Time-Dependent Photoionization of Gaseous Nebulae

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TIME-DEPENDENT PHOTOIONIZATION OF GASEOUS NEBULAE

by

Ehab Elsayed Elhoussieny Ahmed

A dissertation submitted to the Graduate College
in partial fulfillment of the requirements
for the degree of Doctor of Philosophy
Physics
Western Michigan University
June 2017

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We study time-dependent photoionization of gaseous nebulae, i.e. the physical conditions and spectra of astronomical plasmas photoionized by a time-dependent source of ionizing radiation. Our study proceeds in two chief steps: First, we start with a simplified model of plasmas of pure H. Second, we develop a more realistic model of plasmas composed of a mixture of chemical elements. For the first step, we wrote a time-dependent photoionization code (TDP) that solves the coupled system of equations for ionization, energy balance, and radiation transfer in their full time-dependent forms. For the second step, we developed a more realistic code (TDXSTAR) to solve for the excitation, ionization, thermal, and radiative transfer equations in their full time-dependent forms using full atomic model. The TDXSTAR code is based on the well known steady-state code XSTAR and capable of including all chemical elements from hydrogen (Z=1) to nickel (Z=28).

TDP and TDXSTAR simulations of a pure hydrogen nebula with constant density show that ionization and thermal fronts are created due to flux variations and propagate (often supersonic) through the cloud over time scales that vary widely and non-linearly across the nebula. Further, simulations for slabs initially in pressure equilibrium show that thermal and pressure fronts propagate through the plasma, which become particularly pronounced across the ionization front (IF). In addition, periodic variations in the ionizing flux lead to
the following conclusions, (1) the instantaneous physical conditions of the plasma are different from any steady-state solution, (2) the time-averaged conditions are different from any steady-state solution and characterized by over-ionization and a broader IF with respect to the steady-state solution for a mean value of the radiation flux. (3) the dispersions in the physical conditions from their time-averaged values are increase period of variations in the flux, (4) variations in physical conditions are asynchronous along the slab due to the combination of non-linear propagation times for thermal and ionization fronts and equilibration times.

Further, we used TDXSTAR to study the physical conditions in planetary nebulae (PNe) that are experiencing a steady decline in stellar temperature. Simulations show that spectra of different ions respond differently to the stellar evolution; while some lines decay others are enhanced. Differences in initial stellar temperatures don’t affect the spectral lines trend. However, higher initial stellar temperature yield more intense forbidden lines due to the higher electron temperature. Moreover, models with different gas densities show that gas densities determine the time scale of the gas response to the changes in the ionizing radiation. Furthermore, models of different fixed luminosities produce similar conditions throughout the nebulae where luminosities and distances scale in a way such that the radiation field stays nearly the same across the nebulae, with the exception He II lines.

In addition, we studied the time-dependent effects in H II regions and planetary nebulae ionized by binary systems. Simulations of different periods from a few days to decades show that short-period binaries (with periods much shorter than equilibration times in the gas) have no noticeable effects on the gas conditions. In contrast, binary systems with
long periods (comparable to equilibration times in the nebula) have noticeable effects on
gas conditions. The time-averaged temperature profiles are different from the steady-states
corresponding to the mean flux. Further, time-averaged temperature profiles show two
peaks and flatter profiles compared to that of the steady-state corresponding to the mean
of the ionizing flux. The two-peak average temperature profiles suggest binaries as prob-
able sources of temperature fluctuations. Furthermore, the average temperature weighted
by collisionally excited and recombination lines integrated over nebular volume exhibit
clear discrepancies in the temperature. Thus, adopting an average temperature for spec-
troscopic abundances determinations are expected to lead to discordances in the estimated
abundances.
ACKNOWLEDGMENTS

I would like to express my sincere gratitude to my advisor, Prof. Manuel Bautista for his guidance, valuable discussions, and his continued support. Without his guidance there is no way I could accomplish this work. Thank you!

I would also like to thank Prof. Timothy Kallman from NASA for his immeasurably helpful discussions; I would not have been able to get a foothold in his profound code, XSTAR, without his great help.

I would also like to thank Dr. Javier Garcia from Harvard-CFA, for his great help with his code, TDP, which was a milestone in understanding the basics of my research project.

I am grateful to my dissertation committee members, Prof. Kirk Korista, Prof. Thomas Gorczyca, and Prof. Mark Voit for reviewing this dissertation and their valuable comments.

I would like to thank my wonderful wife, Sarah who deserve the credit of this work for giving me the time at home to work on this dissertation and made sure I had plenty of sustenance during the process. I love you and our son, Yusuf dearly.

I would like to thank my dearest friend ever, Carolyn and her family who made life much easier through encouragement and support.

Ehab Elsayed Elhoussieny Ahmed
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CHAPTER I

INTRODUCTION

1.1 Astronomical Photoionized Nebulae

Photoionized gaseous nebulae are one of the most common structures in astrophysics and comprise any situation in which a gaseous cloud is ionized by electromagnetic radiation. They span through a wide range of temperatures and density conditions and appear as illuminated regions with a wide range of sizes extending from a circumstellar nebula to large cosmological structures. They have been observed in a broad range of brightnesses, from bright nebulae that can be easily seen directly from a regular telescope eyepiece to extra galactic structures faint that require longer exposure time and filters to suppress lights from other sources [1].

Incident ionizing photons ionize the gas ejecting electrons (photoelectrons) with wide range of energies, which contribute to the net heating of the plasma. Power of the ionizing source determines the depth of the ionized region within a cloud. A large fraction of the ionizing photons within this volume get absorbed by atoms and ions, beyond this depth the ionization fraction sharply drops forming a thin transition layer, called ionization front (IF), that separates the ionized region from the neutral gas. For example, a star emitting ionizing radiation and embedded in the central region of a spherical cloud, composed of only hydrogen with density $n_H$, ionizes spherical volume (called Strmgren Sphere) with radius given by,

$$ R = \left( \frac{3N_\ast}{4\pi \alpha n_H^2} \right)^{1/3} $$
where $N^*$ is the total rate of ionizing photons in the sphere, $\alpha$ the recombination rate coefficient, $n_H$ is the hydrogen density. Thus, a cloud with density $n_H = 10 \, cm^{-3}$ ionized by a source of radiation emitting ionizing photons with a rate of $N^* \approx 10^{49} \, photons/s$, the recombination rate is $\alpha \approx 3 \times 10^{-13} \, cm^3 \, s^{-1}$, yield a Strömgren radius of 30 ly. Here we review three examples of the most common photoionized astrophysical nebulae [2].

The interstellar medium (ISM) in galactic plane can be either neutral (called HI regions) or ionized (called HII regions or diffuse nebulae). HII regions are of the most common examples of photoionized nebulae in astrophysics. They are large clouds with sizes ranging from tens to hundreds of light years across and characterized by irregular shapes due to the asymmetry of the medium as well as the anisotropy of the incident radiation emitted by different stars from different directions. They appear as bright regions due to their emission lines from various species, such as hydrogen, helium, oxygen, iron etc. They originate in gas clouds associated with newly formed stars, such as clouds in the spiral arms of the spiral galaxies which host a plethora of newly born stars that provide energetic ionizing photons needed for ionization. The ionizing stars (O type or early B type) are luminous and hot with effective surface temperatures ranging from $30,000 \, K$ to $50,000 \, K$. Usually, the hottest ones are the main source of ionization. The typical density of HII regions ranges from $n_H \approx 10 - 10^4 \, cm^{-3}$. This density tends to decrease due to the expansion of the hotter gas in the ionized region pushing the IF toward the surrounding cooler neutral medium, see figure 1.1. Through the nebula the constituent elements are singly to triply ionized. Being rich of hydrogen and helium, spectra of HII nebulae are typically strong in HI and HeI recombination lines. Other strong features in the spectra are collisionally excited dipole
forbidden lines, such as [NII] and [OII] [3].

Planetary Nebulae (PNe) are also examples of photoionized nebulae. PNe are bright shells seen around stars that have recently evolved from the red giant towards the white dwarfs stage. The main source of ionization in PNe is a very hot old star/s lying at their centers. The surface temperature of these stars are typically in excess of about 50,000 K. The free electrons, released by photoionization (photoelectrons), recombine with the ambient ions creating emission lines during the recombination process. Typical PNe are with sizes of order of light year across, and density from $10^2 - 10^4 \text{cm}^{-3}$. Unlike HII regions, PNe are characterized by greater degree of symmetry. They have similar chemical abundances similar to that of their parent stars from which they were originated. PNe originated from stars in the galactic plane are much more metal rich than those originate from stars in the galactic halo. The cloud’s physical properties such as temperature, electron density can be derived from their emission lines. PNe expand with velocities of tens of km s$^{-1}$ which causes a decrease in their densities and emission with time, making them fairly faint over a course of several thousands of years [4].

The above examples of photoionized nebulae experience variability in their emitted radiation on different timescales. For instance, recent observations of HII regions have shown variability in their fluxes on short timescales $\sim 10\text{yr}$. The flux variability in HII regions can be caused by various reasons such as dynamical effects or variability in the ionizing star/s embedded in the HII medium [5]. Similarly, PNe observations show variability in their observed fluxes over timescales as short as $\sim 1\text{yr}$. The variability in PNe can be caused by the stellar evolution of the ionizing source embedded in their clouds [6, 7].
Figure 1.1  NGC 604, a giant H II region in the Triangulum Galaxy. Image Credit: NASA, Hui Yang University of Illinois ODNursery of New Stars
Figure 1.2  The Spirograph Nebula (IC 418) planetary nebula lies in the Milky Way Galaxy with a diameter extending to about 0.3 light-year. Image Credit: NASA and The Hubble Heritage Team (STScI/AURA).
1.2 Photoionization Modeling

Modeling photoionized nebulae is important in order to understand their physical conditions, interpret their observed spectra, and eventually reveal information regarding their hosting systems. For instance, by studying planetary nebulae we understand the structure and composition of the outer shells expelled by a dying star and the physical characteristics of the remaining core. The study of AGN outflows may provide insight into the physical conditions and structure of the hosting black hole.

A successful photoionization model should include all the major micro-physics processes affecting the atoms and ions that make the nebula. These processes include photoionization, recombination, Bremsstrahlung radiation, collisional excitation and ionization, and spontaneous and stimulated radiative transitions. The chief physical difference among various photoionization modeling codes available at present is the treatment of radiative transfer of the diffuse part of the radiation where one of the following methods is adopted, on the spot approximation, outward-only approximation (most of the current codes), or full radiative treatment [8, 9]. The codes may also be different in the geometric treatment, plane-parallel, spherical approximation, or 3D.

Traditionally, modeling of astronomical photoionized plasmas is done from the condition of steady-state statistical equilibrium, which means that gas ionization is balanced by recombination, atomic excitations are balanced by spontaneous and induced de-excitations, and electron heating is balanced by cooling. These conditions result in a set of coupled ionization/excitation balance equations (one for each atom and ion in the plasma) and a general
thermal balance equation. In addition, the models must determine the local radiation field, including direct and diffuse components, which is also coupled to the conditions above through the radiative transfer equation [4]. There has been much progress in steady-state photoionization modeling in the last few decades through increasingly detailed treatment of the microphysics, improvements in the quality and completeness of atomic and molecular data, and growth of computational power. At present, there are several sophisticated photoionization modeling codes in use, e.g., XSTAR [10], CLOUDY [11, 12], TLUSTY [13, 14], and MOCASSIN [15, 16].

The steady-state assumption is appropriate whenever the equilibration time scales for excitation, ionization, and thermal balance are much shorter than variability time scales in either the ionizing radiation continuum or the geometrical structure of the plasma. However, if the ionizing radiation changes at a rate shorter than the equilibration time scales, or if other conditions change on shorter timescales than those of microscopic processes, then it is necessary to take into account the full temporal dependence of the state equations. There are many astrophysical systems in which time-dependent photoionization (TDP) modeling is necessary due to the variability in their emitted fluxes. Some examples include the interstellar medium [17, 18], H II regions [19, 20], planetary nebulae [7, 21, 22, 23, 24], novae and supernovae [25, ?, 26, 27], the reionization of the intergalactic medium [28, 29, 30, 31, 32, 33], ionization of the solar chromosphere [34], Gamma ray bursts [35, 36], accretion discs [37], active galactic nuclei [38, 39, 40], the evolution of the early Universe [?], and low-ionization broad absorption lines of quasars (FeLoBALs) [41]. However, there is as yet no general tool to model time variable photoionized plasmas.
1.3 Current Work

The subject of this dissertation has been to develop a general time-dependent photoionization modeling code. This work is presented in this document, which proceeds as follows. Chapter II summarizes the basic micro-physics processes involved in photoionized nebulae and presents the basic equations needed to solve the steady state photoionization problem considering the simple idealized example of a pure hydrogen nebula subject to a steady state ionizing source of radiation. Chapter III presents our work on developing a time-dependent photoionization code. The first section of this chapter presents our preliminary work on developing a time-dependent photoionization code (TDP) [42]. The following section presents the development of the more realistic code time-dependent photoionization code, TDXSTAR, based on the well known steady state photoionization code, XSTAR [43]. In chapter V we present the results of the non-equilibrium photoionization problem and illustrate its behavior in various cases of general interest in astrophysics: in the first section we introduce the results of the TDP code of a pure hydrogen nebula subject to varying source of ionizing radiation. In the second section we present the results of the TDXSTAR code of a pure hydrogen nebula but with the consideration of multi-level atomic model. The chief difference between TDP and TDXSTAR calculations is that the latter takes into consideration the various atomic processes involved in multi-level atomic models. In the following section we present a qualitative study of the effects of time-dependent photoionization in planetary nebulae, in particular we used a grid of models analogy to those used by [7]. The last section of this chapter presents our study of temperature fluctuations in
planetary nebulae and H II regions due to variability of the ionizing flux. In the present work, we propose that temperature fluctuations do occur naturally in PNe and H II regions due to the binary nature of their ionizing stars.
CHAPTER II

OVERVIEW - PHOTOIONIZED GASEUS NEBULAE

2.1 Introduction

Interpretation of photoionized nebulae spectra is the chief goal in order to understand their physical conditions and structure. This process is usually done via numerical codes to simulate nebular conditions to predict nebular spectrum and match it to observed ones. These photoionization codes rely mainly on plasma physics and the underlying atomic processes. In order to understand the basic physics of photoionization, we review an idealized case assuming a nebula consisting of only hydrogen and subject to a steady ionizing radiation. We outline the equations that govern the nebular conditions used in building photoionization codes. In addition, we overview the main physics processes contributing to the physical conditions of the nebula.

2.2 Basic Atomic Processes

The state of a photoionized nebula is governed by several atomic processes such as photoionization, collisional ionization, recombination, etc. Understanding these processes and finding their occurrence rates is crucial for building computational models of astrophysical plasmas. The quality of a model is highly dependent on the completeness and accuracy of the set of the atomic processes involved in modeling. In this section, we summarize the atomic processes used in building photoionization codes, in particular, we focus on the
atomic processes used in the XSTAR code [10].

2.2.1 Photoionization

Photoionization is the predominant process in photoionized nebulae and it takes place by ejecting bound electrons by incident energetic photons,

\[ X^{(+i)} + h\nu \rightarrow X^{(+i+1)} + e^- \]

where \( X^{(+i)} \) is the element \( X \) in the ionization state \( i \) and \( h\nu \) is the energy of incident photon. The liberated electrons, \( e^- \), are called photoelectrons and have energies equal to the difference between the energy of the ionizing photon and the ionization energy of the bound level from which the electron was ejected. The photoionization rates are found by integrating the radiation field with the photoionization cross-section [44],

\[ \gamma = \int_{\nu_0}^{\infty} \frac{4\pi J_\nu}{h\nu} a_\nu d\nu \tag{2.1} \]

where \( a_\nu \) is the photoionization cross-section of the bound level from which an electron is ejected, \( J_\nu \) is the mean intensity of the ionizing radiation field, \( J_\nu \frac{dc}{d\nu} \) is the density of the ionizing photons in the frequency range \( d\nu \). The integration is performed from the ionizing threshold frequency \( \nu_0 \) to infinity. The photoionization rates calculations needs the cross sections for every level of every ion over a wide range of the ionizing photon energies.

