></td>
</tr>
<tr>
<td>IIb</td>
<td>$4 \times 10^{19}$–$2 \times 10^{20}$</td>
<td>1000</td>
<td>0.2</td>
<td>0.03</td>
<td>0.6</td>
<td>$H^+$, He$^+$, p.e.</td>
<td>H$_2$ lines</td>
<td></td>
</tr>
<tr>
<td>III</td>
<td>$&gt;2 \times 10^{19}$</td>
<td>200</td>
<td>0.03</td>
<td>3 $\times 10^{-4}$</td>
<td>0.9</td>
<td>$H_2$ lines</td>
<td>FIR metal lines</td>
<td></td>
</tr>
</tbody>
</table>
Fig. 2.—Same as Fig. 1, but for an equivalent static model (B00).

principally to the absorption of H$_2$ lines emitted in zone II, while the cooling in zone III is dominated by collisionally excited far-infrared metal lines. Figure 4 (bottom) shows the difference between the heating and cooling rates, which is equal to the net rate of energy transfer from the radiation field to the gas. This can be seen to have a sharp peak at the boundary between zones I and IIa, where it represents a significant fraction of the total heating. Outside this narrow heating front, the gas is everywhere in approximate thermal equilibrium. The fraction of the bolometric stellar luminosity that is converted into thermal and kinetic energy of the gas can be shown to be $\eta = 10^{12} L_{bol} / (1 + L_{bol} / L_{rad})$ (Fig. 5, dashed curve). The dotted line in the figure indicates the maximum fluorescent efficiency, assuming that all FUV radiation is converted into H$_2$ lines.

4. PREDICTED H$_2$ SPECTRUM

Figure 5 shows the radiative efficiency of the models in converting the stellar luminosity into H$_2$ emission lines: $\eta = L_{line} / L_{bol}$. The value of $\eta_{tot}$, corresponding to the sum of all H$_2$ lines, is <0.01 for the static models and rises rapidly with $\lambda_{ad}$ for the advective models, approximately as $\eta_{tot} = 1.1\lambda_{ad}/(1 + \lambda_{ad})$ (Fig. 5, dashed curve). The dotted line in the figure indicates the maximum fluorescent efficiency, assuming that all FUV radiation is converted into H$_2$ lines.
The slope of the excitation diagram is steeper for lower excitation energies, which is demonstrated in Figure 1: the emissivity of the lower pure rotational lines (excitation temperatures <5000 K) peaks in zone IIb, where the gas temperature is \( \approx 1000 \text{ K} \), whereas higher excitation lines have their peak emissivity in zone IIa, where the gas temperature is \( \approx 2000 \text{ K} \).

5. Discussion

Observations of the molecular hydrogen spectrum of the knots in the Helix Nebula (Cox et al. 1998; Hora et al. 2006; OHF07) are indicated as error bars in Figure 6. It can be seen that the two advective models are in broad agreement with the observations, whereas the static model is not. Model C06 best matches the distance of the spectroscopically observed knots from the ionizing star and indeed shows a better agreement than model A06, which corresponds to the closer-in knots. The observed nebular flux in the 1–0 \( S(1) \) line and in the sum of the 0–0 \( S(1) \) to \( S(7) \) lines is \( \approx 1\% \) and \( \approx 4\% \), respectively, of the bolometric stellar flux (OHF07). From Figure 5, this can be satisfied by our models with \( \lambda_{ad} > 0.3/f \), where \( f \) is the area-covering fraction of knots. A strong prediction of our model is that higher excitation lines from the \( v \geq 1 \) levels should show a higher population temperature of \( \approx 2000 \text{ K} \). A recent study of an inner knot (Matsuura et al. 2007) finds a population temperature of about 1800 K for these levels, in agreement with the prediction of our relevant model (A06).

Rovibrationally warm \( \text{H}_2 \) has been detected in other PNe (e.g., Likkel et al. 2006; McCandliss et al. 2007) and has frequently been interpreted as evidence for shocks (Zuckerman & Gatley 1988). However, EUV-dominated advective PDRs may be a promising alternative in these cases too.

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REFERENCES