ADVANCES IN NUMERICAL SIMULATIONS OF GASEOUS NEBULAE

GARY J. FERLAND
Department of Physics & Astronomy, University of Kentucky, Lexington, KY 40506, USA
and
Cerro Tololo Inter-American Observatory, National Optical Astronomy Observatories[1], *Casilla 603, La Serena, Chile*

Abstract

I outline recent advances in numerical simulations of gaseous nebulae. These fall into three major areas; the Opacity Project and its extensions, the role of grains within the ionized gas, and the effects of mechanical heat on the nebula. These advances, together with improvements in stellar atmosphere calculations, should lead to a new generation of more realistic simulations of conditions in planetary nebulae and predictions of their emitted spectra.

1. Introduction

Planetary Nebulae are important both as a stellar phenomena and as a source of chemical enrichment of galaxy. Emission line analysis is the primary way one measures the chemical composition of the ejecta and the luminosity and temperature of the central star. With the continued development of large-scale codes designed to simulate both the central star and surrounding nebula, and ready access to cheap fast computers, numerical simulations of the conditions producing the observed spectrum are increasing being used as a tool to interpret spectroscopic observations. Some of these codes are summarized in the 1985 Meudon Meeting on Model Nebulae (Pequignot 1986), and in previous reviews in this series of meetings (Pequignot 1983 and Harrington 1989).

[1]The National Optical Astronomy Observatories are operated by the Association of Universities for Research in Astronomy, Inc., under cooperature agreement with the National Science Foundation.

R. Weinberger and A. Acker (eds.), Planetary Nebulae, 123–130.

In addition to their astronomical importance, planetary nebulae can be considered to be an especially clean laboratory for atomic molecular physics, and as an opportunity to test our ability to simulate conditions within an ionized plasma. We understand the geometry and the central source of ionizing photons, and the continuum emitted by the central star can be calculated from first principles, although this is in itself a very difficult problem. These are all assets we do not enjoy in extragalactic objects such as the giant HII regions or active nuclei. The ability to reproduce the spectrum of a PN is a necessary first step to validating simulations of far more poorly understood objects.

Although the boundary conditions of a planetary nebula simulation are well posed, there are several major complications which are now altering the standard picture, or answer, developed over the past thirty years. These are a) the results of the Opacity Project, the definitive photoabsorption-recombination data base, but one of almost overwhelming size and complexity, b) the effects of grains on the ionized gas, mainly in adding an additional source of photoelectric heating and opacity, and c) the role played by mechanical heating and ionization.

2. The Opacity Project

Numerical simulations of any non-equilibrium plasma require a wide range of collisional and radiative data. The major advance now occurring is in the photoionization-recombination data base, the result of the Opacity Project (hereafter OP; see Seaton 1987) and its extensions to recombination processes.

2.1. Photoabsorption Data

The original calculations of photoabsorption cross sections were either at only a few energies, or used approximations which resulted in an opacity which was smooth and could be well-fitted by simple power laws (see, for example, Table 2.7 of Osterbrock 1989). For many years the most complete photoionization data base was the central field calculations of Reilman and Manson (1979; RM). These showed some structure and had the great advantage of extending to medium X-ray energies. The OP has changed all this with complete data of high

https://doi.org/10.1017/S0074180900170299 Published online by Cambridge University Press

accuracy, but in a manner which itself presents two serious challenges, its size, and its complexity.

The OP includes all atoms and ions of astrophysically abundant elements, and includes the ground and excited states for n<10 and l<10. The predictions are the result of state-of-the-art R-matrix close coupling calculations, and the effects of auto-ionization resonances are explicitly included. An example of the type of data the OP routinely generates is shown in Figure 1, adopted from Nahar and Pradhan (1992a). The small-scale resonant structure shown there is characteristic of most OP data. Excited states can present even more complicated behavior; the so-called PEC (photoexcitation of core) resonances make excited state cross sections decidedly non-hydrogenic.

