Atomic processes in planetary nebulae
and H II regions

Manuel A Bautista

Department of Physics, Virginia Polytechnic Institute and State University, VA 24061, USA
E-mail: bautista@vt.edu

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Abstract
Spectroscopic studies of planetary nebulae (PNe) and H II regions have driven much development in atomic physics. In the last few years, the combination of a generation of powerful observatories, the development of ever more sophisticated spectral modeling codes, and large efforts at mass production of high-quality atomic data have led to a significant progress in our understanding of the atomic spectra of such astronomical objects. In this paper, I review this progress, including evaluations of atomic data by comparisons with nebular spectra, detection of spectral lines from most iron-peak elements and neutron-capture elements, observations of hyperfine emission lines and analysis of isotopic abundances, fluorescent processes and new techniques for diagnosing physical conditions based on recombination spectra. The review is aimed at the atomic physicists and spectroscopists who are trying to establish the current status of the atomic data and models and need to know the main current issues.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction

Nearly all modern observational research in gaseous nebulae (planetary nebulae (PNe), H II regions and circumstellar nebulae) involves some kind of spectra, whose interpretation requires some understanding of the atomic processes involved and the handling of atomic data. The level of understanding of such processes and the data required for various applications range from phenomenological and statistical studies of common prominent lines, to compilation of raw atomic data for direct inspection (such as line lists), and to modeling of synthetic spectra attempting to fit the observed spectra. On the other hand, the accuracy and quantity of atomic models describing various features of observed spectra have evolved with time, driven by great advances in ground- and space-based observatories, computer technology and experimental techniques. At present there are models and data accurate enough for satisfactory analysis of at least the most prominent spectral features. Also, the advent of on-line databases and spectroscopic tools has revolutionized the dissemination of results of atomic physics research. However, the demands on the quantity and quality of the atomic data will grow as new instruments delivering greater sensitivity and spectral resolution become available.

A review of atomic processes spans an audience that includes specialists in the study of atomic systems utilizing tools capable of providing models and atomic data, astronomers seeking to understand the reliability and accuracy of their modeled spectra, and those who use the models and data to compare synthetic spectra with observations in order to diagnose the physical conditions and compute chemical abundances of nebulae. The present review is aimed at the researchers in atomic physics and spectroscopy who wish to understand the extent of currently available atomic models and to identify present needs.

The physical conditions in gaseous nebulae of interest here are those of photoionized plasmas as observed in the ultraviolet (UV), optical and infrared (IR) bands. Roughly speaking, these conditions are: temperatures of the order of $10^4$ K and electron densities between $10^5$ and $10^8$ cm$^{-3}$. This
The spectrum of hydrogen in H II regions has been studied extensively for quite some time. In principle, the spectrum is determined by the recombination rates into each level and the subsequent radiative cascades. Such a process is accurately modeled in two idealistic situations, the so-called ‘case A’ in which all lines are optically thin and ‘case B’ that assumes that the optical depth of H Lyα goes to infinity. Two complications arise beyond these approximations: (1) a detailed solution to the radiative transfer of H Lyα photons, including the effects of self-absorption, removal of Lyα photons and collisionally induced transitions between the 2s and 2p states, and (2) when the electron temperature and density of the plasma are high enough for effective collisional excitations on to n > 2 states.

Dennison et al [2] discuss the first of these problems and propose an observational test. They claim that radio telescopes will soon be able to detect the 2s1/2–2p1/2 and 2s1/2–2p3/2 lines at 1.1 and 9.9 GHz, respectively. They explain that removal of H Lyα photons by dust would limit the pumping of H atoms into the 2p states, and under these conditions the 2s1/2–2p1/2 transition will appear in stimulated emission, while the 2s1/2–2p3/2 line will appear in absorption. In general, the relative strength of these two lines should serve as a diagnostic of the populations of the 2s and 2p states and the responsible processes. Further, Dennison et al suggest that removal by dust is the dominant mechanism acting on H Lyα photons in H II regions, which if correct would circumvent the need to solve the radiative transfer problem.

With regard to collisional excitation of hydrogen, Péguynot and Tsamis [3] studied the evolution of calculated collision strengths for 1s → n = 3, 4, 5. They point out large variations in the theoretical values up to the last calculation of Anderson et al [4]. Péguynot and Tsamis compare their observations for the planetary nebula G135.9+55.9 with predictions of models using various collisional data sets. They find that the collision strengths of Anderson et al yield the most consistent results, yet these may not have reached ultimate accuracy.