2.2.2 Collisional Ionization

The ionization state of a nebula is increased by collisions of its constituent atoms, ions, protons and electrons. This process becomes more important in hot plasmas, where the
electron kinetic temperature is comparable to the ionization energy of the most abundant ions. This process can be expressed schematically as

\[ X^{(+i)} + e_\varepsilon \rightarrow X^{(+i+1)} + e_\varepsilon' + e_\varepsilon'' \]

where \( e_\varepsilon, e_\varepsilon', \) and \( e_\varepsilon'' \) are free electrons with energies \( \varepsilon, \varepsilon', \) and \( \varepsilon'' \), respectively. Collisions involving atoms with heavy particles are typically negligible in low density nebulae due to their low occurrence rates. Collisions triggered by electrons targeting ions are the most important impact induced atomic transitions. The volumetric rate of electron-ion collisional ionization can be expressed as

\[ C = n(X^i)n_e\alpha_c \]

where \( n(X^i) \) and \( n_e \) are the number densities of the ion \( X^i \) and electrons, respectively, and \( \alpha_c \) is the collisional ionization rate \( (cm^{-3} s^{-1}) \) given in CGS units and is given by,

\[ \alpha_c = 2.649 \times 10^{-8} \left( \frac{I_P}{kT} \right)^{\frac{1}{2}} \sum_i \zeta(i) \int_{\varepsilon(i)}^{\infty} \sigma_\varepsilon e^{-\varepsilon/kT} d\varepsilon, \]  \hspace{1cm} (2.2)  

where \( I_P \) is the ground state ionization potential for the ion, \( k \) is the Boltzmann constant, and \( T \) is the electron temperature. \( \zeta(i) \) and \( \varepsilon(i) \) are the number of electrons in the shell \( i \) and the ionization potential of that shell. \( \varepsilon \) is the electron kinetic energy and \( \sigma_\varepsilon \) is the collisional ionization cross-section [?].
2.2.3 Radiative and Dielectronic Recombination

The recombination process occurs when a positive ion $X^{(i+1)}$ captures a free electron resulting in a lower ionization state ion $X^{(i)}$. The recombination process has two distinct types, radiative and dielectronic. Radiative recombination occurs when a positive ion $X^{(i+1)}$ captures a free electron $e^-$ to one of its bound levels resulting in spontaneous emission of a photon and it can be expressed schematically as,

$$X^{(i+1)} + e^- \rightarrow X^{(i)} + \gamma \epsilon$$

The dielectronic recombination process can be expressed schematically as,

$$X^{(i+1)} + e^- \rightarrow X^{(i)\ast\ast} \rightarrow X^{(i)} + \gamma \epsilon$$

where $X^{(i)\ast\ast}$ is the doubly excited state of the ion $X^{(i)}$.

The total number of recombinations per unit volume per unit time is,

$$\alpha_\epsilon = n_e n_{X^{(i+1)}} \alpha$$

where $n_e$ and $n_{X^{(i+1)}}$ are the electron and ion $X^{(i+1)}$ number densities, respectively, and $\alpha$ is the total recombination rate coefficient ($cm^3 s^{-1}$), the sum of the recombination rates into all atomic states [44].

2.2.4 Milne Relation: Photoionization and Recombination Cross-sections

In this section, we derive the Milne relation defining the relation between the photoionization and recombination cross-sections. The derivation is based on the detailed balance principle assuming thermal equilibrium conditions. In particular, we balance the recombination rate of electrons in the velocity range $v$ and $v + dv$ by photoionization with photons.
in the frequency range \( \nu \) and \( \nu + d\nu \). The electron velocity and the photon frequency satisfy the following relation,

\[
m_e \nu \, dv = h \, d\nu
\]

where \( m_e \) is the electron mass.

The detailed balance of the two processes in thermal equilibrium can be schematically written as,

\[
\text{recombination rate (induced + spontaneous)} = \text{photoionization rate}.
\]

Using equation 2.1 and taking into account the fact that in thermal equilibrium the induced recombination rate is equal to the photoionization rate multiplied by \( e^{-\nu / kT} \), the above balance equation can be written as,

\[
n_e n(X^{i+1}) u \sigma(v) f(v) dv + n(X^i) \frac{4\pi B_\nu(T)}{h \nu} a_\nu e^{-\nu / kT} d\nu = n(X^i) \frac{4\pi B_\nu(T)}{h \nu} a_\nu d\nu \tag{2.3}
\]

where \( n_e \) and \( n(X^i) \) are the number densities of electrons and ions in the ionization state \( i \), respectively, \( v \) is the speed of electrons, \( \sigma(v) \) and \( a_\nu(\nu) \) are the recombination and photoionization cross-sections, respectively, \( f(v) \) is the Maxwell-Boltzmann velocity distribution given by,

\[
f(v) = \sqrt{\left( \frac{m_e}{2\pi kT} \right)^3} \frac{4\pi v^2 e^{-m_e v^2 / 2kT}}{e^{m_e v^2 / 2kT} - 1}, \tag{2.4}
\]

where \( m \) is the electron mass and \( kT \) is the product of Boltzmann’s constant and characteristic temperature \( T \), i.e. the electron kinetic energy. Here, \( B_\nu(T) \) is the Planck function used to substitute the mean intensity of the radiation field in the photoionization rate equa-
tion 2.1 to define the radiation intensity within a frequency range $d\nu$,

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}. \tag{2.5}$$

And the Saha equation is given by,

$$n_e n(X^{i+1}) \frac{n(X^i)}{n(X^i)} = \frac{2g_{i+1}}{g_i} \left( \frac{2\pi kT}{h^2} \right)^{3/2} \exp(-h\nu/kT), \tag{2.6}$$

using equations 2.4-2.6 in equation 2.3 we find the Milne relation,

$$\sigma(\nu) = \frac{g_i}{g_{i+1}} \frac{h^2\nu^2}{m^2c^2v^2} a_\nu. \tag{2.7}$$

Though the Milne relation was derived using the thermal equilibrium concept, it relates the recombination cross-section at electron at velocity $v$ to the photoionization cross-section at the corresponding photon frequency $\nu$ [4].

2.2.5 Charge Transfer

Charge transfer takes place by transporting an electron from ion $Y^i$ or atom $Y^0$ to positive ion $X^i$, where $X$ and $Y$ are two different elements. There are two types of charge transfer, direct (recombination) and inverse charge transfer (ionization). The former occurs when the donated electron is transferred from an atom $Y$ to an ion $X^+$. This process can be expressed schematically as,

$$X^+ + Y \longrightarrow X + Y^+ \pm \Delta E \tag{2.8}$$

where $\Delta E$ is the difference between the binding energies of the two systems, before and after the charge transfer. In this case the charge transfer ionizes the atom $X^0$ and lowers the
ionization state of the ion $Y^i$. The inverse process is called the inverse charge transfer. The position of the new shell to which the electron is transfered relies on the particles impact energy, the larger the collision energy the deeper the shell. There is another type of charge transfer called resonance charge transfer in which an electron is transfered from an atom to an ion of the same element,

$$X^+ + X^0 \rightarrow X^0 + X^+.$$  \hspace{1cm} (2.9)

This process is not significant in astrophysical nebulae. The charge transfer rates most important in astrophysical nebulae are those involving neutral hydrogen and helium due to their high abundances, and therefore high collisional rates. For hydrogen,

$$X^{(i+1)} + H^0 \rightarrow X^i + H^+$$  \hspace{1cm} (2.10)

and for helium,

$$X^{(i+1)} + He^0 \rightarrow X^i + He^+$$  \hspace{1cm} (2.11)

The number of occurrences of these processes (direct and inverse) per unit volume per unit time is given by,

$$\overrightarrow{N}_{ch} = n_{X^{(i+1)}} n_{Y^0} \overrightarrow{r}_{ch}(X^+, Y^+)$$  \hspace{1cm} (2.12)

and

$$\overleftarrow{N}_{ch} = n_{X^i} n_{Y^+} \overleftarrow{r}_{ch}(X^i, Y^+)$$  \hspace{1cm} (2.13)

where $\overrightarrow{r}_{ch}$ and $\overleftarrow{r}_{ch}$ are the direct and inverse charge transfer rates, respectively [4].
2.2.6 Collisional Excitations and Deexcitations

Collisions among the constituent particles of the gas may excite or de-excite the involved atoms or ions. In our case we are concerned with collisions between electrons and atoms or ions where they are the most dominant in astrophysical nebulae. Collisional excitations take place when a free electron, possessing energy equal to the excitation energy or larger, collides with an atom or ion and excites it to a higher energy. While deexcitation may occur when an electron with any energy collides with an atom or ion carrying away energy and lowering the ionization state of the ion without emitting photons.

The rate of collisional deexcitations can be expressed as [44],

\[ R_{ji} = n_e n_j \int_0^\infty \sigma_{ji}(E) v(E) f(E) dE = n_e n_j q_{ji} \]  

(2.14)

where \( n_e \) and \( n_j \) are the number densities of electrons and ions in state \( j \), respectively, \( \sigma_{ji} \) is the collisional cross-section, which is related to the collision strength \( \Omega \) by,

\[ \sigma_{ji}(E) = \frac{\hbar^2}{8\pi m_e E} \frac{\Omega_{ji}}{g_j} \]  

(2.15)

and \( v(E) \) is the electron velocity and \( f(E) \) is the Maxwell velocity distribution given by equation 2.4. Using Equations 2.14 and 2.15, we can write the collisional deexcitation rate coefficient \( q_{ji} \) in the form,

\[ q_{ji} = \left( \frac{\hbar^4}{8\pi^3 k_m c^3} \right)^{1/2} \frac{1}{g_j \sqrt{T}} \int_0^\infty \Omega_{ji}(E) e^{-E/kT} d\left( \frac{E}{kT} \right) \]  

(2.16)

or

\[ q_{ji} = \frac{\beta}{g_j \sqrt{T} \gamma_{ji}} \]  

(2.17)
where $\gamma_{ji}$ is the effective collision strength denoted in Equation 2.16 by the integral of the collision strength $\Omega_{ji}$ over Maxwellian distribution and $\beta = (h^4/8\pi^3kn_e^3)^{1/2}$.

The rate of collisional excitation can be found as follows,

$$R_{ij} = n_e n_i \int_{E_{ij}}^{\infty} \sigma_{ij}(E')V(E')f(E')dE' = n_e n_i q_{ij} \quad (2.18)$$

Note that the integral minimum limit this time limit the selection to electrons with kinetic energies equal to or larger than the excitation energy, i.e. the energy separation between the $i$ and $j$ states. Then, similarly, we can write the rate coefficient $q_{ij}$ in the form,

$$q_{ji} = \left( \frac{h^4}{8\pi^3k_n^3} \right)^{1/2} \frac{1}{g_i \sqrt{T}} e^{-E_{ij}/kT} \int_{0}^{\infty} \Omega_{ij} (E + E_{ij}) e^{-E/kT} d\left( \frac{E}{kT} \right) \quad (2.19)$$

where we replace $E$ with $E - E_{ij}$ in Equation (2.16), and, hence, the integral limits has changed. From Equation (2.18) and Equation (2.19), one can write,

$$q_{ji} = \frac{g_j}{g_i} q_{ij} e^{-E_{ij}/kT}$$

Similarly, equation 2.19 can be written as,

$$q_{ij} = \frac{\beta}{g_i \sqrt{T}} \gamma_{ij} e^{-E_{ij}/kT} \quad (2.20)$$

In the case of thermodynamic equilibrium, $R_{ij} = R_{ji}$, i.e.

$$n_e n_i \frac{\beta}{g_i \sqrt{T}} \gamma_{ij} e^{-E_{ij}/kT} = n_e n_j \frac{\beta}{g_j \sqrt{T}} \gamma_{ji}$$

then,

$$\frac{n_j}{n_i} = \frac{\gamma_{ij}}{\gamma_{ji}} \frac{g_j}{g_i} e^{-E_{ij}/kT} \quad (2.21)$$
Since the system is in thermodynamic equilibrium, the relative populations of levels has to
conform the Boltzman distribution:

\[
\frac{n_j}{n_i} = \frac{g_j}{g_i} e^{-E_{ij}/kT}
\]  

(2.22)

Comparison of the two equations (2.21) and (2.22) yields \( \Omega_{ij} = \Omega_{ji} \), i.e., the effective
collision strengths are symmetric.

### 2.3 Equilibrium State Conditions

In order to understand the basic physics of photoionized nebulae we overview the case
of a homogeneous nebula subjected to steady ionizing radiation, i.e., equilibrium gas con-
ditions. The condition of photoionized nebula is found by determining the temperature and
the ionization state of the gas, from which one can reproduce the emitted spectrum. In the
following subsections, we summarize the main three equations ionization balance, energy
balance, and radiation transfer equations used to determine the physical conditions of the
gas.

#### 2.3.1 Ionization Balance

Steady-state ionization equilibrium at every point in a cloud is attained by balancing
photoionization and collisional ionization with recombination of free electrons with the
ambient ions. Thus, ionization state of the gas depends on both the gas temperature and
the radiation field of the ionizing source. Finding the level populations proceeds in two
main steps: first, find the ionic fractions of the involved ions relative to the parent elements
by solving ionization balance equations using the total ionization and recombination rates
from and into every ion [45, 43],

\[
\begin{aligned}
\left( n_e \alpha_i^{\text{tot}}(T) + K_R^{ij}(T) \right) = \\
n_{ij}(\xi_{ij} + n_e C_{ij}(T) + K_I^{ij}(T)),
\end{aligned}
\] (2.23)

where \( n_{ij} \) is the number density of ion of the element \( i \) in its ionization state \( j \), \( n_e \) is the electron number density, and \( T \) is the temperature of the gas. \( \alpha^{\text{tot}} \) is the total (radiative and dielectric) recombination rate coefficient. The terms \( K_R^{ij} \) and \( K_I^{ij} \) are the recombination and ionization rates due to charge transfer, respectively. \( \xi_{ij} \) is the sum of ionization rates due to photoionization and Compton ionization, and \( C_{ij} \) is the collisional ionization rate. The explicit forms of the above terms are given in section (2.2).

The level populations are found by solving a system of balance equations linking the various atomic levels [43],

\[
\begin{aligned}
n_i^0 \left( \sum_{i \neq j} R_{ij} + \sum_{q>0} \Gamma_i^{0-q} + n_e \alpha_i^{-1} + n_e Q_i^{0-1} \right) = \\
+ \sum_{k \neq i} n_k^0 R_{ki} + \sum_{q>0} \sum_{l>0} n_l^{-q} \Gamma_{li}^{-q-0} \\
+ n_e \sum_{l} n_l^{-1} Q_i^{1-0} + \sum_{s} n_s^1 n_e \alpha_s^0,
\end{aligned}
\] (2.24)

where \( n_i^0 \) is the level population of level \( i \) in the ion of interest denoted by 0, \( n_i \) is the level populations of level \( i \), and \( n_e \) is the electron density. Here, the superindices denote the ionization stages (a single index) or transitions among the different ionization stages (two indices associated with arrows). The subindices are used to denote the levels (a single index) or transitions among the various levels (two indices). For instance, \( 0 \to q \) represents the transition from the ion of interest denoted by 0 to higher ionization stage \( q \), while
\( -q \to 0 \) denotes transitions from lower ionization stage \(-q\) to the ionization stage of interest 0. See section (2.2) for detailed information on the atomic processes above.

