Letter to the Editor

The collision strength of the [Ne v] infrared fine-structure lines*

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Abstract. The calculation of accurate collision strengths for atomic transitions has been a long standing problem in quantitative spectroscopy. Most modern calculations are based on the R-matrix method and problems pertaining to the use of this method have led to a discussion of the accuracy of these results. More in particular, based on an analysis of the spectra of NGC 3918 and NGC 6302, Clegg et al. (1987) and Oliva et al. (1996) have questioned R-matrix calculations for the infrared [Ne v] fine-structure transitions. Using improved flux measurements for the [Ne v] lines, we show that the conclusion that these collision strengths would be too high, is not correct. The discrepancies found by Clegg et al. (1987) can be explained by the inaccuracy of the [Ne v] 342.6 nm flux they adopted. The discrepancies found by Oliva et al. (1996) can be explained by the inaccuracy of the LRS flux for the [Ne v] 14.32 µm line. Based on the data presented in this paper there is no reason to assume that there are any problems with the R-matrix calculations for Ne4+ of Lennon & Burke (1994). We show that the data are accurate at the 30 % level or better. This confirms the validity of the close coupling method.

Key words: atomic data – plasmas – ISM: planetary nebulae: individual: NGC 3918 – ISM: planetary nebulae: individual: NGC 6302 – ISM: planetary nebulae: individual: NGC 7027 – infrared: ISM: lines and bands

1. Introduction

The calculation of accurate collision strengths for atomic transitions has been a long standing problem in the field of quantitative spectroscopy. Any calculation involving atoms in non-LTE conditions requires the knowledge of vast numbers of collision strengths in order to make these calculations realistic and accurate. Until recently the computing power was simply not available to calculate collision strengths in a systematic way. One either had to resort to simpler and more approximate methods or one had to limit the calculations to only the most important transitions. This situation has now changed with the start of the Iron Project (Hummer et al. 1993), which aims to produce a large database of accurately calculated collision strengths.

The collision strength for an atomic transition depends strongly on the energy of the colliding electron and shows many resonances (e.g., Aggarwal 1984). Such resonances occur when the total energy of the target ion and the colliding electron correspond to an auto-ionizing state. In order to calculate these resonances accurately, a fine grid of energy points is necessary. This is a type of problem for which R-matrix methods are very well suited. However, a source of uncertainty in these calculations is that the energies of most auto-ionizing states have not been measured in the laboratory and therefore need to be derived from calculations. It is a well known fact that the resulting energies are not very accurate and hence the positions of the resonances are also uncertain. Since the collision strengths are usually folded with a Maxwellian energy distribution, this is not a major problem for high temperature (i.e., X-ray) plasmas where the distribution is much broader than the uncertainty in the position of the resonances. However, for low temperature (e.g., photo-ionized) plasmas this can lead to problems if a resonance is present near the threshold energy for the transition. If only the high-energy tail of the Maxwellian distribution is capable of inducing a collisional transition, then a small shift in the position of a near-threshold resonance can have a severe impact on the effective collision strength. This effect would be even more pronounced if the resonance shifts below the transition threshold and disappears completely.

The inclusion of resonances in the calculation of collision strengths can lead to much higher values than were previously published (see Table 2 in Oliva et al. 1996). This is also illustrated in Table 1, where we show various calculations of the effective collision strength of transitions within the ground term of Ne4+. One can see that the R-matrix calculations of Aggarwal (1983) and Lennon & Burke (1991, 1994) yield substantially larger results than the previous calculations. This is caused by the presence of a large complex of strong resonances at low

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Table 1. Comparison of various determinations of the effective collision strengths for transitions within the ground term of Ne\(^{3+}\). The values are for \(T_e = 10000\) K.