The first challenge of the OP is the shear volume of data. The full data base requires roughly a gigabyte of storage. Incorporating these data into existing radiative equilibrium codes is the second challenge. It is wrong to simply fit the OP data by a low order polynomial of some sort; the high-frequency resonant structure cannot be ignored. These contribute to the net photoionization rate when the gas is optically thin, and (as a corollary) the resonances will become optically thick in many circumstances. Each resonance must therefore be transferred if the depth-

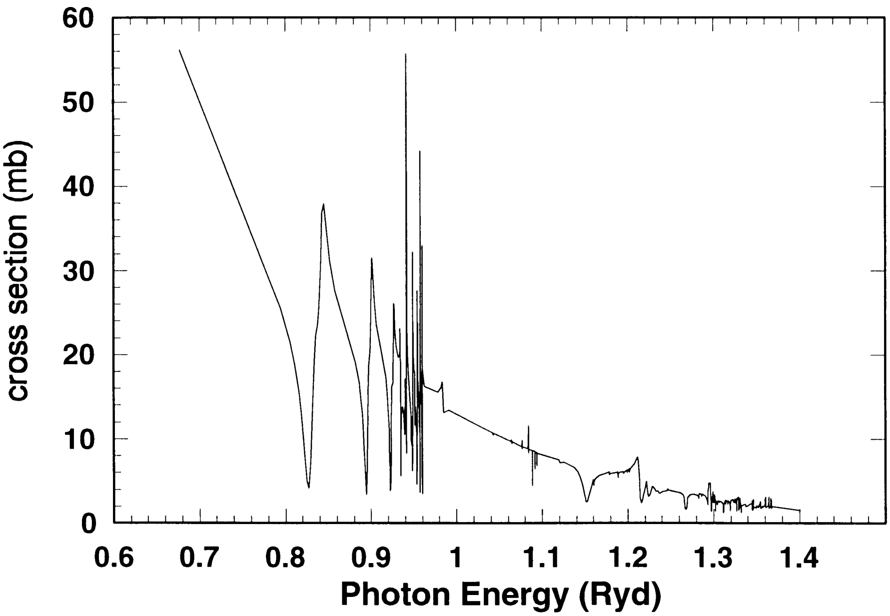

Figure 1, Photoabsorption cross section for the ground term of atomic Si.

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dependent photoionization rate is to be computed. Moreover, if one of these resonances happens to coincide with a major ionizing emission line, such as the HeI or HeII Lyα lines, the photoionization rate of the heavy element could be changed by many orders of magnitude.

It will be necessary to develop new numerical methods to take advantage of the OP. The evaluation of photoioinization rates for a PN model, using this data in its raw form, frequency by frequency, and depth by depth, is beyond the capacity of even today's supercomputers. An obvious solution would be to adopt an opacity distribution function approach to both distill the OP data to a more manageable form and include the resonances in the photoionization rates. This will be the approach I will take, although this is going to take some time.

2.2. Recombination Rate Coefficients

Both radiative and dielectronic recombination rate coefficients can be obtained from OP photoionization cross sections by direct integration with the Milne relations. This effort is now underway (Nahar and Pradhan 1992b) but will be a massive undertaking and is far from complete. It would of course be inconsistent to combine OP photoabsorption data with other sources of recombination rates.

It is difficult to say what affects these changes in the photoionization - recombination database will produce in the computed spectrum. Predictions for lines from atoms of the third row will certainly change; currently there are no calculations of the dielectronic recombination rate coefficients for these elements at all. Furthermore, the OP cross sections sometimes disagree with the RM values by factors of several for these many-electron systems.