### 2.3.2 Energy Balance

The gas temperature in a photoionized nebula subjected to a steady ionizing source of radiation is determined by balancing the heating and the cooling rates, which can be schematically written as,

\[
\text{Heating} = \text{Cooling}
\]

Photoionization is the chief heating source in photoionized nebulae and it takes place by absorbing energetic photons and ejecting bound electrons. The photoelectrons have energy equal to the energy difference between the energy of the absorbed photon and the threshold energy in the hydrogen case. The photoelectrons are quickly thermalized and enhance the average energy in free electrons. In other words, free electrons follow the Maxwell-Boltzmann velocity distribution (see equation 2.4). On the other hand, electrons cool down by radiative energy losses that result from electron-ion recombinations and electron impact excitations. Another source of energy loss is Bremsstrahlung (free-free) radiation. In the case of photoionization equilibrium the temperature is determined by balancing the energy gain by photoionization and the energy loss by recombination and radiation, which can be expressed schematically as

\[
\Gamma_P = \Lambda_R + \Lambda_C + \Lambda_B
\]  

(2.25)
Figure 2.1  The interstellar net cooling rate versus temperature for different fractional ionization $x = n_e/n_H$ indicated on each curve. The curves are distinct for temperatures less than $T = 10^4 \, K$, and identical for higher temperatures due to the contributions of collisional ionizations from all elements at higher temperature, $T > 10^4 \, K$. The figure is taken from Dalgarno & McCray [46].
where \( \Gamma_P \) is the photoionization heating rate in units of \( \text{erg cm}^{-3}\text{s}^{-1} \) and given by

\[
\Gamma_P = n(H^0) \int_{\nu_0}^{\infty} \frac{4\pi J_{\nu}}{h\nu} h(\nu - \nu_0) \sigma_{\nu} d\nu
\]

(2.26)

Cooling by recombination and collisional ionization are given by equations 3.31 and 3.32, respectively.

\[
\Lambda_R = n_\text{e} n \alpha_r(T) g k T
\]

(2.27)

and

\[
\Lambda_C = n_\text{e} n C(T) \varepsilon_{\text{th}}.
\]

(2.28)

where \( n \) is the number density of the ion involved in the process, \( \varepsilon_{\text{th}} \) is the threshold energy for that ion.

The Bremsstrahlung cooling rate is given by,

\[
\Gamma^\text{brem} = 1.42 \times 10^{-27} Z^2 n_z \sqrt{T}
\]

where \( n_z \) is the ion number density and \( Z \) is its charge, and \( T \) is the electron temperature [4].

2.3.3 Radiative Transfer

Determination of the local radiation field at every point within the cloud is necessary in order to find the gas temperature. The energy transfer is governed by the radiation transfer equation given by

\[
\frac{dI_{\nu}}{dx} = -n(H^0) \sigma_{\nu} I_{\nu} + j_{\nu},
\]

(2.29)
where \( I_\nu \) is the local radiation field at depth \( x \) and has units of \((erg cm^{-2} s^{-1} Hz^{-1} sr^{-1})\), and \( j_\nu \) is the radiation emission coefficient and has units of \((erg cm^{-3} s^{-1} Hz^{-1} sr^{-1})\). The local radiation field can be attributed to two sources, the first is from the incident ionizing radiation and the second is a contribution from the diffuse radiation emitted by the local ionized gas. Therefore, the specific intensity at depth \( x \) can be written as,

\[
I_\nu = I_s + I_d,
\]  

(2.30)

where \( I_s \) is the local specific intensity from the ionizing source and \( I_d \) is the specific intensity of the radiation emitted by the ionized gas.

The incident radiation \( I_s \) is altered by two mechanisms, the first is the geometrical dilution and the second is gas absorption,

\[
\pi F_s(r) = \frac{\pi F_s(R)}{r^2} e^{-\tau_\nu}
\]  

(2.31)

where \( F_s(r) \) and \( F_s(R) \) are the radiation flux at distance \( r \) and at the surface of the radiation source, respectively, and have units of \((erg cm^{-2} s^{-1} Hz^{-1} sr^{-1})\). \( \tau_\nu \) is the optical depth to hydrogen ionizing radiation at distance \( r \) and given by,

\[
\tau_\nu(r) = \int_0^r n(H^0, r) \sigma_\nu dr
\]  

(2.32)

The diffusion part \( I_d \) is governed by the radiation transfer equation

\[
\frac{dI_d}{dx} = -n(H^0) \sigma_\nu I_d + j_\nu
\]  

(2.33)

The emission coefficient for radiative recombination, which is the most important source of radiation at temperatures much lower than the ionizing energy, is given by,

\[
j_\nu(T) = \frac{2h\nu^3}{c^2} \left( \frac{h^2}{2\pi m_e kT} \right)^{3/2} \sigma_\nu n_p n_e e^{-h(\nu-\nu_0)/kT}, \quad \nu \geq \nu_0
\]  

(2.34)
The number of photons emitted due to recombination to the ground state of hydrogen can be found by

\[
4\pi \int_{\nu_0}^{\infty} \frac{j_\nu}{h\nu} d\nu = n_p n_e \alpha_1(H^0, T)
\]

where \( \alpha_1(H^0, T) \) is the recombination coefficient to the hydrogen ground state \( 1^2S \) and the local diffuse mean intensity is given by,

\[
J_d = \frac{j_\nu}{n(H^0) a_\nu}.
\] (2.35)

### 2.4 Spectral Formation

The atomic processes involved in astrophysical nebulae are responsible for the observed spectra. Emission spectral lines are a result of bound-bound atomic transitions, and they are classified according to their occurrence mechanisms as recombination lines (RLs) or collisionally excited lines (CELs), sometimes referred to as “forbidden lines”.

#### 2.4.1 Recombination Lines

Spectral lines of allowed transitions between excited levels of H, He, C, N, O, Ne, Si and Mg have been observed in spectra of gaseous nebulae. These lines are mainly formed by recombination to excited states followed by spontaneous decay to the ground level. Theoretical studies have been made to calculate spectral lines intensities formed by transitions between the various atomic levels. The difficulty of such calculations lie in the complexity of atomic levels structure, in particular for heavy ions, as well as the uncertainties resulting from atomic transition rates. In XSTAR, spectral models of H-like and He-like recombination spectra were computed by Bautista et al. [47] and Bautista &
Kallman [48]. The emission coefficient of each line is given by,

\[ j_{nn'} = \frac{h\nu_{nn'}}{4\pi} \sum_{L=0}^{n-1} \sum_{L' \pm 1} n_{nL} A_{nL,n'L'} \]  \hspace{1cm} (2.36)

where \( j_{nn'} \) is the emissivity of the line formed by downward transition between the levels \( nL \) and \( n'L' \), \( n_{nL} \) is the populations of level \( nL \), and \( A_{nL,n'L'} \) is the transition probability. Equation 2.36 calculates the emissivity of recombination lines considering Case A, in which all the emitted lines are allowed to escape from the nebula without absorption. This case is a good approximation in case of optically thin nebulae, but, in fact, the majority of the observed nebulae are optically thick for the hydrogen Lyman alpha line. For instance, in a nebulae with temperature of \( T = 10^4 \) K, the optical depth of (Ly\( \alpha \)) line is about \( 10^4 \) times that of the Lyman limit of the ionizing radiation. In addition, after a few scatterings, there is a probability that some lines are converted to weaker spectral series that can not escape from the medium. For instance, Ly\( \beta \) line is converted to H\( \alpha \) line from the Balmer series plus two photons in the continuum \( 2^2S - 1^2S \). Thus, better treatment for recombination lines should assume optically thick nebulae, which is called Case B. In case B photons are emitted from transitions to the ground level and absorbed somewhere in the nebula to excite another H atom to the same excitation level. Thus, the net radiation spectrum from transitions to the ground level is canceled out in Case B. The total energy irradiated by a recombination line can be found by,

\[ E(\Lambda) = \int n_e n_p \alpha_{eff}^{nn'} h\nu_{nn'} dV \]  \hspace{1cm} (2.37)

where \( n_e \) and \( n_p \) are the number densities of the electrons and the recombining ion, \( \alpha_{eff}^{nn'} \) is the effective recombination coefficient, the total recombination coefficient due to all
recombinations to all levels, and \( h\nu_{nn'} \) energy of the emitted photon with the integral over the nebular volume \( V \).

### 2.4.2 Collisionally Excited Lines

The second mechanism by which spectral lines are formed is when ions are excited by collisions with ambient electrons/ions and then the excited ions spontaneously decays to lower levels emitting photons. Collisional lines of atoms such as C, N, O, Ne, Al, Si, S, Ca, K in various wavelength ranges have been observed, with the strongest often in optical range. These photons escape from the nebula reducing its thermal energy, and thus, are considered very effective in cooling. Similarly, the net radiated energy by a collisionally excited lines at specific wavelength can be found using equation 2.37 where the level populations in either case is calculated by solving the equations for statistical equilibrium of the populations of the various atomic levels. These lines are enhanced by other excitations mechanisms, such as photoexcitations by the continuous spectrum (e.g., [49]) and charge transfer reactions (e.g., [50]).
CHAPTER III
TIME-DEPENDENT PHOTOIONIZATION OF GASEOUS NEBULAE

3.1 Introduction

This chapter consists mainly of two sections to introduce the physical assumptions, the fundamental equations, and the numerical methods used to develop our photoionization modeling codes. In section 3.2, we introduce a simple time-dependent photoionization (TDP) code assuming two-level atomic model to study the effects of the variability of the ionizing radiation on the state conditions of a photoionized nebula with the assumption that the nebula of interest consists of only hydrogen. Although a simple atomic model has been used, our model is important in explaining the general behavior of the gas reaction to a varying source of ionizing radiation. In section 3.3, we present a more realistic time-dependent photoionization code, TDXSTAR, which uses a full chemical model and includes important microphysical processes.

3.2 Two-level Atomic Model: TDP Code
3.2.1 Introduction

The content of this section is based on our published work on time-dependent photoionization [42]. In this section we lay out the basic approach to solve the TDP problem and present an overview of the behavior of non-equilibrium photoionized plasmas. In order to understand the time-dependent effects in photoionized nebulae we start by simple model of optically think pure hydrogen plasma. Though non-equilibrium photoionized plasmas exist in many astronomical objects with complex chemical compositions, studying the simple
pure hydrogen model in detail provides deep insights into the big picture of photoionized nebulae. This similarly will allow us to study the dependence of the time-dependent effects on the individual parameters, such as adopted spectral energy distribution of the continuum (SED), optical depth, density, etc.

In sections (3.2.2-3.2.7), we present the physical model and assumptions used in building our models and introduce the fundamental system of equations representing the ionization balance, energy, and radiative transfer equations and the numerical methods used to solve the coupled system of equations to determine the gas physical conditions at any given time.

3.2.2 Physical Model and Assumptions

Our model comprises a slab of gaseous nebula composed of only hydrogen and exists in the vicinity of a source of varying photoionizing radiation. We approximate the geometry of the system assuming that the thickness of the nebula, \( r \), is much smaller than the distance from the photoionizing source, \( R \), that is \( r/R \ll 1 \). This assumption allows the use of the plane-parallel approximation, which adopts a parallel layers representation for the cloud. Thus, the gas conditions depend only on the radial direction and the depth within the cloud (see figure (3.1) for a schematic diagram of the model). Furthermore, in order to solve such a computationally challenging problem, we assumed a simplified atomic model composed of only two levels representing the ground and continuum states.
Figure 3.1  TDP model of a photoionized nebula with thickness $r$, much smaller than the inner radius of the nebula $R$.

3.2.3 Ionization Balance

Our assumption of the two-level atomic model of TDP code restricts the involved atomic processes to ionization and recombination processes, while neglecting the atomic excitations and deexcitations. Therefore, the population of the ground state can be expressed as

$$\frac{dn_1(x, t)}{dt} = -n_1(x, t) [\gamma(x, t) + n_e C(T)] + n_2(x, t) n_e \alpha_r(T)$$ (3.1)

where $n_e$ is the electron number density, and $n_1$ and $n_2$ are the population of the ground and continuum levels, respectively. $\gamma$ is the photoionization rate, see chapter II. $C(T)$ and $\alpha_r$ are the collisional ionization and recombination rate coefficients, respectively. For the
collisional ionization rate, we adopt the expression given by Cen [51]:

$$ C(T) = 5.83 \times 10^{-11} T^{1/2} (1 + T_5^{1/2})^{-1} e^{-157809.1/T} \quad (3.2) $$

and for the recombination rate we use the fitting formulas given by Badnell [52],

$$ \alpha_r(T) = 8.32 \times 10^{-11} / \left[ \sqrt{\frac{T}{2.97}} \left(1 + \sqrt{\frac{T}{2.97}}\right)^{0.25} \left(1 - \sqrt{\frac{T}{7 \times 10^5}}\right)^{1.75}\right] \quad (3.3) $$

where $T$ is the temperature in Kelvin, $T_5$ is in units of $10^5$ K, and $\alpha_r$ and $\alpha_c$ are both in cm$^3$ s$^{-1}$. In our calculations we consider optically thin nebulae, therefore, we consider Case A recombination. Other scenarios, such as Case B recombination of hydrogen, will be treated elsewhere.

We assume hydrogen plasmas with fixed density, i.e. there is a free electron per every bare proton, i.e. $n_2 = n_e$ and the hydrogen density is conserved $n = n_1 + n_2$. Then Equation (3.1) becomes,

$$ \frac{dn_1(x,t)}{dt} = n_1^2(x,t) [\alpha_r(T) + \alpha_c(T)] $$
$$ - n_1(x,t) \{\gamma(x,t) + n [2\alpha_r(T) + \alpha_c(T)]\} + n_2^2 \alpha_r(T) \quad (3.4) $$

### 3.2.4 Energy Equation

The temperature of the gas can be found from the net gain of thermal energy by the system, which is given by,

$$ \frac{dQ}{dt} = \Gamma^{(\text{heat})} - \Lambda^{(\text{cool})}, \quad (3.5) $$
where \( Q \) is the particle kinetic energy per unit volume, \( \Gamma^{(\text{heat})} \) and \( \Lambda^{(\text{cool})} \) are the heating and cooling rates. Assuming a rapid energy equipartition among atoms, protons, and electrons, one can write the particle kinetic energy per unit volume as \( Q = (3/2)n_t kT \), where \( n_t = n + n_e = 2n - n_1 \) is the total number density, \( k \) the Boltzmann constant and \( T \) the gas temperature. With the assumption of fixed density, \( n \), one can write,

\[
\frac{dT}{dt} = \frac{2}{3(2n - n_1)k} \left[ \Gamma^{(\text{heat})} - \Lambda^{(\text{cool})} + \frac{3}{2}kT \frac{dn_1}{dt} \right].
\]

The last term on the right hand side of equation 3.6 corresponds to the kinetic energy input due to temporal changes in the ionization state of the plasma. This term explicitly couples the ionization and thermal balance equations, but it is zero under steady-state conditions.

The photoionization heating is

\[
\Gamma^{(\text{pho})} = n_1(x, t) \int_{0}^{\infty} \sigma_\varepsilon J_\varepsilon(x, t)(\varepsilon - \varepsilon_{th}) \frac{d\varepsilon}{\varepsilon}
\]

and can be written as

\[
\Gamma^{(\text{pho})} = n_1(x, t) \gamma(x, t) < \bar{\varepsilon} >
\]

where

\[
< \bar{\varepsilon} > = \frac{\int_{\varepsilon_{th}}^{\infty} J_\varepsilon(x, t)\sigma_\varepsilon(\varepsilon - \varepsilon_{th})d\varepsilon / \varepsilon}{\int_{\varepsilon_{th}}^{\infty} J_\varepsilon(x, t)\sigma_\varepsilon d\varepsilon / \varepsilon}
\]

is the mean kinetic energy of free electrons weighted by the photoionization cross section, and \( \varepsilon_{th} = 13.6 \text{ eV} \) is the hydrogen threshold energy.