| ref.            | \(\ ^3P_0 - ^3P_1\) | \(\ ^3P_0 - ^3P_2\) | \(\ ^3P_0 - ^3P_3\) |
|-----------------|----------------------|----------------------|----------------------|
| Blaha (1969)    | 0.251                | 0.132                | 0.611                |
| Osterbrock (1974)| 0.23                 | 0.11                 | 0.53                 |
| Aggarwal (1983) | 1.463                | 1.810                | 5.901                |
| Lennon & Burke (1991) | 1.401               | 1.766                | 5.725                |
| Lennon & Burke (1994) | 1.408               | 1.810                | 5.832                |

Table 2. Log of the SWS observations. The AOT’s are described in de Graauw et al. (1996), SWS01–4 stands for SWS01 speed 4.

| Source    | Date      | Rev. | AOT     | \(F(14.32)\) 10^{-14} W m^{-2} | \(F(24.32)\) 10^{-14} W m^{-2} |
|-----------|-----------|------|---------|-----------------------------|-----------------------------|
| NGC 7027  | 11 Dec 1995| 24   | SWS01–4 | 160.                        | 47.0                        |
| NGC 7027  | 19 Dec 1995| 32   | SWS02   | 136.                        | 40.9                        |
| NGC 7027  | 6 Nov 1996 | 365  | SWS02   | 141.                        | 47.1                        |
| NGC 6302  | 19 Feb 1996| 94   | SWS01–4 | 65.2                        | 29.7                        |
| NGC 6302  | 20 Feb 1997| 462  | SWS06   | 63.4                        | 30.8                        |

energies (see Fig. 5 in Aggarwal 1984). This large difference has led to a discussion of the validity the R-matrix calculations (Clegg et al. 1987, C87; Oliva et al. 1996, O96). Both authors tested the calculations by comparing predicted flux ratios with observations and both concluded that the R-matrix calculations yielded results that are too high. Nebulae offer powerful tests of atomic physics, and have revealed incomplete treatment in the past (Péquignot et al. 1978, Harrington et al. 1980). However, both C87 and O96 base their conclusions on only one nebula and both include LRS data in their analysis. Since the accuracy of LRS data is limited to approximately 30% (Pottasch et al. 1986), a re-analysis based on more accurate SWS data is warranted. In this paper we will present a test of the R-matrix calculations for Ne\(^{3+}\) by applying them to observational data of NGC 3918, NGC 6302 (the nebulae studied by C87 and O96, respectively) and NGC 7027. This will yield a larger and more accurate sample for the discussion.

2. The observational data and analysis

Several SWS observations were obtained for the objects studied in this paper. A log of the observations is shown in Table 2. The instrument is described in de Graauw et al. (1996). The observations used three different templates: SWS01 – a spectral scan from 2.4 \(\mu\)m to 45 \(\mu\)m, SWS02 – a set of grating scans of individual lines, and SWS06 – a high resolution grating scan. All SWS spectra of NGC 7027 were obtained during calibration time. The complete SWS06 spectrum of NGC 6302 is published in Beintema & Pottasch (1999). An SWS spectrum of NGC 3918 was also obtained, but not used. Due to inaccurate pointing the source was partially outside the aperture.

The line fluxes were measured in spectra reduced with the SWS interactive-analysis software. The line fluxes were virtually identical to those derived from the standard ISO auto-analysis products. The various SWS measurements were subsequently averaged. Table 3 shows the dereddened line fluxes we have adopted for our study. The values adopted by C87 and O96 are also shown for comparison. The extinction corrected [Ne \(^{v}\)] 342.6 nm fluxes were taken from the original publications. Both for NGC 7027 and NGC 6302 the dereddening is complicated by the fact that the extinction varies over the nebula. The correction for the blend in NGC 3918 is discussed below. The infrared line fluxes were dereddened using the law from Mathis (1990).

To calculate the diagnostic diagrams we used the effective collision strengths given in Lennon & Burke (1994) and adopted the transition probabilities from Baluja (1985). We used a 5-level atom to calculate the relative level populations. The line flux ratios we included contributions from the absolute calibration accuracy of the UV and IR data, the internal calibration accuracy of the SWS data and the uncertainty in the extinction correction. We will now discuss the results for each nebula separately.

