PHOTOIONIZATION MODELS

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ABSTRACT. A recent comparison of the photoionization models generated by five independent codes run with the same density and stellar radiation shows substantial agreement. Problems are more likely to arise with the defining parameters: the density distribution should be based on observed images, and the ionizing radiation should be from model atmosphere calculations, which, however, are inadequate for stars with winds. Models can be improved by including dust and by incorporating, self-consistently, radiative transfer in optically thick lines. Future work may extend modeling to axially-symmetric objects, to the interface with the hot, shocked, stellar wind, and to the molecular component present around many nebulae.

1. HISTORICAL INTRODUCTION

This talk could well be subtitled "Twenty Years of Nebular Modeling". For it was just 20 years ago that the first nebular models to calculate the ionization of the heavy elements and to incorporate their cooling in the determination of the run of electron temperature were constructed. The first such models published were those of Goodson (1967). Later in 1967, at the first in this series of IAU Symposia on planetary nebulae, similar ionization studies were described by Flower and by Williams, and I published some models shortly thereafter (Flower 1968, Harrington 1968, Williams 1968).

Soon during the first decade of modeling (1967-1977), models were compared with specific objects, and a problem emerged which dominated these studies during this period. It was found that the predicted emission lines from the low ionization stages were too weak when compared to observation. This problem has by now been resolved: the effects of charge-exchange with neutral hydrogen and of di-electronic recombination decrease the ionization level of many of the heavy elements, so that even high excitation nebulae can show strong lines of [N II], [O II], [O I], etc. The solution to this problem was emerging at the 1977 IAU Symposium: it was realized from the few rates then available that charge transfer could have a significant effect (Harrington 1978). Pequignot (1978) went so far as to compute what charge transfer rates would be needed to solve the problems presented by the spectrum of NGC 7027, and his predictions have proven to be in substantial agreement with the subsequent atomic physics calculations.

The first half of the second decade (1977-1982) saw the impact of ultraviolet observations of planetary nebulae on models. The results obtained with the IUE satellite were of especial importance. The ultraviolet data simultaneously made nebular modeling less

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arbitrary and more useful. The strongest UV lines arise in the He^{++} zone of high-excitation PNe. A lack of temperature-sensitive line ratios from this zone encourages the use of models, which provide temperatures based on the energy balance of the gas. The models were in turn constrained by the observed spectra, which were especially useful in establishing the elemental abundance of carbon, the major coolant in the He^{++} zone. The use of models for the analysis of nebular spectra helped illustrate the fact that such models provide a rational basis for the ionization correction factors (i.c.f.'s) needed to account for unobserved stages of ionization when deriving elemental abundances.

Looking over the literature since the last PN Symposium in London (1982), it seems clear that during these last 5 years modeling has finally "arrived" as a standard technique. It is a technique that is now used by a large number of groups and applied to an increasing variety of problems.

2. CURRENT STATE OF MODELING CODES

The task of evaluating the current state of nebular computational techniques was made much easier by the "Workshop on Model Nebulae", which was held at Meudon in July of 1985. This workshop included modelers of active galaxies and H II regions as well as planetary nebulae, and shock codes as well as photoionization codes. A key feature of the conference was the case studies, a set of well defined models which all the participants constructed and subsequently intercompared. Not all codes in use were represented, of course, but the 12 groups which constructed the planetary nebula case represents a substantial fraction of the active workers in this field.

The planetary nebula model consisted of a sphere of gas with a uniform density of 3000 hydrogen atoms cm^{-3} and an inner radius of 10^{17} cm, ionized by a central star with a radius of 10^{10} cm, radiating as a 150,000K black body. The nebula was to be ionization bounded, with the computation carried until the gas became neutral (at about 3.9 10^{17} cm from the star). The abundances, relative to 10^4 H atoms, of He, C, N, O, Ne, Mg, Si, and S, were set at 1000, 3, 1, 6, 1.5, 0.3, 0.3, and 0.15, respectively.