The recombination and collisional ionization cooling rates are given by equation 3.31 and 3.32 as

\[
\Lambda^{(\text{rec})} = n_e n_2(x, t) \alpha_r(T) gkT
\]
and

$$\Lambda^{(col)} = n_e n_1(x, t) C(T) \varepsilon_{th}. \quad (3.11)$$

where $g$ is the Gaunt factor, a constant factor that depends on the spectral energy distribution of the radiation field, typically about 0.6. Then, the thermal balance equation becomes,

$$\frac{dT(x, t)}{dt} = \frac{2}{3(2n - n_1)k} [n_1(x, t) \gamma(x, t) < \varepsilon > \left( \varepsilon + 3kT \frac{dn_1}{dt} \right)] \quad (3.12)$$

The non-linear dependence of the terms $\alpha_r$ and $C$ on $T$ makes the above equation unsolvable analytically, even in the steady state case $dT/dt = 0$.

Equations (3.4) and (3.12) both depend on the local radiation field, which is found by solving radiation transfer equation.

### 3.2.5 Ionization Parameter and Radiative Transfer

We assume variable ionizing flux with fixed spectral energy distribution. Thus, the state of the gas can be determined by the ionization parameter only as shown by,

$$\xi = \frac{L}{nR^2} \approx 4\pi F_x < \varepsilon >, \quad (3.13)$$

where $L$ is the luminosity (in energy units) of the ionizing source, and $F_x$ is the photon flux of ionizing radiation, $< \varepsilon >$ is the mean photon energy and $r$ is the distance from the source. The luminosity $L$ is integrated from the ionization threshold for hydrogen (1 Ry) to 1000 Ry, where the ionizing radiation flux is expected to be very small [53]. $L$ and $F_x$ are related through

$$F_x = \frac{1}{4\pi R^2} \int_{1\text{Ry}}^{\infty} \frac{L_{\nu}}{h\nu} d\nu.$$
This definition for the ionization parameter is related to various other customary ionization parameter definitions, i.e., \( U_H = \Phi_H/n_H c \); \( \Sigma = F_\nu(\nu_L)/(2hc\nu) \), where \( F_\nu(\nu_L) \) is incident specific (energy) flux at 1 Ry; and \( \Xi = L/(4R^2cnkT) \) [54].

The radiative transfer equation defining the interaction between the ionizing radiation and gas particles is given by,

\[
\frac{1}{c} \frac{\partial I_\varepsilon(x, \mu, t)}{\partial t} + \mu \frac{\partial I_\varepsilon(x, \mu, t)}{\partial x} = \eta_\varepsilon(x, t) - \chi_\varepsilon(x, t) I_\varepsilon(x, \mu, t) \tag{3.14}
\]

where \( I_\varepsilon(x, \mu, t) \) is the radiation field intensity at depth \( x \), \( \mu \) is the cosine of the angle with respect to the normal, and \( \eta_\varepsilon(x, t) \) and \( \chi_\varepsilon(x, t) \) are the gas total emissivity and opacity, respectively. Solving this equation is computationally challenging as discussed in the literature. To solve this equation we adopted the one-stream approximation in which the normal direction is the only contributing to the problem. In this case, \( \mu = 1 \) and then \( J_\varepsilon = \int_{-1}^{1} I_\varepsilon d\mu \approx I_\varepsilon \). Further, we ignored photon scattering and the gas local emissivity, hence we can write the radiative transfer equation as,

\[
\frac{1}{c} \frac{\partial J_\varepsilon(x, t)}{\partial t} + \frac{\partial J_\varepsilon(x, t)}{\partial x} = -n_1(x, t)\sigma_\varepsilon J_\varepsilon(x, t) \tag{3.15}
\]

### 3.2.6 Characteristic Times

Time-dependent effects in photoionized plasmas are governed by three time scales: the ionization equilibration time scale, the temperature equilibration time scale, and the propagation time scale. The photoionization time scale can be written as,

\[
t_{pi} = \frac{n}{n_1 \gamma} \tag{3.16}
\]
the recombination time as,

\[ t_{\text{rec}} = \frac{n}{n_2 n_e \alpha_r}, \]  

(3.17)

and the collisional ionization time

\[ t_{\text{col}} = \frac{n}{n_1 n_e \alpha_c}. \]  

(3.18)

where we employed our terms for \( n/n_1 \) and \( n/n_2 \) in the traditional definitions of the time scales. For example, a typical definition of recombination time is \( t_{\text{rec}} = 1/(n_e \alpha_r) \), which is appropriate for steady-state condition in the fully ionized region where \( \alpha \) is . Our present definitions are generally correct for nebulae where the ionization of the plasma may change with time.

The ionization equilibration time, \( \tau_{\text{ion}} \), can be defined as

\[ \frac{1}{n} \frac{(n_1 - n_1^E)}{\tau_{\text{ion}}} = -\frac{1}{t_{\text{ion}}} + \frac{1}{t_{\text{rec}}}, \]  

(3.19)

where \( n_1^E \) is the density of neutral hydrogen at the final equilibrium after the change in radiation field and \( t_{\text{ion}} \) is defined as the ionization time, \( t_{\text{ion}} = t_{\text{pi}} t_{\text{col}}/(t_{\text{pi}} + t_{\text{col}}) \). Thus,

\[ \tau_{\text{ion}} = \frac{n_1^E - n_1}{n} \frac{t_{\text{ion}} t_{\text{rec}}}{t_{\text{rec}} - t_{\text{ion}}}. \]  

(3.20)

Similarly, we can define a temperature equilibration time, \( \tau_T \), as

\[ -\frac{3k(T - T^E)}{2\tau_T} = \frac{d}{dt} \left( \frac{3}{2} kT \right), \]  

(3.21)

where \( T^E \) is the temperature at the final equilibrium after the change in radiation field. Note that \( \tau_T \) is the ratio of the excess of energy density to the net cooling rate assuming constant
Though they are interrelated, the ionization time scale is generally much longer than that of the temperature as seen in section 4.2.1.

In addition to the ionization and temperature time scales governed by the local processes, radiation propagation time is important in determining the time at which local gas will respond to the flux variations causing a delay between the continuum variations and the gas response from point to point across the cloud.

\[
\tau_{\text{prop}} = \int_0^x \frac{n_1(r)}{F(r)} dr \approx \frac{x < n_1 >}{F_x} = \frac{N_H}{F_x},
\]

(3.22)

where \(N_H\) is the neutral hydrogen column density [55]. The propagation time is the characteristic time it takes for the ionization front to move under the assumption that there is one ionization event per incident photon. The above equation shows that the propagation time is short and nearly constant in the ionized region and sharply increase near the ionization front where the neutral hydrogen \(n_1\) increases. Thus, across the IF too the equilibration times reach maximum values, and hence, exhibit the largest departures from equilibrium conditions after changes in the ionizing radiation field.

### 3.2.7 Numerical Approach

The solution of TDP model is found by solving simultaneously the three coupled equations representing ionization, thermal balance, and radiative transfer equations given by (3.4), (3.12), and (3.15), respectively. To do so numerically, we divide space, time, and radiation energy coordinates into grids of finite elements. Thus, the time and spatial derivatives of
physical quantities can be expressed as,

\[
\frac{dy^{i,j}}{dt} = \frac{y^{i+1,j} - y^{i,j}}{\Delta t^{i,j}}, \quad (3.23)
\]

\[
\frac{dy^{i,j}}{dx} = \frac{y^{i,j+1} - y^{i,j}}{\Delta x^{j}}, \quad (3.24)
\]

with \( \Delta t^{i,j} = t^{i+1,j} - t^{i,j} \) and \( \Delta x^{j} = x^{i,j+1} - x^{i,j} \), and \( y^{i,j} \) at the \( i \)-th time step and \( j \)-the spatial step. We used implicit method in which the solution of a given equation involves both the current and a later state of the system. This is due to the stiffness of the used differential equations caused by the large variations expected in the derivatives of the involved physical quantities, making unstable predictions if explicit method is employed. The ionization balance equation (3.4) is then expressed as:

\[
(n_{1}^{i+1,j})^{2} [\Delta t^{i}(\alpha_r^{i+1,j} + \alpha_c^{i+1,j})] - n_{1}^{i+1,j} [1 + \Delta t^{i}(2n_{1}^{i+1,j} + n_{1}^{i+1,j} + \gamma^{i+1,j})] + [n_{1}^{i,j} + \Delta t^{i}n_{1}^{i+1,j}] = 0.
\]

where \( \alpha_r^{i+1,j} = \alpha_r(T^{i+1,j}) \), \( \alpha_c^{i+1,j} = \alpha_c(T^{i+1,j}) \), and \( \gamma^{i+1,j} = \gamma(x, t^{i+1,j}) \). Thus, the population \( n_{1} \) at the \((i+1)\)-th time step is given by the roots of the quadratic equation above, provided that the temperature \( T^{i+1,j} \) is known. The negative solution is non-physical leaving only the positive one. Then, similarly, we use the energy equation (3.12) to find the temperature,

\[
T^{i+1,j} \left[ 1 + \frac{2\alpha_r^{i+1,j}(n_{2}^{i,j})^2}{3(n_{1}^{i+1,j} + 2n_{2}^{i,j})} \Delta t^{i} - \frac{n_{1}^{i+1,j} - n_{1}^{i,j}}{n_{1}^{i+1,j} + 2n_{2}^{i,j}} \right] - T^{i,j} = \frac{-2\Delta t^{i}}{3(n_{1}^{i+1,j} + 2n_{2}^{i,j})k} \left[ n_{1}^{i+1,j} \gamma^{i+1,j} < \xi > - n_{2}^{i,j} n_{1}^{i+1,j} \alpha_c^{i+1,j} \xi_{rh} \right] = 0
\]

The solution to this equation is found numerically by the secant method. Then \( n_{1}^{i+1,j} \) is found from Equation (3.25) for every given temperature, \( T^{i+1,j} \). These solutions de-
pend on the photoionization rate $\gamma^{i+1,j}$ and determined through the radiative transfer Equation (3.15), which in finite differences form becomes

$$J^{i,j,k}_{i+1,j} = J^{i,j-1,k}_{i,j} \left( \frac{c \Delta t^i}{2 \Delta x^j} \right) + J^{i,j,k}_{i,j} \left( 1 - c \Delta t^i \eta^{i,j} \sigma^k \right) - J^{i,j+1,k}_{i,j} \left( \frac{c \Delta t^i}{2 \Delta x^j} \right).$$

This equation needs to be solved for every $k$-th energy interval.

Our solution starts by assuming steady-state conditions at $t = 0$. We impose the boundary conditions at $x = 0$, such that $J^{i,0,k}_{i,0} = J^{i,k}_{i,0} \text{ inc}$, which is the radiation field incident on the illuminated face of the slab. $J^{i,k}_{i,0} \text{ inc}$ is known at all times $i$ and for every $k$-th energy interval.

### 3.3 The Full Chemical Composition Model: TDXSTAR

#### 3.3.1 Introduction

TDXSTAR code is based on the well known steady-state photoionization code, XSTAR [10]. The chief difference between our non-equilibrium codes TDP and TDXSTAR and the steady state models such as XSTAR is that our codes take into account the variability of the ionizing radiation field and hence predict the state of the gas at different times. In this section we present a more realistic numerical code, TDXSTAR, which is developed to solve the energy balance, ionization balance, and radiation transfer equations in a self-consistent fashion in nebulae subjected to rapidly changing ionizing radiation with the consideration of a full atomic model to study the time-dependent photoionization problem. TDXSTAR is a developed version of the well known steady state photoionization code, XSTAR [10], where we extended the excitation, ionization, thermal, and radiative transfer equations to their full time-dependent forms. TDXSTAR is capable of including all chemical elements from hydrogen ($Z=1$) to nickel ($Z=28$).
In this chapter, we describe the model, the physics aspects and assumptions, the theory of operation and the numerical techniques used to develop TDXSTAR.

3.3.2 Physical Model and Assumptions

The physical model encompasses a source of a photoionizing radiation embedded at the center of a spherically symmetric gaseous nebula composed of spherical shells, which is the same model adopted by XSTAR [10]. The ionizing continuum emitted by the central source is absorbed and remitted by the surrounding nebula. Thus, the incident light will be reprocessed by the interfering surrounding gas and its constituent atoms and ions via bound-bound, bound-free and free-free atomic processes. The electron temperature is determined by contributions from all the elements/ions involved in the atomic processes. In steady-state photoionization modeling the conditions of the nebula are determined by imposing the detailed balance between the involved atomic processes (excitations, ionization, and heating) and their inverse (deexcitations, recombination, and cooling). While in our non-equilibrium model, TDXSTAR, the gas conditions is determined by solving a set of coupled ordinary differential equations representing ionic fractions balance, level populations balance, energy equation, and radiative transfer equation assuming non-equilibrium conditions. Therefore, the chief difference between XSTAR and TDXSTAR is that the later takes the variability of the ionizing radiation into consideration, and hence predicts the temporal change of the state of the gas.
3.3.3 The Atomic Models

Photoionization modeling requires having a large database of atomic rates to perform the desired calculations. In our code, TDXSTAR, we used the same atomic models created for XSTAR [10]. Each ion contains a set of about $10 - 50$ ($\geq 100$ for a few ions) spectroscopic bound levels, one or more superlevels, and a continuum level. The spectroscopic bound levels are the low-lying energy levels, such as the ground state and metastable levels, treated individually in full detail. The high-lying energy levels (above the spectroscopic levels and below the continuum) are less important for their observed spectra; therefore, they are consolidated into one or more artificial levels called superlevels. These superlevels are built to contribute the difference in recombination between the total recombination rate to the ion and recombination to the low-lying spectroscopic levels. Finally, the continuum level represents the higher ionization stage of the element.

3.3.4 Ionization Balance and Level Populations

We follow the same procedure adopted by XSTAR to determine the level populations, in which the level populations are calculated over two main steps. First, determination of the ionic fractions of a given element (relative abundances of its ions) by solving the ionization balance equations using the total ionization and recombination rates from and into every ion [45]. Second, determination of the relative level populations by solving the level populations balance equations linking the various bound levels of adjacent and non-adjacent ions. The chief difference between the steady state model, XSTAR and its time-dependent version, TDXSTAR is that the former solves a set of algebraic equations.
representing the ionization balance and relative level populations, while the later uses a set of coupled differential equations to represent the temporal change of the ionic fractions and relative level populations due to the change in the ionizing continuum.

To determine the ionic fractions we developed a system of differential equations to determine temporal change in fractions, one for every ion,

\[
\frac{dn_{ij}}{dt} = n_{ij+1}(n_e\alpha_{ij}^{tot}(T) + K_{ij}^R(T)) + n_{ij}(\xi_{ij} + n_e C_{ij}(T) + K_{ij}^I(T))
\]

(3.26)

where \(n_{ij}\) is the number density of ion of the element \(i\) in its ionization state \(j\), \(n_e\) is the electron number density. \(\alpha^{tot}\) is the total (radiative and dielectric) recombination rate coefficient, and \(T\) is the temperature of the gas. The term \(K_{ij}^R\) and \(K_{ij}^I\) are the recombination and ionization rates due to charge transfer. The term \(\xi_{ij}\) is the sum of ionization rates due to photoionization and Compton ionization. The last term \(C_{ij}\) is the collisional ionization rate. The explicit forms of the above terms are given in section (2.2). Equation (3.26) is a modified version of the steady state model Equation 2.23.