2.1. NGC 7027

We have included this nebula in our sample because it is bright and well studied. This assures that accurate values for the...
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Table 5. The temperature stratification in NGC 7027, derived from our photo-ionization model (Beintema et al. 1996). The temperature is defined as $\int n_e n_{ion} v_{ion} d\nu / \int n_e n_{ion} d\nu$.

| ion | $\chi_{ion}$/eV | $T_e$/K | ion | $\chi_{ion}$/eV | $T_e$/K |
|-----|-----------------|--------|-----|-----------------|--------|
| O$^+$ | 13.62 | 10 450 | O$^{4+}$ | 54.94 | 13 520 |
| N$^+$ | 29.60 | 12 140 | Ar$^{3+}$ | 59.81 | 14 670 |
| Ar$^{2+}$ | 40.74 | 12 990 | Ar$^{4+}$ | 75.02 | 16 180 |
| S$^{2+}$ | 34.83 | 13 100 | Ne$^{3+}$ | 97.12 | 16 350 |
| C$^{2+}$ | 47.89 | 13 440 | Ne$^{4+}$ | 126.2 | 17 990 |

The temperature stratification in NGC 7027, derived from our photo-ionization model (Beintema et al. 1996). The temperature is defined as $\int n_e n_{ion} T_e d\nu / \int n_e n_{ion} d\nu$.

fluxes needed in our analysis are available. Additionally, we have a detailed photo-ionization model (Beintema et al. 1996) which allows us to derive good estimates for the expected electron temperature and density. For a high excitation nebula like NGC 7027, significant temperature stratification of the plasma can be expected. We have illustrated this effect in Table 5 where we show the average electron temperature in various line forming regions. One can see that the electron temperature rises almost monotonically with the ionization potential $\chi_{ion}$. It is important to note that the temperature in the Ne$^{4+}$ region is substantially higher than the temperature in any other line forming region observed in the spectrum. The expected values for the electron temperature and density are based on our photo-ionization model. The analysis of the [Ne v] lines gives a result which deviates less than 3 $\sigma$ from these values.

2.2. NGC 6302

This is the nebula studied by O96. The [Ne v] temperature and density for this nebula were already derived from the SWS06 spectrum by Pottasch & Beintema (1999). In our analysis we will include the SWS01–4 spectrum as well. The expected values for the electron temperature and density are those of O96. Our analysis gives a result which deviates slightly more than 1 $\sigma$ from these values. The preferred temperature of O96 is based on various determinations using ions with lower ionization potentials than Ne$^{4+}$. In view of the discussion in the previous section concerning temperature stratification, this estimate is probably too low. Especially in view of the temperatures derived by O96 from rather low excitation line ratios like [S iii], [Ar iii] and [O iii] which range between 18 100 K and 19 400 K, the [Ne v] temperature may be expected to be considerably higher than 19 000 K. A temperature of 22 000 K is more realistic (see the discussion in Pottasch & Beintema 1999). This value for the temperature is indicated by an arrow in Fig. 1. After this correction the discrepancy is slightly less than 1 $\sigma$.

2.3. NGC 3918

This is the nebula studied by C87. The intensity for the [Ne v] 342.6 nm line is in doubt. C87 quote $I(342.6) = 80$, but it is not clear how this value was obtained. We decided to use the value quoted in Aller & Faulkner (1964) instead. From the discussion in that article it is not clear whether the data were corrected for interstellar extinction. The intensities they quote for other strong blue emission lines compare well with the dereddened intensities given by C87 and we therefore assume that the Aller & Faulkner (1964) data are corrected for interstellar extinction. They give $I(342.6+342.9+344.4) = 60$. The correction for the blend with the O iii 342.9 nm and 344.4 nm Bowen resonance-fluorescence lines is easy, since the O iii 313.3 nm line has been measured by C87. The O iii 313.3 nm, 342.9 nm and 344.4 nm lines all originate from the same upper level $(2s^2 2p 3d^3 P_2^0)$ and the intensity ratio of the lines is simply given by the ratio of the transition probabilities times the photon energy. Using Opacity Project data (Luo et al. 1989) one finds $I(313.3) : I(342.9) : I(344.4)$.