3. The Ubiquitous Grains

The physics of "classical" grains (large-mass particles with a time-steady temperature) is well understood (Spitzer 1948, Draine 1978; Draine and Salpeter 1979, Oliveira and Maciel 1986, Baldwin et al. 1991). Photoionization of grains establishes a floating potential, and the kinetic energy of the photoelectron heats ionized gas. In PNs grains are a source of photoelectric heating at least as important as helium, and in some cases they can be the dominant heating mechanism (Borkowski and

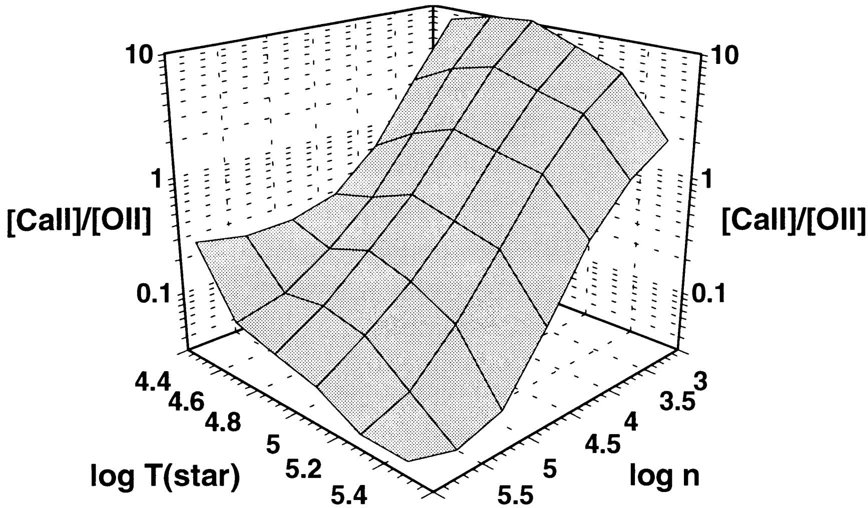

Figure 2. The [CaII]/[OII] ratio as a function of hydrogen density and stellar temperature.

Harrington 1991). No photoionization calculation can safely neglect grains in environments in which they are known to exist.

A simple argument can be used to test for extreme depletions due to the presence of grains (see also Shields 1975). Calcium is among the most highly depleted of the elements in ISM gas (approaching four orders of magnitude for dense gas, see Field 1974; Cowie and Sangila 1986), and thus offers a simple test for the existence of grains.

Figure 2 shows the results of including calcium with a solar abundance (Grevesse and Anders 1989) in a typical PN photoionization calculation (Ferland and Persson 1989; Kingdon and Ferland 1993). A spherical nebula with a small inner radius was assigned various densities. The central star was assumed to have a luminosity near the Eddington limit (10^{38} erg s^{-1}) and assigned various blackbody temperatures. The Figure shows the predicted ratio of the intensity of the [CaII] doublet at λλ7291, 7325 to the nearby [OII] λ7325 multiplet. It shows that the unobserved [CaII] lines would be among the strongest lines in the near infrared spectrum *if calcium had a cosmic gas-phase abundance*. The conclusion is that Ca must be strongly depleted. As a corollary, it seems difficult to imagine circumstances in which any significant fraction of the grains within a nebula could be destroyed without liberating too large an amount of calcium (see also Harrington 1990). Several mechanisms could destroy grains over the lifetime of a

PN. If the calcium carriers are destroyed too, then [CaII] emission should "turn on" as the nebula ages and grains are destroyed. It is because of its extreme depletion that the search for [CaII] emission provides a fairly clean test for the destruction of grains.

4. Mechanical Heating

Photoionization (of both gas and dust) is the primary heating and ionization mechanism for planetary nebulae. Although it dominates the global energetics, this is not to say that there are not situations where other mechanisms come into play. The nuclei of planetary nebulae undergo rapid mass loss. The interaction of this fast wind with the slowly expanding PN envelope must occur, and acts to both heat and ionize the nebula. The effects will be above that provided by photoionizaiton.