After finding the ionic fractions we determine the level populations by solving a matrix of differential equations linking the various bound levels. In order to determine the temporal change of the level populations we developed a differential equations to represent the change in the level population over time. This equation is a modified version of the level
populations balance equation given by Equation 2.24,

\[
\frac{dn_i^0}{dt} = -n_i^0 \left( \sum_{i \neq j} R_{ij} + \sum_{q>0} \Gamma_i^{0\rightarrow q} + n_e \alpha_i^{-1} + n_e Q_i^{0\rightarrow -1} \right) \\
+ \sum_{k \neq i} n_k^0 R_{ki} + \sum_{q>0} \sum_{l} n_l^{-q} \Gamma_{li}^{-q\rightarrow 0} \\
+ n_e \sum_{l} n_l^{-1} Q_{li}^{1\rightarrow 0} + \sum_{s} n_s^{-1} n_e \alpha_s^{0}\]

(3.27)

where \(n_i^0\) is the level population of level \(i\) in the ion of interest denoted by 0, \(n_i\) is the level populations of level \(i\), and \(n_e\) is the electron density. Here, we adopt the same indices used by XSTAR [43], where single index in the superindices denotes the ionization stages, and two indices associated with arrow used for transitions among the different ionization stages. Single index of the subindices is used to denote the levels, and two indices are used for transitions among the various levels. For instance, \(0 \rightarrow q\) represents the transition from the ion of interest denoted by 0 to higher ionization stage \(q\), while \(-q \rightarrow 0\) denotes transitions from lower ionization stage \(-q\) to the ionization stage of interest 0. The various atomic processes involved in the above equation are detailed section (2.2).

### 3.3.5 Energy Balance Equation

To determine the temperature in a nebula, we solve the thermal balance equation. Following the same procedure used in our previous report (Garcia, et.al.2013), a schematic form of the thermal balance equation can be written as

\[
\frac{dQ}{dt} = \Lambda - \Gamma, \quad (3.28)
\]
where $Q$ is the net heat and $\Lambda$ and $\Gamma$ are the heating and cooling rates, respectively. For an ideal electron gas the net heat is equal to the kinetic energy of the electrons $Q = 3/2n_ekT$, where $k$ is the Boltzmann constant and $T$ is the gas temperature. Neglecting hydrodynamics effects, i.e. neglecting mass transport, then $n + ni$ can be assumed to be constant but $n_e$ is variable due to the bound-free atomic processes and their inverse. Hence equation (3.28) can be written as

$$\frac{dT}{dt} = \frac{2}{3kn_e}(\Lambda - \Gamma - \frac{3}{2}kT\frac{dn_e}{dt}).$$

(3.29)

In the above equation we include all the heating and cooling sources adopted by XSTAR [10]. The photoionization heating rate in units of $(erg cm^{-3}s^{-1})$ is given by Equation 2.26 as,

$$\Gamma_p = n(H^0)\int_{\nu_0}^{\infty} \frac{4\pi J_\nu}{\hbar\nu} h(\nu - \nu_0)\sigma_\nu d\nu$$

(3.30)

The cooling processes include radiative recombination, dielectronic recombination, radiative deexcitation, collisional ionization, charge transfer, and bremsstrahlung. The recombination and collisional ionization cooling rates are given by Equations 3.31 and 3.32, respectively, as

$$\Lambda_R = n_e n_\alpha_r(T)gkT$$

(3.31)

and

$$\Lambda_C = n_e nC(T)\varepsilon_{th}.$$  

(3.32)

where $n$ is the number density of ions involved in the process, $g$ is a constant factor, typically about 0.6, that depends on the spectral energy distribution of the radiation field.
In calculating the radiative recombination rate we assume that each recombining electron possesses energy of $\frac{3}{2}kT$. The dielectronic recombination rate is calculated assuming that each recombination yield satellite to resonance line corresponding to the recombining ion. The cooling by collisional ionization is calculated assuming each ionization causes a reduction to the gas energy by the amount of the ionization energy. And heating/cooling by charge transfer is calculated from the change in the system binding energy, see Kallman & Bautista [10] for more detail. The last term in the previous equation represents the change in temperature due to a change in the total number of particles, i.e. change in electron number density. If the gas is undergoing an ionization phase due to increase in the ionizing radiation, $dn_e/dt$ becomes positive leading to a decrease in the temperature. This decreasing temperature has to be compensated by an increase in the heating rate, otherwise the temperature would keep on decreasing even though the energy input by radiation has increased. Equation 3.29 is a modified version of the steady-state thermal balance Equation given by Ross [56].

### 3.3.6 Radiative Transfer

The ionizing radiation emitted by the central source is modified by the ambient gas via photoionization, absorption, emission and scattering. Thus, it is required to determine the radiation field (continuum and diffuse) at every point in space and time through the cloud, in particular in the non-equilibrium case. The radiation field is found by integrating the radiative transfer equation under the assumption adopted by Kallman & Bautista.
that the gaseous nebula is composed of concentric spherical shells with the ionizing source of radiation laying at its center. To solve the radiative transfer problem we adopt the radiation components adopted by XSTAR, incident continuum $L_x^{(1)}$, transmitted continuum $L_x^{(2)}$, emitted continuum, inward $L_x^{(3)}$ and outward $L_x^{(4)}$, and emitted lines, inward $L_i^{(1)}$ and outward $L_i^{(2)}$. The radiative transfer equation for the incident continuum in the non-equilibration case can be written in the form,

$$\frac{1}{c} \frac{\partial L_x^{(1)}}{\partial t} + \frac{\partial L_x^{(1)}}{\partial R} = -\kappa_c L_x^{(1)} + 4\pi R^2 j_x(R)$$

(3.33)

where $c$ is the speed of light, $L_x^{(1)}$ is the local specific luminosity at local region at depth $R$ in the cloud, $\kappa_c$ is the local continuum opacity, and $j_x$ is the local emissivity of the ionized gas. $L_x^{(1)}$ equal to the incident luminosity at the inner boundary of the cloud, $L_x^{(inc)}$. The continuum emissivity due to spontaneous recombination is given by,

$$j_x = n_{upper}n_e \left( \frac{n_i}{n_{i+1}n_e} \right) \frac{\varepsilon^3}{h^3c^2 \sigma_{pho} \epsilon^{(\varepsilon_h-\varepsilon)/kT}}.$$

The transmitted continuum component, $L_x^{(2)}$ is the radiation which would be observed if the incident light is subject to absorption only. This component is important in fitting the calculated spectra to observational data and it can be written in the form,

$$L_x^{(2)} = L_x^{(inc)} e^{-\tau_{cont}(\varepsilon)}$$
where $\tau_{\text{cont}}(\varepsilon)$ is the total optical from the inner to the outer edge of the cloud,

$$
\tau_{\text{cont}}(\varepsilon) = \int_{R_{\text{inner}}}^{R_{\text{outer}}} \kappa_{\text{cont}}(\varepsilon) dR
$$

The total emitted continuum by a model, inward $L^{(3)}_{\varepsilon}$ and outward $L^{(4)}_{\varepsilon}$, can be written in the form,

$$
L^{(3)}_{\varepsilon} = \int_{R_{\text{inner}}}^{R_{\text{outer}}} 4\pi R^2 j_{\varepsilon}(R)e^{-\tau_{\text{cont}}^{(in)}(\varepsilon)} P^{(in)}_{\text{esc,cont}}(R) dR
$$

$$
L^{(4)}_{\varepsilon} = \int_{R_{\text{inner}}}^{R_{\text{outer}}} 4\pi R^2 j_{\varepsilon}(R)e^{-\tau_{\text{cont}}^{(out)}(\varepsilon)} P^{(out)}_{\text{esc,cont}}(R) dR
$$

where $P^{(in)}_{\text{esc,cont}}(R) = (1 + C)/2$ and $P^{(out)}_{\text{esc,cont}}(R) = (1 + C)/2$ are the escape probabilities in both directions, inward and outward, to account for the suppression due to reabsorption of the emitted continua, and $C$ is the covering fraction.

The emitted lines, inward and outward, are calculated over every spacial step and can be calculated using a transfer equation similar to Eq. (3.33),

$$
\frac{1}{c} \frac{\partial L^{(1)}_{i}}{\partial t} + \frac{\partial L^{(1)}_{i}}{\partial R} = -\kappa_{i} L^{(1)}_{i} + 4\pi R^2 j_{i}(R) P^{(in)}_{\text{esc,line}}
$$

$$
\frac{1}{c} \frac{\partial L^{(2)}_{i}}{\partial t} + \frac{\partial L^{(2)}_{i}}{\partial R} = -\kappa_{i} L^{(2)}_{i} + 4\pi R^2 j_{i}(R) P^{(out)}_{\text{esc,line}}
$$

where the line escape probabilities in the inward and outward directions are calculated by,

$$
P^{(in)}_{\text{esc,line}} = (1 - C) P_{\text{esc,line}}(\tau_{i}^{(in)}),
$$

$$
P^{(out)}_{\text{esc,line}} = (1 - C) P_{\text{esc,line}}(\tau_{i}^{(out)}) + CP_{\text{esc,line}}(\tau_{i}^{(in)} + \tau_{i}^{(out)})/2,
$$
where $P_{esc,\text{line}}(\tau_{\text{line}})$ is the line probability given by Kwan & Krolik [57], and

$$P_{esc,\text{line}}(\tau_i) = \begin{cases} \frac{1}{\tau_i \sqrt{\pi} (1.2 + b)} & \tau_i \geq 1 \\ \frac{1 - e^{-2\tau_i}}{2\tau_i} & \tau_i < 1 \end{cases}$$

where $b = \sqrt{\log(\tau_{\text{line}}) / (1 + \tau_{\text{line}}/10)}$, $\tau_i^{(\text{in})}$ and $\tau_i^{(\text{out})}$ are the line scattering optical depth in both directions:

$$\tau_i^{(\text{in})} = \int_{R_{\text{inner}}}^R \kappa_i dR, \quad \tau_i^{(\text{out})} = \int_R^{R_{\text{outer}}} \kappa_i dR$$

and $\kappa_i$ is the line opacity. Since ionized plasmas emits lines that may contribute to re-ionization of the local gas, the lines have to be considered in calculations of the local ionizing radiation. To include the lines effects on the local ionization state of the gas we bin then to the continuum using profile function $\phi(\varepsilon - \varepsilon_i)$ as follows,

$$L_{\text{line},\varepsilon}^{(\text{in})} = \sum_{i \exists |\varepsilon - \varepsilon_i| \leq \Delta \varepsilon} \frac{L_i^{(1)} \phi(\varepsilon - \varepsilon_i)}{\Delta \varepsilon}$$

and

$$L_{\text{line},\varepsilon}^{(\text{out})} = \sum_{i \exists |\varepsilon - \varepsilon_i| \leq \Delta \varepsilon} \frac{L_i^{(2)} \phi(\varepsilon - \varepsilon_i)}{\Delta \varepsilon}$$

Combining Eq. (3.33) and (3.35) yields the final form of the radiative transfer equation to be solved to find the local ionization state of the gas,

$$\frac{1}{c} \frac{\partial L^{(V)}_{\varepsilon}}{\partial t} + \frac{\partial L^{(V)}_{\varepsilon}}{\partial R} = -\kappa_c L^{(V)}_{\varepsilon} + + 4\pi R^2 j_\varepsilon(R) + 4\pi R^2 \sum_{i \exists |\varepsilon - \varepsilon_i| \leq \Delta \varepsilon} \frac{j_i(R) P_{esc,\text{line}} \phi(\varepsilon - \varepsilon_i)}{\Delta \varepsilon} \tag{3.36}$$

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3.3.7 Computational Procedure and Flowchart

Studying the evolution of the conditions of a photoionized gaseous nebula requires a simultaneous integration of system of first order differential equations governing the state of the gas. To perform the numerical integration the computational procedure used to develop TDXSTAR included two main steps: (1) Finding the initial conditions of the gas assuming that the gas is initially in steady-state and the solution at this initial time step is found by the steady-state photoionization code XSTAR.

(2) Performing numerical integration of the coupled differential equations by moving forward in time to find the state of the gas at later time steps. At the beginning of every time step the code checks for the new values of the incident flux and the radiation temperature of the ionizing source via a variability function, which is an input parameter to determine the temporal change of the luminosity and/or the radiation temperature of the ionizing source. The new luminosity and the radiation temperature will be used as boundary conditions at the inner surface of the slab (the initial spacial step of the nebula). Once the boundary conditions of the ionizing flux is determined the code integrates the system of coupled differential equations representing the ionization and level populations balance equations, energy balance equation, and radiative transfer equation moving forward zone by zone staring with the innermost to solve for the state of the gas at the current time step, which in turn will be used as initially values for the following time step. The time loop terminates once the ending time or the maximum number of time steps is reached. The basic computational steps are summarized in the flowchart in Figure 3.2.
Figure 3.2  Basic flowchart for the TDXSTAR code.
The numerical integration is performed by discretization of the ordinary differential equations by defining the time and spacial derivatives of the physical quantities as follows [42],

\[
\frac{dy^{i,j}}{dt} = \frac{y^{i+1,j} - y^{i,j}}{dt}, \quad \frac{dy^{i,j}}{dx} = \frac{y^{i,j+1} - y^{i,j}}{dx}
\]

where \(dt^i = t^{i+1} - t^i\) and \(dx^i = x^{j+1} - x^j\).

The ionization balance equations

\[
\frac{n_{i+1,j} - n_{ij}}{t^{i+1} - t^i} = (\text{rates into ion}) - (\text{rates out of ion})
\]

Similarly the level populations balance equations

\[
\frac{n_{i+1} - n_i}{t^{i+1} - t^i} = (\text{rates into level}) - (\text{rates out of level})
\]

By solving the ionization balance equations we obtain the ionic fractions (relative ion abundances), which are used to calculate the relative level populations of the various bound levels. The integration of the level populations equations is performed using the fourth order Rung-Kutta method, see for example [58].

To find the temperature of the gas we need to solve the energy balance equation (??), which can be written in the form,

\[
\frac{T^{i+1,j} - T^{i,j}}{dt^i} = \frac{2}{3k n_e^{i+1,j}}(\Lambda^{i+1,j} - \Gamma^{i+1,j} - \frac{3}{2}kT^{i+1,j}n_e^{i+1,j} - n_e^i)
\]

Or,

\[
T^{i+1,j}(1 + \frac{n_{e}^{i+1,j} - n_{e}^{i}}{n_e^{i+1,j} dt^i}) - T^{i,j} - \frac{2}{3k n_e^{i+1,j}}(\Lambda^{i+1,j} + \Gamma^{i+1,j})dt^i = 0
\]

The above equation is solved numerically for \(T^{i+1,j}\) using the secant method, see for example [59].
CHAPTER IV

RESULTS AND DISCUSSION

4.1 Introduction

This chapter presents our findings on time-dependent photoionization of gaseous nebulae using our photoionization codes, TDP and TDXSTAR (see Chapter III). The current chapter includes mainly two sections. In the first section (4.2), we introduce the preliminary results of our two energy levels models of non-equilibrium photoionization of gaseous nebulae composed only of hydrogen using our code TDP ([42]). We studied the time-dependent effects in a constant density slab consisting of only hydrogen due to a rise in the ionizing flux by a factor of 3 for different ionization parameters. In this case we use a step-like function to represent the variation in the intensity of the ionizing flux, see figure 4.1. In subsection 4.2.1, we present the results of calculating the ionization and temperature equilibration time scales through the constant density slab. In subsection 4.2.2, we present the effects of varying the ionizing flux on a slab in pressure equilibrium across the slab. In section 4.3.2 we present the results of studying the time-dependent effects in a slab at constant density subjected to a periodically varying incident ionizing flux. In this case we use a sinusoidal function to represent the flux variation.