Fig. 1. In these graphs the electron temperature and density derived from the [Ne v] lines is marked with a +. The solid, dashed and dotted lines are the 1 $\sigma$, 2 $\sigma$ and 3 $\sigma$ contours respectively. The expected value of the electron temperature and density, based on either photo-ionization modeling or other line-ratio diagnostics, is indicated with an x. An arrow indicates the estimated increase of the electron temperature if temperature stratification is taken into account. The top row was obtained using the effective collision strengths $\Upsilon$ given by Lennon & Burke (1994), the bottom row was obtained by lowering the $\Upsilon$'s for transitions within the ground term by 30%.
I(344.4) = 10.94 : 1.00 : 2.94. C87 gives I(313.3) = 85. Hence
I(342.9 + 344.4) = 30.6 and I(342.6) = 29.4. This result is
substantially lower than the value used by C87. We were
not able to correct the SWS spectrum accurately for aperture
effects and therefore preferred to use the LRS flux for the [Ne v]
14.32 μm line. To complete the data set, we assumed a value
for the 24.32 μm flux such that the resulting density agreed
with the expected value. None of the flux values we adopted
for this nebula can be considered accurate and re-measurement
is warranted. The expected values for the electron temperature
and density were determined by averaging the data in Table 12
of C87. For the temperature we only used the values derived
from the [Ar v], [Ne iv] and [Ne v] line ratios, for the density
we used all values except those derived from [Mg i], [N iv] and
[O iv] lines. One can see that there is a slightly more than 2 σ
discrepancy for the electron temperature. Again the expected
value for the electron temperature may be underestimated due
to temperature stratification. We think 15 000 K is in all probability
a more realistic, though still conservative, estimate. This value
for the temperature is indicated by an arrow in Fig.1 After this
correction there is a 1.5 σ discrepancy.

3. Discussion
A major advance in atomic theory in the past decade has been
close coupling calculations that include resonances. These new
calculations (carried out with an R-matrix code) can raise the
collision strength by an order of magnitude or more compared to
older calculations. These large differences have led to a discussion
of the validity of these calculations. Nebulae offer powerful laboratories for verifying atomic processes, and two studies
(C87 and O96) used this approach to test the R-matrix calcula-
tions for Ne4++. They found that spectra of planetary nebulae
did not agree with the R-matrix results. This casted doubt on
the validity of close coupling calculations.

In this paper we have redone the analysis carried out
by C87 and O96 using newer, more accurate data. We also
included the well studied nebula NGC 7027 in the analysis to
obtain a larger sample. We found that the expected values of
the electron temperature and density all were within 3 σ of
our results. Hence there is no proof for significant problems
with the R-matrix calculations. On closer inspection one sees
that the largest discrepancy is for NGC 7027, the best
studied nebula. Also the electron temperature derived from our
analysis is systematically higher than the expectation value for
all nebulae. This could point to inaccuracies in the collision
strengths. To check this point further, we have re-analyzed
our sample using effective collision strengths which were
lowered by 30 % for transitions within the 2P ground term.
The results are shown in the bottom row of Fig. They
are in good agreement with the expected values. Hence the
R-matrix calculations for Ne4++ could be off by 30 %, but
certainly not more. We point out that this is significantly
less than the factor ~2.7 suggested by O96. An alternative ex-
planation could be that the [Ne v] 342.6 nm fluxes are system-
atically overestimated due to a problem with the extinction curve,
or a combination of the two effects.

We reach the following main conclusions:

1. The discrepancies found by C87 can be explained by the
inaccuracy of the [Ne v] 342.6 nm flux they adopted. The
discrepancies found by O96 mainly stem from the inaccu-
acy of the LRS measurement of the [Ne v] 14.32 μm line.
2. Based on the data presented in this paper there is no reason

to assume that there are any problems with the collision
strengths for Ne4++ calculated by Lennon & Burke (1994).
Our analysis has shown that the data are accurate at the 30 %
level or better. This confirms the validity of close coupling
calculations.

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