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Photoionization modelling of planetary nebulae with realistic density distribution using detailed method for diffuse radiation calculation and Outward Only approximation

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The approximate methods to calculate the diffuse ionizing radiation (DIR) during the photoionization modelling (PhM) of the nebular environments are frequently used with purpose to increase the calculation speed of modern photoionization codes as well as for simplification of their calculation algorithms. The most popular Outward Only method in many cases gives the satisfactory calculation precision and speed. However, in our previous studies it was shown that even for nebular environments with constant density the calculation errors, related to usage of approximate method of DIR, are significant for spatially extended or optically thin objects. However, constant density is a bit rough assumption. In present work to compare the detailed method of DIR calculation with Outward Only one we used more realistic density distribution for planetary nebulae proposed by Golovatyy & Mal'kov [6]. Using optimal photoionization models for IC 5117 and NGC 7293, obtained by Melekh et al. [8] and calculated in Outward Only approximation, we recalculated them using detailed method of DIR calculation. While IC 5117 is the most compact (young) and dense planetary nebula from sample used by Golovatyy & Mal'kov [6], NGC 7293 is the most extended (old) with lowest density one from the same sample.

We compared PhM results for these PNe obtained using Outward Only approximation and detailed method of DIR treatment. It was concluded that largest differences in ionization structure of nebula caused by differences in DIR calculation methods are in outer part of PN – at radii larger than maximal density radius. Therefore, [N II], [O II] and [S II] and other emission lines, that achieve the maximal emissivities in outer part of PNe, are the most sensitive to DIR calculation method.

Key words: planetary nebulae: individual: IC 5117, NGC 7293, diffuse ionizing radiation, photoionization modelling.

INTRODUCTION

Physical conditions in nebulae (planetary nebulae, large H II regions) are usually obtained using so-called diagnostic method, that allows to obtain the average electron temperature T_e and density N_e from different emission line intensities ratios (see, i.e., DIAGN method [5]). However, in the case of diagnostic methods values of T_e and N_e are constant within investigated ionization zone. For detailed analysis of the ionization structure of nebular environment the transfer of the ionizing radiation should be calculated, taking into account all elementary processes in nebular plasmas important for such transfer. Such calculations are performed during PhM of nebular environment.

In the case of nebulae with compact ionization source (i.e star, compact stars cluster, etc.) radiation can be separated into two components:

- direct component, comming from ionizing source;
- diffuse component, originating in nebular environment.

While transfer of the direct component of the ionizing radiation can be easily calculated (because of no source terms), the diffuse radiation transfer calculation is a very time consuming even for modern supercomputers, since it requires the iterative process of ionizing radiation flux integration over volume in each elementary cell of nebula environment. For time saving purposes the approximate methods of diffuse radiation calculation are frequently used. The most popular are On The Spot (OTS) approximation, based on the assumption that ionizing radiation is consumed in the same volume where it was emitted, and Outward Only approximation, based on the assumption that ionizing radiation is propagating only in radial direction – from ionizing source to outer surface of object. However, OTS method is

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good only in the case of optically thick objects. Outward Only approximation is more precise, however it can be inaccurate in case of objects with complicated morphology. For example, dense clumps cause shaded regions behind of them and non-radial DIR can play main role in formation of the ionization structure of these shaded regions.

Detailed methods for DIR calculation require much more computer time than approximate ones. The detailed review of previous methods applicable for DIR calculation in precise way can be found in our previous paper [1]. The most modern methods aiming to the reduction of computational time during DIR calculation can be found in papers of Lucy [7] and Ercolano et al. [3] (code `Mocassin`) where problem of DIR transfer was solved by considering the propagation within nebular environment of the ionizing photons packages, on the base of Monte Carlo approach. But, from our point of view, statistical basement of these methods does not allow to treat them as detailed.

To avoid usage of approximate methods for DIR calculation and reduce time, required for PhM, we developed our method (so-called `DiffRay`) of diffuse ionizing radiation calculation transfer in detailed way.

In paper [1] we used this method to test the reliability of Outward Only approximation for planetary nebulae (PNe) and H II regions. It was shown that usage of detailed method is more important for H II regions than for PNe, because of lower density and, correspondingly, optical thickness for DIR. But all calculations in [1] were done for constant density of nebular gas ($n_e = 3000$ cm^{-3} for PNe and $n_e = 100$ cm^{-3} for H II regions correspondingly).