As such models go, this one is fairly demanding of the ionization program, for the high temperature star produces significant radiation at high frequencies where the absorption coefficients of H and He are small. As a result, the model must be continued to optical depths in the Lyman continuum of several hundred before the gas is predominately neutral. If the computation is terminated too soon, some of the $H\beta$ radiation is missed and the normalization of all the lines is affected.

Table 1 is a partial list of the line intensities (on a scale of $H\beta$ = 100) from 5 independent model codes. The agreement is overall rather good for the lines from major ionization stages and for temperature sensitive line ratios, with some problems apparent for the highest ionization stages. Differences can arise from a wide variety of sources: atomic data, numerical techniques, radiative transfer effects, ect. In fact, it emerged that the greatest problem was the treatment of the diffuse ionizing radiation which arises in the He^{++} zone. Codes used for clouds illuminated from the outside (as in the modeling of active galaxies) normally let this diffuse radiation escape from the inner face, while the planetary nebula codes assume such radiation crosses the interior and reenters the opposite side. This made a surprising difference, and it was necessary to re-run some codes assuming this radiation did not escape. But since many real nebulae (as opposed to this ideal case study) may allow leakage of such radiation, it is clear that there is an uncertainty in modeling real objects introduced by the extent of leakage. A further problem affecting the strengths of the high excitation lines from the He^{++} zone is different methods used to treat the line radiation which constitutes part of the diffuse field in the form of the He^{+} $L\alpha$ line and its degradation products, the Bowen fluorescence lines.

The complete list for this and other case studies (as well as the identities of the modelers!) can be found in the Workshop proceedings (Pequignot, 1986). I would urge anyone running photoionization codes to examine these proceedings and compare the results of their code with those presented there. While the workshop did not attempt to define a "standard" model, nevertheless, as Pequignot concluded, "..significant departure from these tables should reasonably call for a comment".

TABLE 1. Comparison of Independent Photoionization Codes.

Line		- Model Program -				
		(1)	(2)	(3)	(4)	(5)
Hβ	(ergs/sec)	2.64E+35	2.51E+35	2.67E+35	2.29E+35	2.01E+35
He I	5876 Å	9.7	11.	11.	9.6	8.7
He II	4686	33.6	35.0	31.6	35.0	43.4
C II	2326	49.8	31.0	32.3	44.0	32.3
C III	1909	167.	173.	170.	226.	291.
C IV	1549	170.	119.	202.	212.	207.
N I	5200	2.0	1.0	1.7	0.9	1.8
N II	6548,84	149.	146.	137.	153.	145.
N III	17492	11.8	9.0	11.2	14.5	13.7
N IV	1487	11.6	9.0	16.0	15.3	23.7
N V	1240	7.9	4.0	14.8	12.0	13.8
O I	6300,63	15.5	15.0	13.4	15.2	17.6
O II	3726,29	228.	224.	218.	252.	256.
O III	5007,4959	2015.	2105.	2160.	2470.	1990.
O III	4363	15.9	15.0	15.6	21.0	17.9
O III	52 mμ	144.	142.	143.	149.	136.
O IV	1403	14.9	7.0	17.9	15.0	21.7
O V	1218	7.3	3.0	17.8	13.2	23.5
Ne II	12.8 mμ	2.35	3.0	3.2	2.5	5.2
Ne III	15.5 mμ	256.	244.	254.	256.	238.
Ne III	3869,3968	268.	252.	259.	344.	278.
Ne IV	2423	61.9	43.0	62.0	52.6	83.9
Ne V	3426,3346	65.9	60.	94.3	94.6	106.

It is perhaps worth noting that by present-day standards, the construction of photoionization models does not require "big" computers. This came to my attention recently when the Astronomy Program at Maryland acquired several SUN 3/50 workstations. These are desktop computers. I find that my code, running on this machine, can generate a full 36 zone model, iterating four times to converge the diffuse radiation field, in less than 20 minutes. The implication is that on a big computer, a full photoionization calculation can become a subroutine in a more general problem.