Abell 30 provided one of the first examples of the possible influences of heating by a wind (Harrington and Feibelman 1984). Ultraviolet spectra revealed collisionally excited lines that were very strong relative to recombination lines. The ratio of these two is proportional to the mean ionizing photon energy through the Stoy (1933) ratio:

$$\frac{I(\text{strong collisional line})}{I(\text{recombination line})} \propto \frac{\text{cooling rate}}{\text{recombination rate}} \propto \frac{\text{heating rate}}{\text{photoionization rate}} \propto \langle h\nu - \text{IP} \rangle$$

The observation is that no reasonable choice of stellar continua can provide the amount of heat deposited per photoionization. Mechanical heating could provide this additional heating (although grain photoionization is a second possibility, see the work by Borkowski and Harrington in this volume).

The outer halo of NGC 7662 provides a second possible example of winds heating the nebula (Middlemass et al 1991). Observations of high electron temperatures and inferred anomalous heating could be explained with the interaction of the windy central star with the surrounding outer nebula.

A second line of evidence for mechanical heating may be provided by the Type 1 PN NGC 6302. Ashely and Hyland (1988) discovered the presence of significant emission from the high-ionization species Si^{+5} and Si^{+6}. If the result of photoionization then the central star would need a temperature of roughly half a million degrees.

Lame and Ferland (1991; LF) pointed out that photoionization by a star this hot would produce very strong [OI] λ6300 emission, the result of penetrating X-rays heating neutral gas. The argument is a general one, and could be used to set an upper limit to the temperature of the population of radiation-bounded nebulae. Figure 3, adopted from LF using their parameters but solar abundances, shows how the [OI]/Hβ ratio increases with depth for photoionization by a very hot star. The geometry of NGC 6302 is exceedingly complex, well-shielded regions are evidenced by H_2 emission, and the reddening is large. However, if a continuum hard enough to produce the silicon emission also strikes the region with neutral hydrogen, then strong [OI] emission would result. LF argued that mechanical heating and ionization could produce the weak high-ionization lines, and would be consistent with the evidence of strong mass loss from the central star of this object.

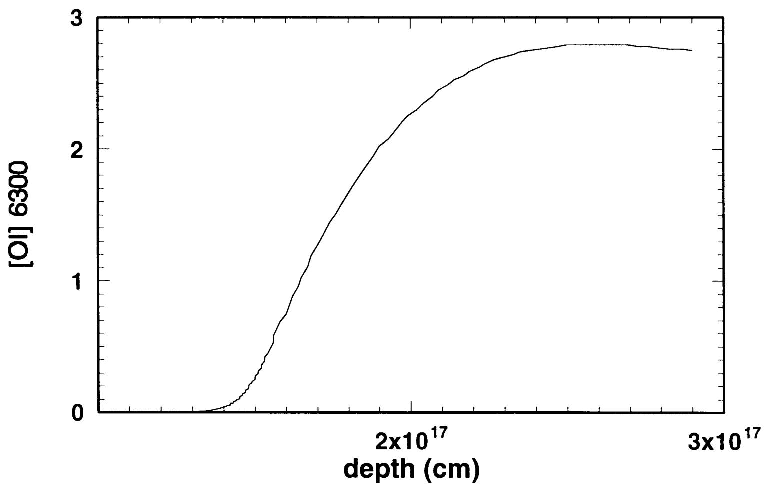

Figure 3. The intensity of [OI] 6300 relative to Hβ is shown as a function of depth for a gas with solar abundances irradiated by a blackbody with a temperature of 450,000K.

https://doi.org/10.1017/S0074180900170299 Published online by Cambridge University Press

5. Summary

Three major advances in the numerical simulations of ionized gas within Planetary Nebulae are now occurring. The predictions for even the simplest photoionization models will change once the results of the Opacity Project have been fully incorporated. Another advance is the inclusion of the thermal/opacity effects of grains within the ionized gas, which depletion patterns suggest are a general feature of PNs. Grain photoionization can sometimes be the dominant heating mechanism. Finally, mechanical heating due to stellar winds may account for weak or anomalous emission in some cases.

I thank the National Science Foundation for support, most recently through grant AST 90-19692 and by NASA through GO-2306. I acknowledge helpful conversations with Robin Clegg, Pat Harrington, Anil Pradhan, and Kevin Volk.

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