In present work we continue the work on testing the reliability of Outward Only approximation for PNe. For this purpose we use more realistic density distribution for PNe proposed by Golovatyy & Mal'kov [6].

METHOD FOR DIFFUSE RADIATION CALCULATION

The detailed description of PhM algorithm as well as our approach to calculate the DIR in nebular objects can be found in paper [1], therefore in this section we describe only the main points of our approach to calculate the DIR in a detailed way.

In our approach the procedure of integration of DIR over various paths in nebula is performed outside of PhM code's core with its internal iterations. It allows us to reduce the computer time consumption due to decrease the number of calls of integration per model calculation.

The scheme of algorithm of method is shown in Figure 1. Let's consider briefly the steps of this algorithm:

1. Reading the data, such as required precision, maximum iterations, etc.
2. Running PhM code in Outward Only mode, generating and saving emissivity and opacity maps.
3. Running integration procedure using previously generated emissivity maps.
4. Running PhM code using fluxes obtained after step 3. Generating and saving the new emissivity and opacity maps.
5. Check the difference $\delta T(r)$ between average electron temperature distributions obtained in current iteration and in the previous one, $T_{prev}(r)$. If $\delta T(r)/T_{prev}(r) \geq 2\%$ (adopted precision in current research), then go to step 3.
6. Printing radiative fluxes and ionization structure obtained from PhM on last iteration.

For implementation of integration procedure (DIR fluxes calculation – step 3 in Figure 1) the `DiffRay` procedure was developed. The algorithm of `DiffRay` is given in Figure 2. It consists of the following steps:

1. Initialization of integration steps $\Delta\phi$ and $\Delta\theta$ for angles (see detailed description of these parameters in paper [1]), reading emissivity and opacity maps that should be integrated.
2. Integration of emissivities (DIR fluxes calculation) for each elementary volume of nebula environment.
3. Comparison of differences between fluxes ΔJ, obtained during current iteration and in previous one. If required precision is satisfied (2% in current research), then go to step 5. Elsewise go to step 4.
4. Decreasing of the integration step 4 and transition to step 2.
5. Printing the diffuse radiative fluxes for PhM code. Exit.

Such approach provides us couple of obvious following advantages:

1. *Universality.* This method can be implemented into various PhM codes without serious interventions into its core.
2. *Speed.* Putting the large procedure for diffuse radiation integration beyond the core of PhM code with its inner iterative calculations. It provides faster calculations.
3. *Safety.* Minimal interventions into code's core minimize the risk of making some mistakes.

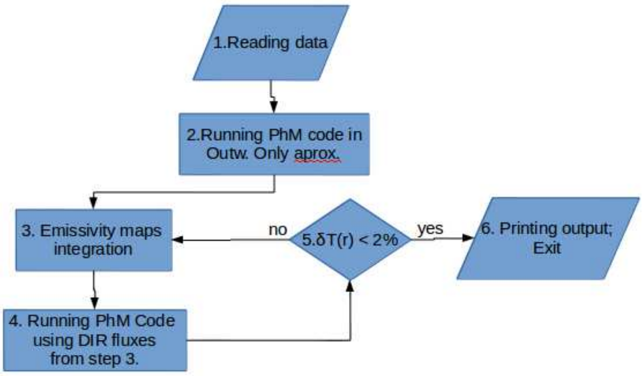

Fig. 1: Our algorithm for DIR calculation.

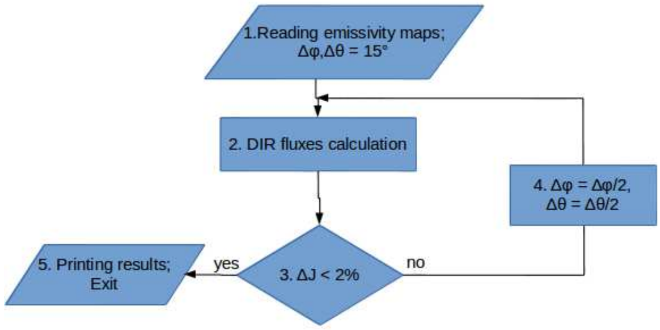

Fig. 2: `DiffRay` algorithm (step 3 in Figure 1)