Modern high signal-to-noise optical spectra allow for accurate measurements of lines and continuum around the Balmer and Paschen recombination series. By fitting the results of detailed spectral models to these measurements, it is possible to determine the electron density and temperature in the nebula [5]. Surprisingly, temperatures obtained from the Balmer series often disagree with the temperatures derived from line ratios of collisionally excited lines, such as the ratio of nebular to auroral lines of [O III]. Moreover, for a large sample of PNe studied by Zhang et al the hydrogen Balmer temperatures are typically lower than the collisional oxygen temperature by several thousand degrees. These temperature differences are used in support of the so-called ‘temperature fluctuations’ or ‘temperature variations’ in nebulae. However, a warning flag on the use of hydrogen temperatures comes from the fact that in four PNe where temperatures from the Paschen series were determined, these disagree with the Balmer temperatures at the three sigma level or more.

3. Helium

Modeling the He I recombination spectrum has become increasingly more reliable, with an accuracy in line emissivities of the order of a few per cent (see [6–8]). Yet, this is not at the 1% accuracy level needed to place useful constraints on the primordial helium abundance in cosmological studies [9, 10]. Recently, Bauman et al [6] worked out the recombination problem in fine structure in the low-density limit. They found no significant effects on the recombination spectrum from spin–orbit coupling. However, they found that some lines may be uncertain due to the use of poor-quality atomic data, specifically the photoionization cross sections for states with 9 < n < 20 and L < 3.

A practical test on the accuracy of models and observations of He I lines came from Porter et al [11], who compared model predictions with measured fluxes for 100 lines with n < 20 from the Orion nebula. They found an average difference of 6.5% between all observed and predicted lines and 3.8% difference for the 22 most accurately measured lines.

Zhang et al [12, 13] present a method to diagnose temperatures from He I line ratios. They write parametric forms for He I line ratios versus temperature and conclude that the best diagnostic is obtained from the λ7281/λ6678 ratio. The results of the diagnostics have an intrinsic uncertainty of ∼ 1000 K at about 10 000 K owing to optical depth effects on the He I λ3889 (2s2 → 3p3P0) line. When comparing the results from the λ7281/λ6678 ratio with those from λ7281/λ5876, a systematic error of (−500 K) arises, which may be related to the uncertainty in the optical depth of the λ3889 line. Interestingly, in a sample of 48 PNe the helium temperature is systematically lower than that obtained from the hydrogen Hβ decrement by an average of 4000 K.

4. The second and third row elements (C–Ar)

Density and temperature diagnostics in PNe are commonly based on line ratios among collisionally excited lines. The best known density diagnostics are [S II] λ6717/λ6731 and [O II] λ3729/λ3726, which are sensitive to densities of the order of \( N_e \sim 10^5 \text{ cm}^{-3} \), [Cl III] λ5557/λ5537 for \( N_e \sim 10^6 \text{ cm}^{-3} \) and [Ar IV] λ4711/λ4740 for \( N_e \sim 10^6-10^8 \text{ cm}^{-3} \).

The [O II] ratio that arises from transitions among the S3/2 ground level and the D3/2 and D5/2 levels was a subject of controversy for the last few years. It was commonly assumed that LS coupling was a valid approximation for terms of the ground configuration of the O+ system; thus the ratio of collision strengths from the ground levels to the D3/2 and D5/2 levels was given by the statistical weights, i.e. 1.5. However, McLaughlin and Bell [14] claimed that relativistic effects enhanced the ratio of collision strengths to 1.93, with profound
 effects on \( N_e \) determinations for low-surface-brightness H \( \text{ii} \) regions. Such claims were contested by evidence from the extensive literature survey of Copetti and Writzl [15] and the observational campaign of Wang et al [16]. The issue seems settled now with a new calculation by Pradhan et al [17] that accounts for all dominant relativistic effects and confirms the earlier predictions of the \( LS \)-coupling approximation. The spectroscopic survey by Wang et al also served to test the \( A \)-values for dipole forbidden transitions of \([O \text{ ii}])\). They found that the transition probabilities of Zeippen [18] best fit the observations, the differences being of only a few per cent, while the results of later calculations by the same author ([19]) and by Wenaker [20] look problematic. This latter set is what is currently available through the database of the National Institute of Standards and Technology (NIST) ([21]).