3. SOME REPRESENTATIVE STUDIES

As a sample of the problems which have been considered in the last few years using photoionization codes, in this section I will review a few papers from two categories: studies which apply to PNe in general, and studies of specific nebulae. This is not intended as a comprehensive survey, rather, the citations are used to illustrate particular ideas.

3.1. General Studies

Several papers applied models to evaluate the Zanstra method for determining the temperatures of central stars. Henry and Shipman (1986) constructed a large grid of models to investigate the photon-counting characteristics of optically- thick nebulae. They considered stellar radiation with a variety of dilution factors, and with flux distributions from model atmospheres computed with various He/H ratios. They found that the traditional approach is sound but that, for thick models, the hydrogen Zanstra temperature may be more useful than the He II temperature because the latter is extremely sensitive to the He/H ratio of the atmosphere.

A more unusual situation was investigated by Stasinska and Tylenda (1986), who asked whether the traditional analysis would reveal the true temperature of extremely hot central stars, i.e., $T_{eff} > 200{,}000K$. They found that the methods break down in this regime - the central star is so faint that the only viable method is to use the ratio of He II lines to H lines. However, the He^{++} recombinations produce H ionizing radiation that swamps the direct ionization of H by the stellar radiation in the 13.6 - 54.4 eV interval, so that the intensity of He II lines relative to Hβ levels off: the He II 4686/Hβ ratio never rises above about 0.6, even for a 500,000K central star. Furthermore, the exact value is sensitive to the treatment of the diffuse radiation from the central He^{++} zone and to the possible escape of this radiation as discussed above.

Models may also be used investigate the sort of errors that are introduced by the assumptions of uniform temperature and density which are implicit in the use of diagnostic line ratios (at least when the fluctuation parameter $< t^2 >$ introduced by Peimbert (1967) is not used). Mihalszki and Ferland (1983), for example, investigated the effects of large fluctuations in density (and the corresponding temperature fluctuations) on the abundance ratios that would be obtained by a naive analysis. They found that the fluctuations cause the carbon abundance as determined from the collisionally excited UV lines to be higher than those inferred from recombination lines, just the opposite of what is frequently observed.

Models may be used to investigate specific physical processes. For example, Clegg and Walsh (1985) used models of nebulae to predict the strength of the O III 5592Å line in several PNe. This faint line is of interest because it arises mainly by charge transfer from H^0 to O^{+3}, and comparison with the observed value provides a check on the calculated rate of charge transfer into the ^1P channel. They found agreement to within a factor of 2, which, in view of the errors inherent in this approach, constitutes a verification of the theoretical rate.

3.2. Studies of Specific Objects

Studies of specific nebulae reveal some of the problems that have to be confronted for successful modeling. Adam and Koppen (1985) constructed two models, one of NGC 4361 and another of NGC 1535. Using the central star temperatures and gravities determined by Mendez et al. (1981) from profiles of the stellar absorption lines, they found that a consistent model of NGC 4361 could be constructed, but that NGC 1535 could not be modeled with the atmosphere flux implied by the stellar line analysis - the flux beyond 54.4 eV had to be raised by a factor of $> 10^3$.

Aller et al. (1987) used modeling techniques to derive physical parameters for 12 PNe in the Magellanic Clouds. The model atmosphere fluxes were taken from the NLTE calculations of Husfeld et al. (1984). This study found lower luminosities for the central stars of the brightest of these nebulae than an earlier study of Stecher et al. (1982), a revision due in large part to the choice of stellar fluxes.

While the previous studies encountered problems with the selection of atmosphere fluxes, the main obstacle that had to be overcome in the study of NGC 3918 by Clegg et al. (1987) concerned the density distribution. It was found that this nebula - which was selected partly because of its symmetrical appearance - could not be represented by a spherical nebula of any optical depth. Instead, it was necessary to adopt "dumbbell" density distribution with the nebula optically thick along the axis but optically thin, even in the He II continuum, in the equatorial plane. This structure allows a leakage of stellar photons in the equatorial plane and, consequently, the adoption of a stellar temperature which exceeds the He II Zanstra temperature.