RADIAL DENSITY DISTRIBUTION

In our previous paper [1] the photoionization models of PNe and H II regions with constant density distribution were calculated using both Outward Only approximation and detailed method for DIR calculation. Obtained results showed that detailed method is recommended for large and optically thin objects. However, constant density assumption is a bit idealistic. In present work the more realistic radial density distribution in PNe, proposed by Golovatyy & Mal'kov, was used :

$$n_H(r) = \frac{x^2\left(1+3e^{-1.2x}\right)}{\left(x^2-1\right)^2+0.36r_c^{-0.43}}\frac{A}{r_c^2}, \qquad (1)$$

where r_c corresponds to a radius that is close to the maximum of gas density radial distribution, $x = r/r_c$, A – parameter that characterizes the intensity of outflow of matter from the progenitor star in the process of PN envelope formation. Details on this distribution can be found in [6]. To derive the Eq. (1) Golovatyy & Mal'kov have used the sample of spherical-symmetrical PNe with various sizes and densities.

For our calculations we used Garry Ferland's code `Cloudy` [4] upgraded by our procedure for detailed calculation of DIR.

RESULTS

In order to test the reliability of Outward Only approximation in the case of PhM of PNe with density distribution defined by Golovatyy-Mal'kov's semi-empirical law (Eq. (1)) we used values of input parameters from the optimal photoionization models, obtained in [8], of the most compact (young) and dense PN IC 5117 as well as the most extended (old) PN NGC 7293 with lowest density from the PNe sample by Golovatyy & Mal'kov [6]. Adopted density distribution parameters in these models are following: $r_c = 0.0032$ pc, $A = 2.05$, $n_H(r_c) = 90074\,\mathrm{cm}^{-3}$ for IC 5117, and $r_c = 0.27$ pc, $A = 1.60$, $n_H(r_c) = 67\,\mathrm{cm}^{-3}$ for NGC 7293. Thus, we tested the reliability of Outward Only approximation in the case of PhM of PNe in a very wide range of densities using only two PNe.

For each of these two PNe we have calculated two photoionization models: (i) with the use of Outward Only approximation, and (ii) applying our detailed method for DIR calculation. In integration procedure of detailed method the precision of 2% was adopted.

It must be noted, that during PhM in Outward Only approximation using code `Cloudy C08.00` we strongly recommend to set the maximal allowed width of zone manually (i.e. we have set this value of $10^{13.5}$ cm), because at large density gradients adaptive algorithm in `Cloudy` works incorrectly.

As a result, the synthetic emission line spectra from photoionization models as well as the maps of ionization structure for both cases of DIR calculation mentioned above were obtained and compared. In Table 1 the comparisons of outer radius, R_{ion}, luminosities in H_β line, L(Hβ), and relative intensities (adopted I(Hβ) = 1) of some important recombination (He I λ4471, He I λ5876, He II λ4686) and nebular ([O II] λ3727, [O III] λ5007, [O III] λ4959, [N II] λ6548, [N II] λ6584, [S II] λ6716, [S II] λ6731, [S III] λ9532, [S III] λ9069) and auroral ([O III] λ4363, [N II] λ5755, [S II] λ4070, [S II] λ4078) emission lines, obtained from PhM of PNe IC 5117 and NGC 7293 in Outward Only approximation and using our Detailed method for DIR calculation are given.

It can be seen that for more extended (old) and low density PN NGC 7293 (see Figure 3 and Table 1) the deviations between results obtained using different methods for DIR calculation are within 4.4%. Maximal deviations were obtained for [S II] (up to 4.4%). For oxygen emission lines the maximal deviation was obtained for line [O II] 3727 Å (3.1%), differences between [O III] and [S III] lines are within 2%. The deviations between recombination lines of H I, He I and He II are practically absent.

Table 1: Comparison of PhM results (see text) of PNe IC5117 and NGC7293, obtained in Outward Only approximation and using Detailed method for DIR calculation. The deviations of Outward Only models from corresponding Detailed ones are given in %.