Wang et al also compared the electron densities obtained from various line ratios and obtained very good agreement between \( N_e ([O \text{ ii}])\), \( N_e ([S \text{ ii}])\) and \( N_e ([Cl \text{ iii}])\). By contrast, \( N_e ([Ar \text{ iv}])\) values yield densities systematically higher than those from the other diagnostics, which places doubt on the accuracy of the \([Ar \text{ iv}])\) \( A \)-values.

### 5. The iron-peak elements

Iron-peak elements are important constituents of gaseous nebulae. Depending on the excitation of the nebula, iron is frequently seen in stages from Fe i to Fe vii. The observed ions of nickel span about the same range. Other less abundant elements of the group are occasionally identified as well. An extreme example of rich spectra is the \( \eta \) Carinae ejecta (see the paper by Nielsen and Gull in this volume).

On this subject, the contributions of Svenseric Johansson could hardly be overstated. He has been the driver of extensive and detailed research on energy levels and transition rates for the low ionization stages of iron-peak species. These data are often taken for granted as they become easily available through various databases, yet their determination from laboratory work requires very skillful people and substantial funding. Johansson’s publications on the subject are too numerous to list here, but some of the most important contributions are: on the spectra of Sc ii [22], Fe i [23], Fe ii [24], Ti ii [25] and Co ii [26] and on the determination of \( f \)-values, lifetimes and radiative rates for forbidden transitions (e.g. for Fe ii [27–30], Ti ii [31] and Ni i [32]). Johansson has also done seminal work on understanding the Ly\( \alpha \) excitation mechanism of Fe ii and other iron-peak species in astronomical spectra (e.g. [33–35, 39]).

Spectra of singly ionized iron-peak species are particularly complex as they respond to a variety of excitation mechanisms. These are H Ly\( \alpha \) fluorescence, continuum fluorescence, self-fluorescence by overlapping Fe ii transitions and collisional transitions among low and high levels. In moderately dense plasmas \((N_e \sim \! 10^7 \text{ cm}^{-3},\) the populations of high levels involved in fluorescence are redistributed by collisionally induced transitions through highly excited pseudo-metastable levels [36]. Furthermore, proper modeling of Fe ii requires the atomic data for large systems to be complete and accurate. This has led to a diverse set of models with little consensus among them and limited understanding about their accuracy. For ions other than iron and nickel the first detailed spectral models are now being created, e.g. [37, 38]. A good part of this work has been done under the auspices of the IRON Project [40]. A summary of the data is presented in figure 1. More work is also in progress by various groups such as the IRON Project, the FERRUM Project at Lund University, at NIST, and the group at Queen’s University Belfast.

Another modeling challenge in dealing with dense spectra of iron-peak species is the treatment of the transfer of line radiation from the point of emission to the boundary of the atmosphere. For iron-peak species, in addition to continuum opacity and resonant scattering, one must consider fluorescence by line overlaps, such as the well-known H Ly\( \alpha \) effect in Fe ii [39]. While writing the present review, I have

|    | Sc | Ti | V | Cr | Mn | Fe | Co | Ni |
|----|----|----|---|----|----|----|----|----|
| I  |    |    |   |    |    |    |    |    |
| II | [49]| [38]| Proc.| [75]| Proc.| [37, 41, 42, 43]| Proc.| [46]|
| III|    |    |   |    |    | [44] |    |    |
| IV |    |    |   |    |    | [45] |    | [48]|

Proc.: in progress

future work

Figure 1. References for spectral models of low ionization iron-peak species.
estimated the number of overlaps between absorption lines arising from low-excitation levels, typically populated under nebular conditions, of Fe ii–iv and lines from H i, He ii, O ii and O iii, dominant species in typical nebular spectra. Line wavelengths were taken from the NIST database and do not represent the entire spectra. For line widths of 20 km s⁻¹ the number of overlaps is 592, 243 and 49 for Fe ii–iv, respectively, whereas for widths or 60 km s⁻¹ the number of overlaps is 1722, 762 and 524 for the same ions. This is the range of line widths in nebular spectra. The huge number of line overlaps demonstrates the need for a detailed treatment of radiative transfer of iron spectra. The case also applies to other iron-rich species.