In the second section of this chapter, we present the results of our full atomic time-dependent photoionization code, TDXSTAR. As initial verification of the code, we present in section 4.3.1 a comparison of TDXSTAR results with the results of TDP model using the same assumptions used in subsection 4.2 except for the fact that TDP code is a two-
Figure 4.1  Step-like function used to represent sudden rise/drop in the ionizing flux by a factor of 3 (top panel), and rectangular function used to represent periodic variation in the ionizing flux (bottom panel).
level energy model while TDXSTAR simulate a more realistic case by adopting full atomic model. In subsection 4.3.3, we qualitatively investigate the effects of time-dependent photoionization in planetary nebulae by constructing a grid of models analogy to those used by Harrington & Marionni [7] to investigate FG Sagittae planetary nebula. Further, in section 4.3.6 we investigate the long-standing problem of temperature fluctuations in Planetary Nebulae and H II Regions using our TDXSTAR code. Our results propose that temperature fluctuations in PNe could be a result of long period binary central stars, and, hence, temperature fluctuations are an evolutionary effect, characteristic of binary systems during the early stages of PNe evolution.

4.2 TDP Model: Step Flux Function on a Constant Density Slab

In this section we present simulations of photoionized slabs with constant hydrogen density, \( n = 10^4 \text{ cm}^{-3} \), subjected to a sudden change in the ionizing radiation. The spectral energy distribution of the ionizing radiation field is assumed to be a power-law. It is also assumed that the slabs are in steady-state equilibrium at \( t = 0 \).

Figure 4.2 shows the level populations and temperature in a slab subjected to sudden change in the ionizing flux. The initial steady-steady solution shows that the neutral hydrogen is minimum when the temperature is maximum at the inner face of the slab and both continue to be roughly constant for a depth at which the majority of the ionizing photons have been absorbed. Then the temperature drops and the neutral hydrogen increases sharply, forming an ionization fronts at \( 7.9 \times 10^{16} \text{ cm} \). At a given time the flux increases suddenly by a factor of 3 and we follow the temporal evolution of state conditions. The gas
conditions for two different ionization parameters show that the models are qualitatively very similar, but the size of the ionized region scales up with the ionization parameter $\zeta$. After sometime, set by ionization and temperature equilibration times, the gas conditions relaxes to a final steady-state conditions corresponding to the flux maximum. Between the final and initial state the temperature increase and the neutral hydrogen decreases gradually until they reached their final steady states.

The temperature profiles show the temporal change in the temperature with a sharp spike in the temperature near the ionization fronts just after rising the flux. This spike tend to decrease gradually until it is completely flattened when the gas reaches the final steady-state. This is due to the fact that most of the photons that are able to reach near the ionization front are high-energy photons, while low-energy photons were absorbed in the ionized region. This process is called radiation hardening. The ionization using energetic photons generates faster photoelectrons. In addition, cooling is reduced by the fewer number of ions available for recombination. Then cooling increases gradually with increasing ionization to flatten the temperature spike when it reaches the final equilibrium state.

Figures 4.3 and 4.4 show the ionization/recombination rates and heating/cooling rates when the flux rises by a factor of 3. The rates are shown at four different times, the initial and final steady-states and two intermediate time steps. At the initial and final steady states the rates are in equilibration at all points across the slab. After the sudden increase in the flux, the state of the gas becomes out of equilibrium forming ionization and heating fronts propagating through the slab leaving the plasma behind out of equilibrium. The ionization and heating fronts are found at $3 \times 10^{16}$ cm after $7.8 \times 10^5$ s and reach the IF at time
Figure 4.2  Time dependent simulation for a slab with constant density of $n = 10^4 \text{cm}^{-3}$ and initial flux of $F_x = 7.95 \text{erg cm}^{-2} \text{s}^{-1}$. At $t = 0$ s the flux is increased by a factor of 3. The upper and lower panels show the neutral hydrogen density and the gas temperature along the position within the slab, respectively. In both cases, each curve corresponds to the profile at a different moment in time. The initial/final steady state conditions are plotted in red/green.
\[ t = 1.1 \times 10^7 \text{ s}. \] By this time the plasma behind has evolved significantly toward final equilibrium state.

Figures 4.5 and 4.6 are similar to Figures 4.3 and 4.4 for a flux reduced by a factor of 3. In this case, cooling and recombination fronts are formed and propagate through the cloud leaving the gas behind out of equilibrium. Later, by the time the cooling and recombination fronts reach the IF the gas behind has mostly reached equilibrium.

### 4.2.1 Timescales and Rates

The results above show that at the intermediate time steps between the initial and final steady states the gas is out of equilibrium and is different from any state solution with different ionization parameter, and hence, the evolution of the states can not be represented by a sequence of steady-state solutions. This is because the gas at different depths respond at different times to variations in the ionizing radiation due to the ionization/thermal or recombination/cooling fronts propagation times. Moreover, different depths evolve at different rates depending on ionization (recombination) and thermal (cooling) equilibration time scales.

Figure 4.7 shows the propagation, ionization equilibration, and temperature equilibration times as a function of depth across the cloud. It is shown that the flux propagate with roughly constant speeds, \( \sim 20,000 \text{ km s}^{-1} \), in the ionized region and then slows down non-linearly by order of magnitude across the ionization front. It is clear that the propagation times are inversely proportional to the flux variation magnitude.
Figure 4.3  Ionization (solid line) and recombination (dotted line) rates versus depth inside the slab with $\log \xi = 0$ after a sudden increase of the ionizing flux by a factor of three. The rates are plotted at $t = 0$ (initial steady-state conditions), $t = 3.4 \times 10^8$ s (when the slab has reached equilibrium again), and two instants in between.
Figure 4.4  Heating (solid line) and cooling (dotted line) rates versus depth inside the slab with log $\xi = 0$ after a sudden increase of the ionizing flux by a factor of three. The rates are plotted at $t = 0$ (initial steady-state conditions), $t = 3.4 \times 10^8$ s (when the slab has reached equilibrium again), and two instants in between.
Figure 4.5  Like Figure 4.3, but for sudden drop in the ionizing flux by a factor of three.
Figure 4.6  Like Figure 4.4, but for sudden drop in the ionizing flux by factor three.
Figure 4.7  Propagation time (top panel), ionization equilibration time (middle panel), and temperature equilibration time (bottom panel) versus depth within the slab for a plasma with \( \log \xi = 0 \) and \( f_x = 3 \).
The ionization equilibration time scale can be found from the relative change in ionization and the ionization and recombination rates. It was found that at the steady-state conditions of our models for $T = 10^4$ K and $n_e = 10^4$ cm$^{-3}$ the ionization and recombination times are of the order of $\sim 100$ yrs, in particular across the IF. This is because the neutral hydrogen fraction experiences the largest changes, from $\approx 1$ to 0, near the IF. In contrast, in the ionized region the gas is nearly fully ionized and the relative change in the ionization state of the gas is small, and thus it has shorter equilibrium times.

Similarly, the temperature equilibration time scale is short, of order of a few years, in the ionized region and peaks at $\sim 35$ yrs at the IF. It is interesting that while in the ionized region the equilibration time scale for temperature is longer than that for ionization, the situation is reversed across the IF.

4.2.2 TDP Model: Step Flux Function on a Slab in Pressure Equilibrium

In this section we show the results of a slab initially at pressure equilibrium at a pressure of $4 \times 10^{-8}$ dyn cm$^{-2}$. For the cloud to be in pressure equilibrium the gas density has to increase as $1/T$ from the outer to the inner face of the cloud toward the ionizing source, which means the density has to increase sharply across the IF.

In Figure 4.8 we follow the temporal change of the the temperature and the pressure when the ionizing flux increase by a factor of three while the gas is kept at fixed density. The IF is initially found at $x \approx 10^{17}$ cm. It is shown that ionization and thermal fronts are formed after the increase in the flux. These fronts propagate through the slab and heat the gas beyond the original IF, leaving the gas behind out of equilibrium. This will
trigger dynamical effects in the cloud. If the thermal fronts propagate at subsonic speed the gas will expand and the density profile will be redistributed in a form which maintains pressure equilibrium across the cloud and with its surroundings. Note that if the thermal front propagates at subsonic speed it will remain constant across the cloud, in the ionized region and across the ionization front. This is because across the IF the thermal front propagation speed is proportional to $T$ and sound speed goes as $T^{1/2}$. On the other hand, if the thermal front propagates at supersonic speed the gas will have no time to adjust its density to maintain the pressure equilibrium leading to strong imbalances, as seen in Figure 4.8. Thus, shock waves will be formed in the cloud, which can ultimately result in the fragmentation of the cloud [41].

Further, we ran several models to simulate the gas conditions when the ionizing flux varies by a factors of $f_x = 0.3, 0.5, 0.8, 1.2, 1.5$ and 2. To follow the pressure front we used the inflection point, the point at which the term $dP/dx$ becomes most negative, as a reference on the pressure profiles. It is shown in the figures that when the flux increases, ionization fronts are created and propagate away from the ionizing source. In contrast, recombination fronts are created and propagate toward the source when the flux decreases.

Figure 4.10 shows the speeds of ionization and recombination fronts. It is shown that ionization fronts move forward with speeds proportional to the flux increment, $v_{pro} = 10^3 \text{ km s}^{-1}$ for $f_x = 3$, which is consistent with $v_{pro} = F_x/H_H$ given by equation 3.22. On the other hand, when the ionizing flux decrease recombination fronts propagate with speeds of order of $\sim 100 \text{ km/s}$ for a decrease in the flux by a factor of 20%. The speed of sound is given by $v_s = \sqrt{\gamma p/\rho}$, where $\gamma$ is the adiabatic index, $p$ is the pressure and
Figure 4.8  Ionization and temperature for a slab initially in pressure equilibrium at $P_o = 4 \times 10^{-8} \text{ dyn cm}^{-2}$. The initial flux corresponds to $\log \xi = 0$, which is suddenly increased by a factor of 3 ($f_x = 3$). The initial condition is plotted in red, and the final state of the system is plotted in green. The black curves depict the physical conditions at different times. The gas density obtained from the pressure equilibrium solution is shown in the upper panel with the dashed-blue line.
Figure 4.9  Pressure profiles in the region where the IF is formed (black lines). The red-dots indicate the position of the IF at different times. Each panel corresponds to a different flux variation factor \( f_x \), as indicated.
Figure 4.10  Propagation speed of the IFs due to flux increases (top panel) and recombination fronts due to flux drops (bottom panel). Each curve corresponds to a different flux variation factor $f_x$, as indicated in each panel.
\( \rho \) the mass density of the gas. For an ideal gas \( \gamma = 5/3 \) and temperature range \( T = (1 - 4) \times 10^4 \text{ K}, v_s = 12 - 24 \text{ km s}^{-1} \). Thus, even small change in the ionizing flux can trigger ionization/recombination fronts to propagate at supersonic speeds.

### 4.2.3 TDP Model: Periodically Varying Flux on a Constant Density Slab

In previous section we have shown that equilibration time scales varies non-linearly by a factor of order of magnitudes across a nebula. That means variations in the ionizing radiation occurring over a wide range of time scales, comparable to equilibration times, will drive the nebula out of equilibrium conditions. Thus, periodic or quasi-periodic variations of ionizing continua, as seen in a large variety of astronomical nebulae such as binary systems, quasars and AGN, are likely to result in non-equilibrium conditions at some point in the nebula. Thus, we studied the time-dependent effects in slabs with hydrogen density \( 10^4 \text{ cm}^{-3} \) and subjected to a periodic change in the ionizing flux; the change in the flux is represented by a periodic square function.

In Figure 4.11 we show the neutral hydrogen fraction and temperature for various flux variation periods. The figures show the initial steady-state solution corresponding to the mean flux, the time-average of the instantaneous conditions, the maximum and minimum conditions corresponding to the flux maximum and minimum, respectively, and the dispersion of the instantaneous conditions from the time-average. Several conclusions can be drawn:

1. The time average of the state conditions differs from the mean of the two steady states solutions corresponding to the maxima of the ionizing flux. The time average solution is
Figure 4.11  Ionization and temperature solutions for constant density slab subjected to periodically varying fluxes with periods of 3, 9, 15, and 40 yrs. The initial hydrogen density is $10^4 \text{ cm}^{-3}$, the radiation flux corresponds to $\log \xi = 0$, and the flux variations are of $f_x = 0.5$. The green curves show the steady-state equilibrium conditions at the low and high states of the flux. The red curves depict the steady-state equilibrium solutions for a radiation flux at the media between the low and high states. The blue solid line shows the time average conditions, while the dashed lines show the dispersion in that average.
over-ionized with respect to the mean solution of the maxima of the flux. In addition, the time average of the temperature is lower than that corresponding to the mean value of the ionizing flux.

(2) The dispersion of the physical conditions from their time average increases with the period. This is expected where at short periods of variation, much shorter than equilibration time scales, the gas conditions would be forced to remain close to the mean steady state. On the other hand, at large periods the gas would have enough time to react for being driven to the final steady states corresponding to the maxima of the flux.

(3) Ionization fronts are much wider than under steady-state conditions. This is due to the fact that the physical conditions at the IFs experience the largest dispersion from the average allowing for smoother transition across the ionization front, from the ionized to the neutral regions, than under steady-state equilibrium.

Full animations of ionization and temperature across the slab can be found at http://hea-www.cfa.harvard.edu/javier/tdp for various flux variability periods.

Figures 4.12 and 4.13 show a few snapshot of ionization and temperature relative to their average values. The simulations of different periods show that the gas is out of equilibrium at the whole time of simulations. In addition, the size of the ionized region varies synchronously with the continuum flux. However, there is a delay between the continuum and the gas response along the depth of the cloud due to the propagation times of thermal and ionization fronts when the flux increases, as well as that of the cooling and recombination fronts when the flux decreases. This will cause the gas conditions to be above the average conditions in some regions and below the average in others. The IF region experi-
Figure 4.12  Instantaneous ionization relative to time averaged values for instants along 1000 years simulations for various radiation flux variability periods. Here, the radiation flux corresponds to \( \log \xi = 0 \) and the amplitude if variations is \( f_x = 0.5 \).
Figure 4.13  Instantaneous temperatures relative to time averaged values for instants along 1000 years simulations for various radiation flux variability periods. Here, the radiation flux corresponds to \( \log \xi = 0 \) and the amplitude if variations is \( f_x = 0.5 \).
ence the largest dispersion from the time-averaged conditions. This due to the fact that the equilibration and propagation times are maximum at the IF.

4.3 TDXSTAR Models

In order to validate our TDXSTAR code we run simulations similar to those excited using TDP code in section 4.2. The results of TDXSTAR code are in good agreement with those done by TDP code.

4.3.1 TDXSTAR Model: Step Flux Function on a Constant Density Slab

In this section we present the results of TDXSTAR of simulation of a constant density gaseous nebula consisting of only hydrogen with density of $10^4 \, \text{cm}^{-3}$ and subject to a sudden change in the ionizing flux. As in TDP simulation, the nebula is assumed initially at steady-state equilibrium. The chief difference between the results of TDP code and those done by TDXSTAR is that the later takes into account the various atomic processes involved in a multi-level atomic model causing excitations and de-excitations among the various atomic levels.

Figure 4.14 shows the time evolution of the number density of hydrogen and the temperature through the slab at different ionization parameters $\xi$. At the initial steady-state, the neutral hydrogen fraction is minimum at the illuminated face of the nebula and it remains relatively constant until most of the ionizing photons are absorbed. At this point, the neutral gas increase sharply, forming the ionization front. The opposite is true for the temperature which is maximum occurs at the illuminated face and remain relatively constant across the ionized region and then drop sharply at the ionization front. Essentially the qualitative be-
behavior is the same at the different ionization parameters except for the fact that the size of
the ionized region scales up with the ionization parameter.