Model:	IC 5117			NGC 7293		
Parameter	Outward Only	Detailed	Deviation, %	Outward Only	Detailed	Deviation, %
R_{out}, [pc]	0.013	0.013	0.0	0.448	0.448	0.0
lg L(Hβ)	30.56	30.56	0.0	31.83	31.83	0.0
[O II] λ3727/H$_\beta$	0.123	0.162	24	7.511	7.748	3.1
[O III] λ5007/H$_\beta$	12.55	12.52	−0.2	5.172	5.083	−1.8
[O III] λ4959/H$_\beta$	4.163	4.153	−0.2	1.718	1.688	−1.8
[O III] λ4363/H$_\beta$	0.200	0.201	0.5	0.049	0.049	0.0
He I λ4471/H$_\beta$	0.054	0.054	0.0	0.067	0.067	0.0
He I λ5876/H$_\beta$	0.184	0.185	0.5	0.185	0.185	0.0
He II λ4686/H$_\beta$	0.096	0.095	−1.1	0.049	0.049	0.0
[N II] λ6548/H$_\beta$	0.209	0.283	26	2.463	2.533	2.8
[N II] λ6584/H$_\beta$	0.612	0.837	27	7.270	7.467	2.6
[N II] λ5755/H$_\beta$	0.029	0.037	22	0.125	0.129	3.1
[S III] λ9532/H$_\beta$	0.630	0.646	2.5	0.136	0.135	−0.7
[S III] λ9069/H$_\beta$	0.253	0.259	2.3	0.054	0.054	0.0
[S II] λ6716/H$_\beta$	0.012	0.015	20	0.101	0.105	3.8
[S II] λ6731/H$_\beta$	0.032	0.032	0.0	0.074	0.077	3.9
[S II] λ4070/H$_\beta$	0.032	0.039	18	0.109	0.114	4.4
[S II] λ4078/H$_\beta$	0.010	0.013	23	0.036	0.037	2.7

Large discrepancies between the Outward Only PhM results and DIR were obtained for very dense and compact (young) PN IC 5117 (see Table 1 and Figure 3). The largest deviations (up to 27%) were obtained for [N II], [O II], and [S II] lines. In the case of [S II] lines these deviations can be explained by the difference between electron density values, obtained using different methods of diffuse radiation treatment. In the case of detailed method the electron density in outer part of object is lower, and, consequently, [S II] 6716 / [S II] 6731 ratio is higher. It can be easily seen in Table 1 that line [S II] 6716 Å is slightly higher in the case of detailed method, while [S II] 6731 line intensity has the same value as in the case of Outward Only one. Due to high electron densities used to model PN IC 5117 the [S II] 6716 / [S II] 6731 ratio decreases much more slower with radius, than at lower values of n_e (see for example Table 3.2 in [2]). It is because at higher electron densities the collisional deactivation of corresponding levels is much more effective than at lower ones. Actually, the values of this ratio are very close to lowest values of n_e available for determination. For this electron densities range the difference in n_e values causes only the difference in populations of level $^2D_{5/2}$ of S II, while $^2D_{3/2}$ one has actually the same population (line [S II] 6716 corresponds to the transition $^2D_{5/2}$ — $^4S_{3/2}$, while line [S II] 6731 corresponds to $^2D_{3/2}$ — $^4S_{3/2}$ one).

On the other hand, the recombination lines as well as high excitation forbidden lines have much lower deviations: not larger than 0.5% in the case of [O III] and not larger than 2.5% for [S III] lines.

While the best reproduced recombination emission lines as well as [O III] ones originate mainly from inner parts of nebula (see Figures 4 and 5), the emissivities of [N II], [O II] and [S II] lines are increase in outward directions. The discrepancies between results DIR calculations by two methods are expected to rise in outer part of nebula, therefore these emission lines have maximal deviations. In the case of NGC 7293 [S III] 9532 line forms mainly close to the density maximum, while in the case of IC 5117 this line emissivities have plateau beyond the density maximum. While the best reproduced recombination emission lines as well as [O III] ones originate mainly from the inner parts of nebula (see Figures 4 and 5), the emissivities of [N II], [O II] and [S II] lines are increase in the outward directions. The discrepancies between results of DIR calculations by two methods are expected to rise in the outer part of nebula, therefore these emission lines have maximal deviations. For example, [S III] 9532 emission line forms mainly close to the density maximum in

NGC 7293, while in the case of IC 5117 this line emissivities have a plateau beyond the density maximum and along this plateau one cannot distinguish emissivities obtained by two different methods for DIR calculation.

In the case of low density PN NGC 7293 direct ionizing radiation dominates over the DIR across all nebular volume. On the other hand, in the case of very dense (at maximum — see Figure 3) PN IC 5117 situation in outer part (at radii higher than denity maximum) is opposite. Therefore, the difference in DIR calculations plays in the case of IC 5117 much larger role in formation of emission line emissivities causing the larger deviations of PhM results obtained in Outward Only approximation from Detailed one.