In modeling spectra one also needs to solve the problem for ionization equilibrium of each element. For that reason, detailed level-specific photoionization cross sections, which account for complex resonance structures, are being computed for both ground and excited states using the R-matrix method. Cross sections are available for Fe i–iv [48–51] and Ni ii [52]. Recently, much progress has been made at the Instituto Venezolano de Investigaciones Científicas (IVIC) by our group on the calculation of cross sections for Sc i, Ti i and Cr i.

6. Hyperfine-induced spectra

Observations of hyperfine-induced transitions in PNe have been of great interest in recent years. This is because these spectra allow us to determine relative isotopic compositions to be compared with predictions of nucleosynthesis. This, in turn, enables us to disentangle enrichment by stellar nucleosynthesis from the primordial composition in observed present total abundances. For example, the abundance of ³He in the Galaxy could be used to test big-bang nucleosynthesis and constrain the baryonic density of the universe. However, the evolution of ³He in the Galaxy is a longstanding open problem due to the observed discrepancy (by two orders of magnitude) between theoretical yields of low-mass stars and the measured abundances in H ii regions [53, 54]. A proposed solution of this problem could be in suppressing, by nonstandard mixing mechanisms, the production of ³He during the red giant branch and/or asymptotic giant branch (AGB) phases of stars of mass up to ∼ 2 M☉ [55, 56]. An observable consequence of such a scenario is that the ratio ¹²C/¹³C in the ejecta of PNe should be much lower than in the standard case. For a 1 M☉ star, the predicted ratio is ∼ 5, in contrast with the standard ratio of 25–30 [57].

Isotopic abundances can be derived from beryllium-like ions through observations of the hyperfine-induced transition 2s2p ⁴P⁰⁰ → 2s ¹S₀ within the UV0.01 multiplet. This transition can only occur through coupling of the electronic total momentum with nuclei of nonzero spin. This happens in spectra involving ¹³C (with nuclear spin ½) but not with ¹²C. Thus, ¹²C/¹³C abundance ratios can be derived from spectra showing the hyperfine transitions together with the stronger 2s2p ⁴P⁰⁰ → 2s ¹S₀ (M2) and 2s2p ⁴P⁰⁻ 2s ¹S₀ (IC) transitions. Palla et al [58] observed these lines in NGC 3242 using the Space Telescope Imaging Spectrograph (STIS) on board the Hubble Space Telescope. From this, they derived ¹²C/¹³C = 38. The same lines from the isoelectronic ion N iv were measured by Brage et al [59] from an STIS spectrum of NGC 3918. In this case both stable isotopes of nitrogen (¹⁴N and ¹⁵N) have nonzero nuclear spin. Although no abundances were derived, this work served to confirm the theoretical A-value for the hyperfine transitions. More recently, Rubin et al [60] analyzed spectra of PNe in the archive of the International Ultraviolet Explorer (IUE) satellite and determined ¹²C/¹³C = 4.4 ± 1.2 for one object and established lower limits to this isotope ratio in 23 objects.

Another study of hyperfine-induced transitions, but this time in Ne-like Al iv, was reported by Casassus et al [61]. The two stable isotopes, ²⁷Al and ²⁶Al, have nuclear spins ⁵ and ⁷, respectively. Thus, hyperfine structure causes the ³P₂→³P₁ transition at 3.66 µm to split into nine components, five of which could be resolved spectroscopically. From the observations, Casassus et al calculated an upper limit to the ²⁶Al/²⁷Al abundance ratio of 1 : 33 in NGC 6302, which is in good agreement with the predicted value of 1 : 37 from stellar evolution models.

7. Neutron capture elements

One of the frontiers of spectroscopy of PNe is the study of neutron-capture elements presumably synthesized by the AGB progenitor of the nebula. The progress in this area since the seminal work of Péquignot and Baluteau [62] has been slow owing to the need for high spectral resolution (Δλ/Δλ > 10,000) and the absence of atomic data and models. Despite the difficulties, Dinerstein [63] was able to identify lines of [Kr iii] and [Se iv] in the K-band of the near-IR spectra of NGC 7027 and IC 5117. Soon after, Dinerstein and Geballe [64] also detected [Zn iv] lines in the near-IR spectrum of NGC 7027. To date, these lines have been identified in almost 100 PNe [65, 66].