Another instance where the density distribution was of critical importance was in the study of the halo planetary DDDM-1 by Clegg, Peimbert, and Torres-Peimbert (1987). In this case, the density based upon the surface brightness in Hβ was higher than that based upon the density sensitive [S II] 6716,31Å line ratio. Fitting these observations required the adoption of a density distribution with a high density core and a lower density envelope: the envelope is of lower excitation and hence is the site of most of the [S II] line emission. This object has extremely low abundances of the heavy elements, in common with other halo objects, but also has a uniquely low carbon abundance. As a consequence of the low abundances, collisional excitation from the metastable He I 2 ^{3}S level, which would normally be insignificant compared to collisional excitation of the elements such as C, N, and O, makes some contribution to the cooling of the nebular gas.

4. CURRENT CONCERNS

From the preceding discussion of recent work, we can see some of the issues that worry the modeler. While most of the computational aspects of the problem seem well enough in hand, the definition of the model often presents a challenge.

4.1. Good Models Demand Good Density Distributions

The distribution of nebular material in space is extremely important. While a simple model is better than no model at all, we should, if at all possible, use a density distribution that is consistent with the appearance of the object in the sky. The beautiful CCD images we have seen in the talks by B. Balick and Y.-H. Chu show the quality of data that is now available to the modeler. If we fail to make use of such information, then the dilution factor of the nebular material may take on unrealistic values. For many nebulae, it will not be possible to construct satisfactory models until departures from spherical symmetry are taken into account.

4.2. What Should We Use for the Stellar Flux ?

The choice of the stellar atmosphere flux is basic to any model. The Zanstra temperatures provide powerful constraints. The Stoy temperature, computed from the ratio of collisionally excited to recombination lines, is also helpful. But the detailed shape of the flux distribution should come from a model atmosphere computation. The recent NLTE models of Husfeld et al. (1984) and of Clegg and Middlemass (1987) are a welcome addition to the classic grid of LTE models by Hummer and Mihalas (1970). Even these models, however, often fail to represent central stars in the intermediate temperature range of 50,000K - 90,000K, where large deviations from predicted flux distributions seem to occur (e.g., Harrington and Feibelman 1983, and Adam and Koppen 1985, as mentioned in § 3.2 above). These stars may have strong stellar winds, which can drastically alter the emergent flux beyond 54.4 eV. The discussion in this Symposium by R. P. Kudritzki indicates that a satisfactory resolution of this long-standing problem may finally emerge as the result of self-consistent NLTE computations which explicitly include the line transfer in the accelerating wind.

Observations of x-rays from some central stars may help discriminate between different model atmosphere predictions of the far-UV fluxes. For example, NGC 1360 has been detected by EXOSAT. The implications of these data were discussed by de Korte et al. (1985). They concluded that no blackbody distribution was consistent with the x-ray data but that fluxes from LTE atmosphere models, with O V and Ne V absorption edges, were consistent. Unfortunately the analysis is complicated by the breadth of the EXOSAT filters. A further concern is that, although the nebula must be optically thin beyond 54.4 eV to see the x-ray emission at all, a small amount of absorption by He^+ could greatly affect the interpretation.

4.3. Other Concerns

Some of the other problems which make modeling less satisfactory than we might hope include incomplete atomic data and deficiencies in the treatment of optically thick lines.

The atomic data are generally good for C, N, O, and Ne, but when we turn to the next row of the periodic table, the data are less complete. Models often have difficulties with sulfur lines, for example. Without reliable charge-transfer and dielectronic recombination rates, we will not be able to model correctly the relative abundances of the different ions. While these elements have relatively little effect on the nebular conditions, we often would like to derive their abundances relative to the CNO group to help trace the nucleosynthetic processes in the progenitor star. Models could provide valuable ionization correction factors if we had more complete atomic data.

We also need to incorporate improved treatments of the transfer of optically thick line radiation in our PNe models. The prototype of such lines is the Lα line of hydrogen. It was originally thought that trapped radiation in this line could become so intense that the radiation pressure would dominate the dynamics. It is now recognized that the universal presence of dust in PNe suppresses the line intensity in those objects with higher optical depths. This diminishes the dynamical importance of Lα, but the transfer of this line radiation is still important as an integral part of the problem of dust heating.