CONCLUSIONS

We developed our approach to calculate the diffuse ionizing radiation of nebular environments in a detailed way and used it to test the reliability of Outward Only approximation during PhM of planetary nebulae. For this purpose we used radial density distribution defined by Golovatyy & Mal'kov [6] after analysis of isophotes maps in Hβ line. Golovatyy & Mal'kov [6] compiled the sample of PNe close to spherical symmetry with different sizes (ages) and densities. For our task we selected two PNe from this sample – the most compact (young) and dense IC 5117 as well as the most extended (old) with lowest density NGC 7293. We used values of input parameters from optimal photoionizaion models of these PNe obtained in [8].

From analysis of modelling results it was concluded that the largest distinctions in ionization structure of nebula due to the differences in DIR calculation methods are in the outer part of PN – at radii larger than maximal density radius. Lines of larger ionization stages ([O III] etc.) originate mainly from the inner part of the nebula and close to the density maximum, so discrepancies in their intensities, obtained in Outward Only approximation and from Detailed method are very low. On the other hand, the emissivities of [N II], [O II] and [S II] lines are increasing in outward directions in nebula. Therefore, they are very sensitive to differences in DIR calculation methods. In PNe with higher maximal densities in its radial distributions, the role of DIR in outer parts increases, because of higher optical thickness for direct ionizing radiation.

It should be noted that deviations of PhM results obtained in Outward Only approximation (see columns Deviation in Table 1) from Detailed one must be taken into account during comparison of modelling results with observed data or during derivation of chemical compositions determination using PhM in Outward only approximation.

REFERENCES

[1] Buhajenko O. S., Melekh B. Ya. 2016, Journal of Physical Studies, 20/4, 4901.

[2] Dopita M. A., Sutherland R. S. 2002, *Astrophysics of the Diffuse Universe*, Springer Science & Business Media.

[3] Ercolano B., Barlow M. J., Storey P. J., Lui X.-W. 2002, MNRAS, 340, 1136.

[4] Ferland G. J. 2008, *Hazy, a Brief Introduction to Cloudy*, Physics Department Internal Report, University of Kentucky[1].

[5] Golovatyi V. V., Dmiterko V. I., Mal'kov Yu. F., & Rokach O. V. 1993, Astronomical Report, 37, 346.

[6] Golovatyi V. V., Mal'kov Y. F. 1992, Soviet Ast., 36, 599.

[7] Lucy L. B. 1999, A&A, 344, 282.

[8] Melekh B. Ya., Demchyna A. V., Holovatyi V. V. 2015, Kinematics and Physics of Celestial Bodies, 31/ 2, 73.

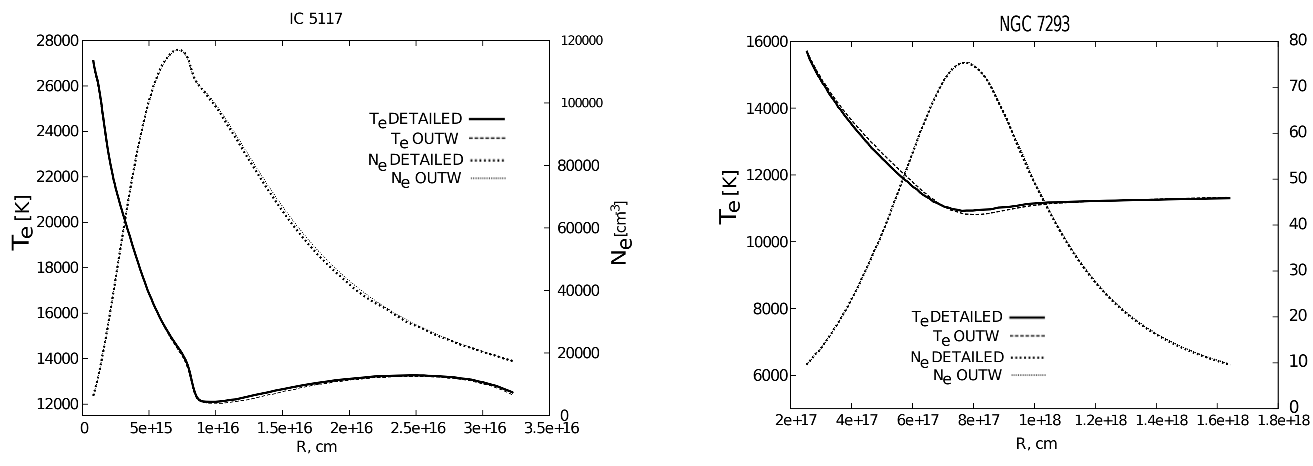

Fig. 3: Radial distributions of T_e and N_e from PhM of PNe IC 5117 and NGC 7293, obtained using Outward Only approximation (OUTW) and Detailed method for DIR calculation.