On the theoretical side, the calculation of collisional data for heavy species represents an important challenge because intermediate coupling representations are inappropriate in many cases, at the same time that relativistic effects become too large to treat in the Breit–Pauli representation. Thus, researchers must turn to fully relativistic codes in the Dirac formalism. Recently, Badnell et al [67] put the Dirac–Coulomb R-matrix package of Berrington et al [68] on the same footing as the traditional Breit–Pauli R-matrix codes developed by the IRON/RnA team. Nonetheless, these sorts of calculations are still far from routine work, owing to the size of the atomic representations in J K-coupling.

8. Additional considerations

This review would not be complete without pointing out some important general issues of relevance to the present subject as well as recently developed tools for atomic spectroscopy.

The accuracy of recombination rate coefficients was in recent years an important source of concern for modelers for their effects on calculations of ionic fractions. The issue, however, seems to have reached a point of stability as different theoretical methods, e.g. the unified R-matrix approach of Nahar and Pradhan and the Thomas–Fermi–Dirac approach in the version of Badnell and collaborators [69], begin to yield consistent results and to release large amounts of data. Such
theoretical results also seem to agree with recent experimental determinations (e.g. [69]). A warning must be raised though regarding low-temperature dielectronic recombination, which is dominated by near threshold autoionizing channels, whose positions are difficult to determine accurately from theory. More experimental work in this area is needed to benchmark current and forthcoming data (e.g. [70]).

On its origins, one of the explicit objectives of the IRON Project was to provide a complete and reliable set of data for positive ions of interest in nebular IR spectroscopy. A comprehensive review of these data is presented by Badnell et al. [71]. The entire data set produced by the IRON Project will soon be available through TIPbase [72].

A very useful tool for nebular spectroscopy, the EMILI package for emission line identification, has been developed by [73]. This tool should expedite the analysis of high-spectral-resolution and high signal-to-noise spectra and enable the identification of faint, poorly known features.

9. Conclusions

The question of what fractions of Lyα photons are self-absorbed and removed by dust in photoionized regions is rather important, as the treatment of hydrogen spectra in photoionization models is one of the main limitations to their accuracy. There are also various questions with regard to heating and photoevaporation of grains in PNe. Further research on this topic is fundamental for entering a new level of detailed understanding of PNe and H II regions.

Temperature diagnostics utilizing H and He are very important as they yield new information on the long-lasting problem of temperature fluctuations in gaseous nebulae. It is important, though to sort out the apparent inconsistencies between temperature diagnostics from different recombination series of lines or line ratios. Moreover, it seems plausible that temperature fluctuations in nebulae could be accompanied by density variations. Thus, it is important that both quantities be derived simultaneously from the same diagnostics.

As atomic models have become available for essentially all of the most prominent species in spectra of gaseous nebulae, it is important to check that diagnostics of temperature and density of the various species all yield consistent results. This would allow us to determine whether the atomic data have reached their ultimate accuracy. A warning flag must be raised, however, with regard to neutral species and ions with ionization potentials below that of hydrogen, because their spectra could be affected by photoexcitation by continuum radiation. This is the case with Ni I [74] that Copetti and Writzl [15] tried to analyze on the same grounds as ionized species.

Iron-peak ions are as important as ever, particularly Fe II, which is prominent throughout astronomy. These ions, however, still pose great challenges. The open 3d structure of these species is difficult to describe owing to various factors: (i) large numbers of strongly correlated LS terms closely spaced in energy from the ground state; (ii) strong angular correlations among configurations such as 4s2, 4p2, 4d2, 4p4f that lead to very demanding computations; (iii) strong core-valence interactions in the vicinity of excitations of 3p electrons onto the unoccupied 3d orbital, leading to the so-called giant 3p → 3d resonance; and (iv) correlations among 3d electrons, such as the radial distribution of electrons in a 3d10N configuration, differ from that of electrons in a 3dNnl. More experimental work is needed, particularly in the measurement of cross sections that guide theoretical work (e.g. [75]).

The importance to modern astronomy of studying isotopic abundances and neutron-capture elements can hardly be overstated. Yet, such work imposes extreme demands on spectroscopic instruments and astronomers. Carefully coordinated efforts between atomic physicists, astronomers and instrument designers would be desirable on this subject.

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