At a given time the flux increased by a factor of 3, and then we follow the temporal
change of the state conditions of the nebula. The temperature is observed to increase gradu-
ally with a small spike at the IFs due to hardening of the ionizing radiation due to the
fact that low energy photons are absorbed in photoionizing the inner regions of the nebula
leaving mostly higher energy photons to ionize deeper regions at the IFs. Faster photoelec-
trons emerging at the adjacent regions to the IFs find fewer number of protons available
for recombination making recombination cooling inefficient, resulting in the spike in the
temperature near the IFs. Later in time, recombination takes on near the IF, which in-
creases cooling and smooths out the temperature spike and the whole nebula comes to a
new equilibrium state.

Figure 4.15 shows heating/cooling rates across the nebula at four different instants of
time. Initially, the gas is at steady state equilibrium, and, hence, heating and cooling rates
are equal everywhere across the nebula. Then, the flux rises by a factor of three and pro-
duces heating front propagating across the nebula leading the gas to a non-equilibrium state.
The figure show that, at time $t = 0.3 \text{ year}$ the heating front is found at $10^{16} \text{ cm}$ leaving the
gas behind in a non-equilibrium state. The heating front continue to propagate across the
nebula to reach the IF at time $t = 35 \text{ yr}$. After about $10 \text{ yr}$, the gas eventually evolves to a
new steady-state equilibrium.

Figure 4.16 shows the heating and cooling rates across the nebula when the flux drops
by a factor of three. Cooling fronts propagate across the nebula leading to a non-equilibrium
Figure 4.14  Time dependent simulation for a slab with constant density of $n = 10^4 \text{cm}^{-3}$ and initial flux of $F_x = 7.95 \text{erg cm}^{-2} \text{s}^{-1}$. At $t = 0 \text{s}$ the flux is increased by a factor of 3. The upper and lower panels show the neutral hydrogen density and the gas temperature along the position within the slab, respectively. In both cases, each curve corresponds to the profile at a different moment in time. The initial condition is plotted in red, and the final state of the system is plotted in green.
Figure 4.15  Heating (solid line) and cooling (dotted line) rates versus depth inside the slab with log $\xi = 0$ after a sudden increase of the ionizing flux by a factor of three. The rates are plotted at $t = 0$ (initial steady-state conditions), $t = 3.4 \times 10^8$ s (when the slab has reached equilibrium again), and two instants in between.
Figure 4.16  Like Figure 4.15 but for sudden drop in the ionizing flux by factor three.
state and, eventually, evolve to new steady-state equilibrium.

4.3.2 TDXSTAR Model: Periodically Varying Flux on a Constant Density Slab

In this section we present the results of time-dependent effects in a slab with constant density of $10^4 \text{cm}^{-3}$ of only hydrogen subject to periodically varying flux. We use a square function with periods of 3, 9, 15 and 40 years with amplitude of 50%. Similar conclusions to those in section 4.3.2 can be made. We find that the time average is characterized by cooler and over-ionized conditions than those of the steady-state corresponding to the mean solution of the flux maxima. The dispersion of the instantaneous conditions from the time-average scales up with the period of the flux variation; periods much shorter than equilibration will force the gas conditions to remain close the time-average with minimal dispersions. The ionization fronts are much wider than stead-state solutions, where in time-dependent simulations the physical conditions at the IFs experience the largest dispersion from the average allowing for smother transition across the ionization front.

Figures 4.18 and 4.19 show snapshots of the neutral hydrogen density and the temperature relative to their average values across the nebula. It is clear that, as observed before with the TDP code, the physical conditions at the IFs experience the largest dispersion from their average values leading to a time delay in the response of the gas across the nebula. The instantaneous physical conditions of the nebula crosses their average values in the sense that the instantaneous conditions oscillate around the average, i.e., it is possible to simultaneously find regions above and others below the average. On the other hand, the instantaneous conditions are out of equilibrium at all times, except when the period of the
Figure 4.17  Ionization and temperature solutions for constant density slab subjected to periodically varying fluxes with periods of 3, 9, 15, and 40 yrs. The initial hydrogen density is $10^4 \text{ cm}^{-3}$, the radiation flux corresponds to $\log \xi = 0$, and the flux variations are of $f_x = \pm 0.5$. The green curves show the steady-state equilibrium conditions at the low and high states of the flux. The red curves depict the steady-state equilibrium solutions for a radiation flux at the media between the low and high states. The blue solid line shows the time average conditions, while the dashed lines show the dispersion in that average.
Figure 4.18  Instantaneous ionization fraction relative to time averaged values for instants along 1000 yrs long simulations for various radiation flux variability periods. Here, the radiation flux corresponds to log ξ = 0 and the amplitude if variations is $f_x = 0.5$. 
Figure 4.19  Instantaneous temperatures relative to time averaged values for various instants along 1000 yrs long simulations for various radiation flux variability periods. Here, the radiation flux corresponds to log $\xi = 0$ and the amplitude of variations is $f_x = \pm 0.5$. 
ionizing source is much longer than equilibration times, giving the gas enough time to relax to the final steady-states corresponding to the flux maxima.

4.3.3 **TDXSTAR Model: Time-dependent Effects in FG Sagittae Planetary Nebulae**

We have constructed a grid of models similar to those adopted by Harrington & Marionni [7] to simulate FG Sagittae planetary nebula. This is a super-giant variable star embedded in a gaseous nebula that appears as a uniform disk photoionized by the central star. It is difficult to determine the change in the star’s intrinsic luminosity due to the fact that only photographic apparent magnitude is present during the observational interval 1894-1955, therefore, the models are constructed assuming constant luminosity and a steady decrease in the stellar temperature. The stellar temperature is assumed to decrease linearly with time as used by Harrington & Marionni [7],

\[ T_*(t) = T^i_* - R(t - t_0), \quad t > t_0 \]  (4.1)

where \( T_*(t) \) and \( T^i_* \) are the stellar temperatures at times \( t \) and \( t_0 \), respectively, and \( R = 250 \, K/yr \) is the temperature decline rate of the stellar temperature. In our models we have adopted the same physical conditions as those used by Harrington & Marionni [7] except for the hydrogen densities and stellar luminosities where we used 10 folds of their original values to meet TDXSTAR’s minimum standard density, which is set to 1000 \( cm^{-3} \). Black-body spectral energy distribution is adopted for the stellar spectrum of the central star. The basic model, called B, has hydrogen nucleus density \( N_H = 2000 \, cm^{-3} \), stellar temperature \( T^* = 56,000 \, K \), and stellar luminosity \( L^* = 40,000 \, L_\odot \). The models A and C are like B but with stellar temperatures of 49,000 K and 63,000 K, respectively. Model E is the same
as model B but with different density of 4000 cm$^{-3}$. Models F and G are the same as the model B but with stellar luminosities of 15,000 $L_\odot$ and 100,000 $L_\odot$, respectively. All of our models have the same chemical composition as those used by Harrington & Marionni [7].

Direct comparison between our present results and those of used by Harrington & Marionni [7] are complicated by the fact that it is unclear from their paper what ionization parameter they used. Hence, we adopted $\log \xi = 0.5$ dex for model B and scaled the rest of the models according their given luminosities and densities using the definition of the ionization parameter adopted in XSTAR [10]. The physical parameters and ionic abundances used in our models are summarized in tables 4.1 and 4.2.

<table>
<thead>
<tr>
<th>Model</th>
<th>Hydrogen Density $n_H$ (cm$^{-3}$)</th>
<th>Effective Stellar Temperature $T_{eff}$ (K)</th>
<th>Luminosity $(L_\odot)$</th>
<th>Ionization Parameter $\log \xi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2000</td>
<td>49,000</td>
<td>40,000</td>
<td>0.5</td>
</tr>
<tr>
<td>B</td>
<td>2000</td>
<td>56,000</td>
<td>40,000</td>
<td>0.5</td>
</tr>
<tr>
<td>C</td>
<td>2000</td>
<td>63,000</td>
<td>40,000</td>
<td>0.5</td>
</tr>
<tr>
<td>E</td>
<td>4000</td>
<td>56,000</td>
<td>40,000</td>
<td>0.3</td>
</tr>
<tr>
<td>F</td>
<td>2000</td>
<td>56,000</td>
<td>15,000</td>
<td>0.07</td>
</tr>
<tr>
<td>G</td>
<td>2000</td>
<td>56,000</td>
<td>100,000</td>
<td>0.9</td>
</tr>
</tbody>
</table>

We used our TDXSTAR code to run the models A-G to study the effects of changing
Table 4.2  Elements abundances in FG Sagittae models.

<table>
<thead>
<tr>
<th>Element</th>
<th>Abundance</th>
</tr>
</thead>
<tbody>
<tr>
<td>He/H</td>
<td>$1.1 \times 10^{-1}$</td>
</tr>
<tr>
<td>C/H</td>
<td>$2 \times 10^{-4}$</td>
</tr>
<tr>
<td>N/H</td>
<td>$3 \times 10^{-4}$</td>
</tr>
<tr>
<td>O/H</td>
<td>$3 \times 10^{-4}$</td>
</tr>
<tr>
<td>Ne/H</td>
<td>$7.5 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

the different physical parameters such as stellar temperature, gas density and luminosity on the fluxes of some of the important observed emission spectral lines. We should emphasize that this study is not intended to investigate FG Sagittae nebula, it is rather to qualitatively validate our code’s performance through comparison with available work.

4.3.4 Results for FG Sagittae Models

Figure 4.20 shows the effects of changing the initial stellar temperatures starting with 49,000 K, 56,000 K, and 63,000 K in models A-C, respectively. The figures show the fluxes of emission lines He II $\lambda$4686, [Ne III] $\lambda$3869, [O III] $\lambda$4959, and [O II] $\lambda$3726 + 3729 relative to the flux of I(H$\beta$)=100. Our results show trends consistent with those calculated by Harrington & Marionni [7], where the line fluxes of He II $\lambda$4686, [Ne III] $\lambda$3869, [O III] $\lambda$4959 decline continuously with time. This trend is the same in all the models despite changes in the initial temperature. It is interesting that, though models A, B, and C have the same gas density, the lines fluxes are different. This due to the fact that these models start with different initial effective stellar temperature for the ionizing star, leading to more
intense lines for models with higher stellar temperature causing the deviation seen in these models.

Figure 4.21 presents the effects of varying stellar temperature on emission spectral lines for various densities \((1000 \, cm^{-3}, \, 2000 \, cm^{-3} \, \text{and} \, 4000 \, cm^{-3})\) for models B and E. Though recombination and cooling rates scale as \(n_e^2\), our results show that models with higher density decline slower because of reabsorption of \(Ly\alpha\) lines in such optically thick models with densities ten times higher than that found in Harrington & Marionni models [7]. Thus, cooling is suppressed by absorption of \(Ly\alpha\) lines at such high densities.

Figure 4.22 shows the result of models F,B and G of varying the stellar temperature at different fixed luminosities. The \([Ne \, III]\) lines are very similar in the different models. The \([O \, II]\), \([O \, III]\) and \([N \, II]\) lines are not graphed because they remain the same in the different models [7]. This is due to the fact that luminosities and distances scale in a way such that the radiation field stays nearly the same at the inner face of the nebulae, and hence the conditions throughout the nebulae are very similar, with He II lines as exception.

From Figures 4.20-4.21, it is clear that different lines from different ions behave differently. This is mainly due to the difference in the ionization energy of the parent ion and the mechanism by which they are produced (e.g., recombination or collisional excitation). Let us start with the two lines \([Ne \, III]\) and \([O \, III]\) showing similarities in their behavior. At the beginning, over the first \(\sim 60 \, years\), is seen that the two lines decay slowly where at this interval the star is able to emit ionizing photons and heats the gas, but after \(\sim 60 \, years\) the effective stellar temperature drops to temperatures at which the star ceases to produce ionizing photons giving the gas a chance to cool down much faster, leading to a faster decay
Figure 4.20  Time-dependent effects in models A (green), B (black), and C (red) with different initial stellar temperatures of 49,000 K, 56,000 K, and 63,000 K, respectively, on He II $\lambda$4686 (solid lines) and [Ne III] $\lambda$3869 (dotted lines) in the top panel, and on [O III] $\lambda$4959 (solid lines) and [O II] $\lambda$$\lambda$3726, 3729 (dotted lines) in the bottom panel. The line fluxes are calculated relative to $F(H\beta) = 100$. 

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Figure 4.21  Time-dependent effects in models B (black) and E (red) with different hydrogen densities of 2000 $cm^{-3}$, and 4000 $cm^{-3}$, respectively, on He II $\lambda 4686$ (solid lines) and [Ne III] $\lambda 3869$ (dotted lines) in the top panel, and on [O III] $\lambda 4959$ (solid lines) and [O II] $\lambda\lambda 3726 - 3729$ (dotted lines) in the bottom panel. The line fluxes are calculated relative to $F(H\beta) = 100$. 

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Figure 4.22  Time-dependent effects in models F (green), B (black), and G (red) with different stellar luminosities of 15,000, 40,000, and 100,000 $L_\odot$, respectively, on He II $\lambda$4686 (solid lines) and [Ne III] $\lambda$3869 (dotted lines) in the top panel, and on [N II] $\lambda$6584 in the bottom panel. The line fluxes are calculated relative to $F(H\beta) = 100$. 
Figure 4.23  Time-dependent effects on the ionic relative abundances of H, He, N, and O (denoted in the figure), integrated over the nebular volume for model B.
rates in the flux of the two lines, [Ne III] and [O III] as seen in Figure 4.20. Note that, in the same figure, He II follows the same trend as that of [Ne III] and [O III] lines, except for the fact that H II is a recombination line, from its decay rate one can infer the recombination rate for doubly ionized species in such nebulae. On the other hand, the two lines [O III] and [O II] behavior is readily understood. Before $\sim 60$ years the decay of the flux of [O III] line infers the depletion of $O^{+2}$ to $O^+$, which leads to enhancement in the flux of [O II] line. After $\sim 60$ years, the star has ceased to produce enough ionizing photons and the nebula has cooled down, which leads to a decay in the flux of both [O II] and [O III] lines.

Figure 4.23 shows the time-dependent effects due to a decaying stellar temperature on the ionic relative abundances for model B. The model starts with effective stellar temperature of $56,000 \, K$, which decays later with a decay rate of $250 \, K/yr$. Following the behavior of the neutral factions of the different elements, one can notice that the gas is becoming more neutral with time. This again, mainly due to the decay in the effective stellar temperature that leads to drop in the number of the ionizing photons and lower temperature for the gas. To explain this let us use $O$ ions as an example, the depletion of $O^{2+}$ leads to enhancement in $O^+$, and a portion recombines and become neutral $O^0$. This behavior is very similar for all the species, higher ions recombine producing lower ions, portion of which will become neutral driving the gas as a whole toward higher neutral state. The sudden increase seen in $He^0$ at $\sim 60$ years can be interpreted as a result of the sever drop in the helium ionizing photons due to the drop in the effective stellar temperature which shifts the peak of the black-body to frequencies below the ionization threshold for $He^0$. 
4.3.5 TDXSTAR Model: Time-dependent Effects in Planetary Nebulae and H II Regions Ionized by Binary Systems

Time-dependent photoionization effects are triggered by variations in the ionizing flux. Such variations can be a result of a change in the ionizing source luminosity/temperature, or as a result of some dynamical activity such as binary system emitting ionizing radiation. Traditionally, planetary nebulae are defined as a late stage of intermediate-mass star life; i.e., a star which has recently evolved from the red giant towards the white dwarf stage. This model can explain spherically symmetric PNe, but it is not sufficient in explaining the wide range of morphologies seen in PNe. In fact, a large fraction of PNe of intermediate-mass stars are known to be in binary systems [60]. Light curves of binaries show periodic variations in their observed flux due to the eclipsing nature of the binary system, see for example [61]. The light flux is maximum when the two stars are side-by-side and minimum when the primary star (more luminous) is eclipsed by the secondary one. Nebulae ionized by binary systems experience such variations in the ionizing flux. In case of short-period binary systems the variations in the ionizing flux occur over short time-scales (much shorter than gas equilibration times), and thus the variations will not significantly impact the ionization state of the gas because it would have no time to respond to the flux variations, forcing the gas conditions to remain close to the time-averaged conditions. In this case, dispersions from time-averaged conditions will be minimal. On the other hand, in case of long-period binaries 1year (comparable to the gas equilibration times) the gas has enough time to react to the flux variations allowing the gas conditions to go farther from their time-averaged values toward equilibrium states correspond to the flux maxima. Therefore, time-dependent
effects are expected in nebulae photoionized by binary systems, in particular when the pe-
riod of the binary system is comparable to the equilibration times scales for the excitations,
ionization, and temperature balance.