While we cannot observe H I Lα directly, there are optically thick lines which can be observed. The C IV 1549Å line is very prominent in the UV spectra of high-excitation PNe, and the trapping of these photons will greatly enhance their absorption by dust. To model the degree of this attenuation requires both a solution of the line transfer problem and a model for the UV dust extinction. The solution of the problem should provide us with the expected emission line profile and the distribution of the emission over the face of the nebula - which in the case of optically thick lines is not just a projection of the emitting region. Unfortunately, IUE observations do not have quite the spatial or frequency resolution to determine much more than the total flux in this line, but the Hubble Space Telescope will be able obtain spatial maps and line profiles.

Another optically thick line which is important for the emission line spectra of PNe is the He+ Lα line. This line, and the O III lines coupled to it by the Bowen fluorescence process, is an important contributor to the photoionization heating in high-excitation PNe. The question is not only one of what fraction of the line radiation is absorbed by photoionization, and hence heats the gas, but also of how far this radiation diffuses from its point of origin. The distribution of absorption will affect the temperature structure in the inner region of the nebula, and the collisionally excited UV lines are quite sensitive to this structure. The transfer problem depends upon the velocity field in the nebula because the O III resonance lines, with only half the Doppler width of the He II Lα line, constitute a major escape channel. But information on the velocity fields in many PNe is becoming available (e.g., H.-Y. Chu, this Symposium) and there is no reason why the models cannot incorporate this data. A by-product of the solution of this problem would be the prediction of the intensities of the O III Bowen fluorescence lines for the specific object.

The methods for solution of such transfer problems exist, but have been applied to general models rather than specific objects. Thus, we have long had solutions to the Bowen fluorescence problem (Weyman and Williams 1969). But now, with advances in computing power and algorithms, we should be able to incorporate such line transfer calculations into the photoionization codes and solve the ionization and line-transfer problems self- consistently.

5. FUTURE DIRECTIONS

Looking to future work in this field, one can predict with little risk that models will continue to be used, with varying degrees of elaboration, to obtain i.c.f.'s for chemical abundance determinations in PNe.

More interesting perhaps is the likelyhood of extending photoionization calculations into situations where other physical processes must be considered. I deliberately do not touch upon the dynamical models where the photoionization computation is carried out in conjunction with the hydrodynamic expansion of the nebula - this topic will be discussed by J. Koppen. Nor I will discuss the time-dependent ionization effects to be expected as a result of the rapid evolution of the most massive central stars, as R. Tylenda will mention this topic. In this section I will just briefly indicate a few other extensions which should be explored.

5.1 Dust in the Ionized Gas

One aspect of PNe which I feel has been somewhat neglected by modelers is the presence of the dust. Not only is the dust responsible for the IR emission, but it also causes attenuation of some observable UV resonance lines, notably C IV 1549Å as discussed above. The introduction of dust into photoionization models places a physical constraint on the dust model: the same radiation field that explains the ionization structure must be able to heat the dust to the temperature required by the observed far IR emission. The IRAS satellite observed a large number of PNe, so observational data is available for most of the bright objects. An attempt to explore this type of modeling for NGC 3918 has been presented by Harrington, Monk, and Clegg (1988). Also, see the contributed paper in this Symposium by M.G. Hoare, who has used similar techniques to model IC 418 and other objects. It is not hard to see why modelers have avoided routine inclusion of the dust. The difficulty, of course, is our poor knowledge of the optical characteristics of the dust particles.

Dust can potentially affect any of the optically thick lines in nebulae, and so should be included in treatments of the Bowen fluorescence lines and the He I 10830Å line.