[1] http://www.nublado.org

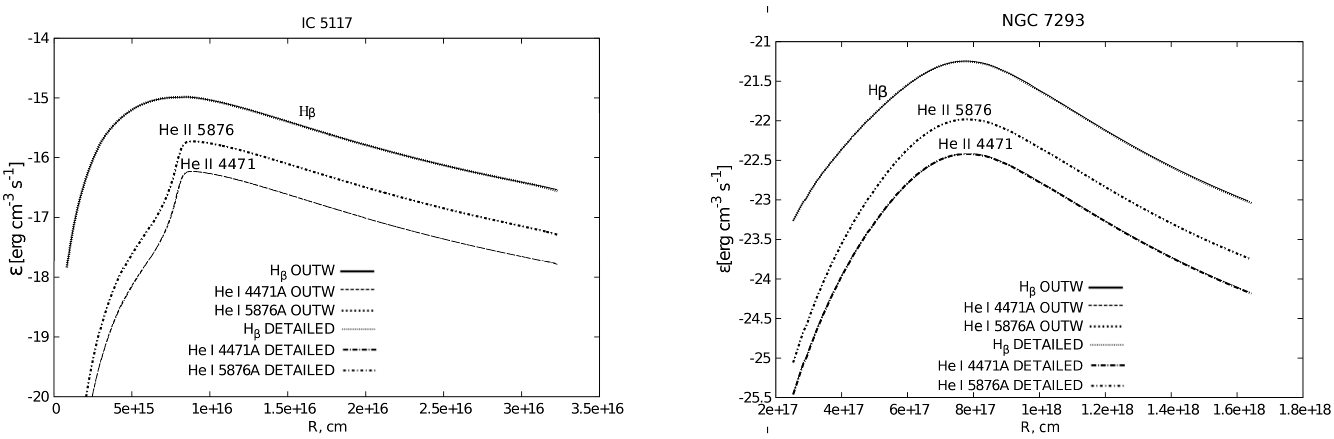

Fig. 4: Radial distributions of important recombination emission line emissivities obtained during PhM of PNe IC 5117 and NGC 7293 in Outward Only approximation (OUTW) and using Detailed method for DIR calculation.

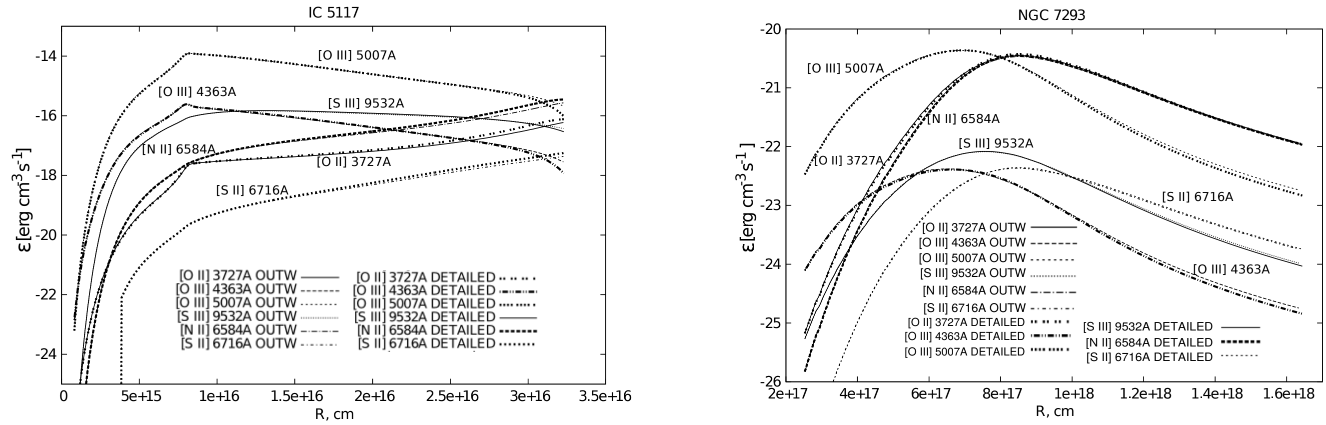

Fig. 5: Radial distributions of important forbidden (nebular and auroral) emission line emissivities obtained during PhM of PNe IC 5117 and NGC 7293 in Outward Only approximation (OUTW) and using Detailed method for DIR calculation.