In order to investigate the time-dependent photoionization effects in PNe associated
with binaries, we used our TDXSTAR code to simulate PNe models powered by binaries.
The physical model of the nebulae consists of spherical shells of gas with constant density
$10^3 \text{ cm}^{-3}$ and of solar chemical composition. The nebulae are ionized by a central system
of binary stars emitting black body radiation, the primary star (compact and bright main
sequence star) with stellar temperature of $50,000 \text{ K}$ and the secondary star (much cooler
and relatively larger) with stellar temperature of $30,000 \text{ K}$. Figure 4.24 shows a schematic
diagram depicting a gaseous shell ionized by a central binary system. The ionization pa-
rameter adopted for the primary star is 0.1. We assume the gas is initially in steady-state
conditions and ionized by the primary star while eclipsing the secondary. Then we follow
the gas conditions in later times accounting for the variations in the ionizing flux due to the
eclipsing nature of the binary system. For simplicity, we adopt a rectangular function to
represent the light curve for the binary system, see figure 4.25.

We study the conditions of the gas in the binary plane, edge-on to the binary system
with different periods for the system, from a few days to decades and eclipsing times from
$1/10$ to $3/8$ of the period. The eclipsing time, $t_e$, is proportional to the orbital period and
the diameter of the secondary star. The period of a binary system is given by,

$$P = \frac{2\pi}{\omega} = \frac{2\pi}{\sqrt{\frac{G(M_p+M_s)}{a^3}}}$$
where $\omega$ is the angular frequency, $G$ is the gravitational constant, $M_p$ and $M_s$ are the masses of the primary and secondary stars, respectively, and $a$ is the separation between the two stars. Assuming masses of $\sim 2M_\odot$ and $\sim 1M_\odot$ for the primary and the secondary stars, respectively, and a separation between the two stars of $\sim 2AU$, one deduces orbital period of $\sim 1.5years$.

The timescale for a sound wave $\tau_s$ in a nebula can be written as,

$$\tau_s = \Delta r/V_s$$

where $\Delta r$ is the depth of the nebula, and $V_s$ is the sound speed in the medium of the nebula. Typical value for the sound speed in a nebula with density $n_H = 10^4 cm^{-3}$ and $T = 10^4 K$ is $V_s \approx 10Km/s$, which implies sound wave timescale of $\sim 300years$, which implies that dynamical effects are not important in our models, given that our models periods are of order of $\sim 10years$

4.3.6 The Results for the Central Binary-star Models

In each model we investigate the median electron temperature and the temperature averages weightd by recombination and collisionally excited lines from the conditions of the gas along the radial direction in the orbital plane.

Figure 4.26 show the initial steady-state temperature profile when the slab is ionized by the primary star emitting black body radiation with effective temperature of 50,000 $K$ and ionization parameter of 0.1. The steady-state temperature profile is minimum at the illuminated face of the nebula and increase gradually across the nebula to reach its maximum at the IF. Later, we account for the variations in the ionizing radiation emitted by
Figure 4.24 Schematic diagram of a cloud ionized by an eclipsing binary system.
Figure 4.25  Rectangular function used to represent the variations in the ionizing flux in PNe and H II regions ionized by binary systems.
the binary system with different periods and different eclipsing times and follow the effects on the gas conditions. It was found that the time-averaged temperature profiles of the different periods are different from any steady-state solution at all times during the simulations. Time-averaged temperature profiles are characterized by two peaks and flatter profiles compared with the steady-state corresponding to the mean flux. The peaks are due to the varying Strömgren radii between the high and low states of the ionizing source. When the flux drops the gas tend to cool down and recombine showing smaller Strömgren radius, the opposite is true when the flux rises showing the other peak of temperature at the larger Strömgren radius. This is due to the fact that binaries with longer periods of order of 10 years allow enough time for the gas to fully respond to the flux maximum/minimum reaching the highest/lowest possible temperatures. The opposite is true for binaries with short periods, of order of days, which have no noticeable effects on the gas conditions due to the inability of the gas to react to the flux variations on such short time scales. Thus, the dispersions in the instantaneous conditions from their time-averages explain the same point, where the gas conditions become more disperse from the time averaged conditions as the period increase.

Figure 4.27 shows the results of a model of a binary system with period of 15 yrs and occultation time of 6 yrs. The figure shows the temperature profiles over a complete cycle for the binary system when it is face-on to the observer, i.e. the temperature profiles along radial directions with different angles in the binary plane. We assign the zero angle to the flux maximum, i.e. when no light is blocked from either of the stars, and the angles for the different radial directions are considered with respect to that zero angle. The tem-
Figure 4.26  Temperature profiles of a constant $10^3 \text{cm}^{-3}$ density PN ionized by a 50,000 K black body primary star, eclipsed by a secondary 80% dimmer than the primary. The binary periods, $P$, and eclipsing times, $t_e$, are indicated in each panels. The green lines are the steady-state solutions when ionized by the primary star. The blue lines are the average temperatures from the time-dependent calculation. The red lines indicate the maximum and minimum instantaneous temperatures.
perature profile of the spectral maximum shows the lowest inner peak and flatter profile. The other lines show the temperature profiles as seen from different angles. Note that the spectral maximum showing the lowest peak in temperature profiles is out of phase with the binary cycle due to the thermal front propagation time. Thus, one can expect to see large temperature fluctuations in symmetric PNe powered by binaries near face-on to the observer.

In Figure 4.28 we show the time-dependent effects in the time-averaged temperature weighted by the emissivity of collisionally excited lines, such as [N II], [O III], and [S III], as well as that of recombination lines, such as H I and He I. Here we consider two cases, one with constant stellar temperatures in the two stars and luminosity dropping by 80\% during eclipsing time, the other case with constant luminosity, but varying black body temperature (50,000 K principal and 30,000 K secondary). In either case, we use the rectangular function shown in figure 4.25 to represent the variations in the ionizing flux. The results show that the average temperature weighted by the emissivity of the different lines fluctuate about their averages on different scales, with the collisional lines, such as [N II], showing larger amplitudes.
Figure 4.27  Temperature profiles of PN ionized by a binary with period 15 yrs and occultation time of 6 yrs. The temperatures are for various radial directions starting with the spectral maximum (black curve) and three additional radii rotated from that maximum by the angles indicated in the figure.
Figure 4.28  Temperature averages along the radial direction weighted by the line fluxes of H I and He I (recombination) and [N II], [O III], and [S III] (collisional). The left panels show the case of constant temperature in the two stars and luminosity dropping by 80\% during occultation. The right panels show the case of constant luminosity, but varying black body temperature (50,000K principal and 30,000K secondary)
CHAPTER V

SUMMARY OF MAJOR CONCLUSIONS

Non-equilibrium nebular conditions are triggered by variations in the ionizing flux, which can be a result of variations in the intrinsic luminosity/temperature of the ionizing source or some dynamical activity. Thus, non-equilibrium time-dependent photoionization (TDP) is found in a large variety of astronomical objects, yet it has received little attention thus far. In the absence of a time-dependent photoionization treatment, it has been assumed that the time-averaged conditions are the same as the steady state corresponding to a mean flux. However, this is not correct because the response of a photoionized gas to variations in the ionizing flux is highly non-linear. Therefore, our research aimed to study the time-dependent photoionization of astrophysical plasmas. As a first approach to the problem, we have developed a basic time-dependent photoionization code (TDP) to study the behavior of non-equilibrium, pure hydrogen photoionized plasmas. Furthermore, in order to build deeper understanding of the time-dependent photoionization problem, we have developed a more realistic general purpose time-dependent photoionization modeling code (TDXSTAR) capable of making quantitative predictions of the physical conditions of nebulae composed of mixtures of chemical elements from hydrogen (Z=1) to Zinc (Z=28) and subjected to varying ionizing flux. We used the two codes (TDP and TDXSTAR) to run simulations of non-equilibrium photoionized nebulae, and here we summarize the major conclusions.
• **TDP Code:**

The physical model of the problem is assumed as a slab of pure hydrogen subjected to varying ionizing flux. The TDP code solves the energy balance, ionization balance, and radiation transfer equations in their full time-dependent form. Though simple model was used to develop the TDP code, it was important in building a general picture of the rather complex photoionization modeling problem.

TDP simulations of constant density slabs show that ionization/heating fronts are formed and propagate at different time scales across the slab, from the illuminated face of the cloud to the Ionization Front (IF). It was shown that the size of the ionized region scales up with the ionization parameter and the evolution of the physical conditions of the plasma is very different from steady-state conditions, thus the instantaneous physical conditions can not be reproduced by assuming sequence of steady-state solutions.

Simulations of slabs initially at pressure equilibrium show that thermal and pressure fronts are formed and propagate across the slab at speeds proportional to the magnitude of the change in the ionizing flux. In contrast, a sudden drop in the ionizing flux yields cooling/recombination fronts recede at speeds proportional to the recombination rates. In either case, these fronts often travel at supersonic speeds and form large pressure imbalance that is expected to trigger important dynamical effects in the nebula.

In addition, we carried out simulations assuming periodic variations in the ionizing radiation. The results show that time averaged conditions are different from any steady-state solution and are characterized by over-ionization and much wider IFs compared with
the steady-state conditions corresponding to the mean flux. The instantaneous physical conditions are, roughly, fluctuating about the time averaged conditions with dispersions, which are asynchronous along the cloud and proportional to the period of the ionizing flux. This is due to the non-linear nature of the ionization/thermal front propagation times and the equilibration time across the cloud.

- **TDXSTAR Code:**

As initial verification of the TDXSTAR code, we carried out simulations of models similar to those performed by TDP code with constant density slab subjected to varying ionizing flux. TDXSTAR results are qualitatively in a good agreement with the TDP, code leading to the same general conclusions. Here we summarize some of the most important common conclusions.

1. A rise in the flux yields thermal/ionization fronts propagating along the cloud at different time scales across the slab.

2. The instantaneous conditions of the gas are different from any steady-state solution and can not be reproduced by a sequence of steady state solutions.

3. Periodic variations in the ionizing flux yield time-averaged conditions different from the steady-state corresponding to the mean flux; the time-averaged conditions are characterized by over-ionization and much wider IFs compared with the steady-state pertaining the mean flux.

4. The instantaneous conditions are asynchronous along the slab and disperse around their time averages with dispersions proportional to the period of the ionizing flux.
Further, we used TDXSTAR code to run a grid of models, modified versions of Harrington & Marionni [7] models of planetary nebulae ionized by a central star with a fixed luminosity but decreasing stellar temperature. Our models are intended for a qualitative study of the general behavior of the time-dependent effects in PNe as well as further validation of our results of TDXSTAR code. It was found that spectral lines experience different effects, while some lines intensities rise, others decline, and some may initially rise and then later in time decline. For instance, the recombination line He II $\lambda$ 4686, continue to decline at roughly the same rate, making it a good indicator for the recombination rates of the doubly ionized species. While the recombination lines [OII]$\lambda$ 3726 + 3729 experience two phases of variations, the flux of the line increases due to the increasing number of O$^{2+}$, and then declines due to the fact that the star has ceased to emit ionizing photons and consequently the gas temperature has decreased. In contrast, the collisionally excited lines, such as [Ne III] $\lambda$ 3846 and $\lambda$ 3846, continue to decline, mainly, due to decrease in the gas temperate. They start to decline slowly because the star still able to emit ionizing photons and heat the gas, and then they decline faster due to the decrease in the gas temperature when the star ceases to emit ionizing radiation.

Further, we studied the effects of the different physical parameters on the evolution of the observed spectra. Though recombination and cooling rates scales as $n_e^2$, our results show that the models with higher density decline slower because our models are optically thick with ten times higher densities than that in Harrington & Marionni [7] models. Thus, cooling is suppressed by absorption of $Lyman_\alpha$ lines at such high densities. Furthermore, we studied different models with different inner radii, the distance from the ionizing source
to the illuminated face of the nebula, and found no major difference on the spectral lines
evolution rates due to the fact that, at a fixed ionization parameter, luminosity and inner
radius scale in a way such that the radiation field at the inner face remains constant, thus
maintaining similar conditions across the nebula. In addition, we studied the effects of
the initial stellar temperature on the evolution of the spectral lines and found that higher
initial stellar temperature yield more intense forbidden lines due to the higher electron
temperature.

We studied the temperature fluctuations and the systematic discrepancies in ionic abund-
dances derived from recombination and collisionally excited lines in H II regions and PNe.

We used TDXSTAR to study the physical conditions of PNe and H II regions ionized
by binary systems. Our model comprises concentric spherical shells of gas with constant
density and solar chemical composition ionized by central binary system. A rectangular
function was used to simulate the ionizing flux variations. We investigated the physical
conditions of the gas with the binary edge-on to the observer, in particular, the gas elec-
tron temperature and the temperatures averages weighted by the flux of collisionally and
recombination excited lines.

Simulations of PNe ionized by central binary stars of various periods and eclipsing
times showed that, unlike monotonically increasing temperature in the steady-state temper-
ature profile, temperature profiles of nebulae ionized by binary systems leads to a double
peaked and, in average, flatter profile. The size of the peaks and duration are proportional
to the period of the central binary and inversely proportional to the occultation time of the
primary (brighter) star. This is due to the fact that longer exposure to the ionizing flux
drives the gas conditions to states corresponding to the flux maximum. In contrast, binaries with short periods, in order of days, did not affect the conditions of the gas for the fact that the gas did not have enough time to respond to the flux variations.

We studied the temperature profiles along the radial direction from different angles in the binary plane over a complete cycle and the results show that temperature profiles are out of phase with the binary cycle due to the propagation times of thermal/cooling and ionization/recombination fronts produced by the flux variations.

In addition, we studied the time-dependent effects of binaries with different periods on the temperature averages weighted by collisional and recombinational lines. The results show that all the temperature averages fluctuate around mean values. However, temperature averaged over collisional lines, such as [N II] emission, have larger amplitudes. This leads to the conclusion that using single temperature to reproduce the observed spectra of such systems is expected to yield discrepancies in the elemental abundances. Thus, temperature fluctuations and discrepancies in elemental abundances could be a result of time-dependent effects triggered by the central binary stars.

To sum up, our above studies illustrate that effects of non-equilibrium photoionization of gaseous nebula are present and of significant importance in various cases of general interest in astrophysics. This has emphasized the crucial need for time-dependent photoionization modelings. Therefore, we developed our TDXSTAR code to be used for analysis of non-equilibrium systems, photoionized by a varying ionizing flux.
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