The line transfer of H I Lα, C IV 1549, etc. in the paper by Harrington, Monk and Clegg (1988) is solved - or rather avoided - by the escape probability method. It is possible improve upon this treatment. If the optical depths are not too large, then partial redistribution in the line wings can be neglected, and the resulting complete redistribution problem can be solved by the powerful accelerated lambda-iteration procedure (Olson, Auer, and Buchler 1986). With this method, taking proper account of the spherical geometry is not difficult. I have obtained solutions by this method which confirm the global accuracy of the escape probability approximation, while at the same time indicating that in objects of non-uniform density structure, there are interesting effects which can only be seen when the transfer problem is solved properly. For example, the absorption by dust depends upon the dust/H^0 ratio, which is highest in low density regions, while the generation of Lα photons is highest in high density regions. Thus there is a transport of energy from the higher density to lower density regions.

5.2 The He I Spectrum

A paper by Ferland (1986), suggesting that collisional excitation of helium atoms in the metastable 2 ^{3}S state was more important than previously supposed, and that as a consequence, He abundances in PNe might have been overestimated by up to 50%, has reawakened interest in the He I spectrum. Recent discussions by Clegg (1987) and by Peimbert and Torres- Peimbert (1987) have shown that the abundance revisions are not in fact large. The discussion by Peimbert and Torres-Peimnert (1987) indicates, moreover, that the population of the 2 ^{3}S state determined empirically from the He I spectrum (the He I 10830Å line is produced chiefly by collisional excitations from 2 ^{3}S) is only about half what one expects based on the rates of recombination, radiative decay, and collisions. This suggests that depopulation by photoionization may be important, and in fact computations show (Clegg and Harrington, 1988) that the population can be reduced by up to 20% in compact objects. In addition to direct photoionization by stellar radiation, the H I Lα radiation field is important. This introduces a further complication since the Lα intensity is controlled by the dust content of the nebula, so that a self-consistent treatment of the He I 10830 line brings us back to the dust problems discussed above.

5.3 Axially Symmetric Nebulae

With all the new CCD images we have seen at this Symposium, there is clearly an explosive growth in information on the structure of PNe. Unfortunately, not too many of them are "theorist's planetaries"! B. Balick has presented the case for an evolutionary sequence of axially symmetric objects, with expansion driven by the pressure of the shocked stellar wind, which forms a hot, thin gas trapped inside the denser nebular shell. Whether or not this picture is universally valid, it is clear that axially symmetric objects in various orientations can explain most of the forms we see. We will have to generalize our codes to deal with such structures. We should be grateful for any symmetry we can get!

5.4 The Interface With the Shocked Stellar Wind

When a 2000 km/sec wind from the central star strikes the virtually stationary nebular material, or rather, the previously stopped wind material, the shock results in temperatures of the order of 10^7 K. We expect that there will be some transfer of this heat into the adjacent nebular gas, either through conduction across the contact discontinuity, or if this is too strongly inhibited by magnetic fields, perhaps by conduction into small parcels of material mixed into a (mass- loaded) flow of the shocked wind. Such a flow past the nebular torus would form when the wind-blown bubble bursts, and would explain the material seen to be moving at velocities of hundreds of km/sec in some nebulae. Radiation from such a region would generally be swamped by the normal nebular spectrum, but spectra of high spatial resolution might reveal some signature of the interface. To complement the observational search for interaction of the 10^7 K component and the 10^4 K component, we need models of such an interface zone, defining the volume occupied by the various ionization species and the power radiated in different spectral lines.

5.5 The Molecular Component

Finally, we will want to consider the molecular gas which is being discovered in more and more objects. How do CO (and presumably H_2) molecules survive in such an evolved object as NGC 7293? Can we balance the heating and cooling to determine the temperature and hence predict the CO emission? The simplest questions, such as the effectiveness of self-shielding and the consequent lifetime of molecules in PNe have yet to be determined. In cases where the line ratios indicate that the H_2 IR emission may be due to fluorescence rather than shock heating, we will want to model this process. Once again, planetary nebulae may emerge as the best laboratories for the investigation of a whole set of physical processes, this time processes which have hitherto been hidden in amorphous, dark clouds.

The construction of ionization models should be regarded as the meeting ground for all the varied data we are able to collect. When thus brought together, the whole should be greater than the sum of the parts.

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