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[O II] line ratios

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ABSTRACT

Based on new calculations, we reconfirm the low- and high-density limits on the forbidden fine-structure line intensity ratio [O II] $I(3729)/I(3726)$: $\lim_{N_e \to 0} = 1.5$ and $\lim_{N_e \to \infty} = 0.35$. Employing [O II] collision strengths calculated using the Breit–Pauli **R**-matrix method, we rule out any significant deviation due to relativistic effects from these canonical values. The present results are in substantial agreement with older calculations by Pradhan, and validate the extensive observational analyses of gaseous nebulae by Copetti & Writzel and Wang et al. that reach the same conclusions. The present theoretical results and the recent observational analyses differ significantly from the calculations by McLaughlin & Bell and Keenan et al. The new Maxwellian averaged effective collision strengths are presented for the 10 transitions among the first five levels to enable computations of [O II] line ratios.

Key words: atomic data – atomic processes – line, formation – ISM: general – H II regions – planetary nebulae: general.

1 INTRODUCTION

The most prominent density diagnostics in astrophysics come from the forbidden fine-structure lines [O II] λλ3729, 3726 and [S II] λλ6716, 6731. Their utility stems from several factors, such as (i) they respectively lie at the blue and the red ends of the optical spectrum, (ii) their atomic structure and hence the density dependence are essentially the same, and (iii) they are quite strong in the spectra of most H II regions owing to the relatively large abundances of oxygen and sulphur. Seaton & Osterbrock (1957) have described the basic physics of these forbidden transitions. High-accuracy calculations using the then newly developed computer programs (IMPACT) based on the close-coupling method (Eissner & Seaton 1972, 1974; Crees, Seaton & Wilson 1978) were later carried out by Pradhan (1976, hereafter P76) for the collision strengths, and by Eissner & Zeippen (1981) and Zeippen (1982) for the transition probabilities. These atomic parameters subsequently enabled a consistent derivation of electron densities from observations of [O II] and [S II] lines in a wide variety of H II regions (e.g. Keyes, Aller & Feibelman 1990; Kingsburgh & English 1992; Aller & Hyung 1995; Aller, Hyung & Feibelman 1996).

More recently McLaughlin & Bell (1998, hereafter MB98) repeated the [O II] calculations of collision strengths using the **R**-matrix method (Burke et al. 1971; Berrington, Eissner & Norrington 1995), also based on the close coupling approximation and widely employed for a large number of atomic calculations (Hummer et al. 1993; The Opacity Project Team 1995). They included a much larger target wavefunction expansion than P76, and relativistic effects not considered in the earlier calculations. Their electron impact collision strengths and rate coefficients were markedly different for the relevant transitions $^4S^o_{3/2} \rightarrow {}^2D^o_{5/2,3/2}$ than those of P76, which led the theoretical density diagnostic line ratio $I(3729)/I(3726)$ to be up to 30 per cent higher and ≈2.0 in the low-density limit $\lim_{N_e} \rightarrow 0$. Keenan et al. (1999, hereafter K99) recomputed the [O II] line ratios to analyse several planetary nebulae using these MB98 results.

However, other extensive observational studies (e.g. Copetti & Writzel 2002; Wang et al. 2004) have noted the discrepancy between electron densities derived from [O II] and other density indicators, notably [S II] λλ6716, 6731. In particular, the recent analysis of a sample of over 100 nebulae by Wang et al. (2004) shows that the collision strengths of MB98 are not supported by observations, and that the earlier results of P76 are to be preferred. However, these observational studies leave open the question of what precisely are the collision strengths? Given that P76 used a small basis set to describe the O II target, considered no relativistic effects, and could not fully resolve the resonance structures in the collision strengths owing to computational constraints, it seems puzzling that the new MB98 results which do account for all of these factors appear to be inaccurate.

To address this important issue and to resolve the outstanding discrepancy, we recently undertook new calculations for [O II] using the same Breit–Pauli **R**-matrix (BPRM) method as employed by MB98 and including relativistic effects. While the details of

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the atomic calculation and comparison of collision strengths with different basis sets of target wavefunctions will be presented elsewhere (Montenegro et al. 2005), we present the final results of astrophysical interest in this Letter.

2 THEORY AND COMPUTATIONS

Forbidden lines are often sensitive to ambient electron density; as the Einstein spontaneous decay rates of the upper levels are small, they may be collisionally excited to other levels by electron impact before radiative decay (Osterbrock 1989; Dopita & Sutherland 2003). This is likely to happen when there is a pair of lines originating from closely spaced metastable energy levels, especially in ions of the $2p^3$ and the $3p^3$ outer electronic configurations as exemplified by O II and S II. The first five levels are: $^4S^o_{3/2}$, $^2D^o_{5/2,3/2}$, $^2P^o_{3/2,1/2}$. The pair of [O II] transitions of interest are $^2D^o_{5/2,3/2}$–$^4S^o_{3/2}$ at λ3729 and λ3726 respectively.

The basic physics of the limiting values of the line ratio $I3729/I3726$ is quite simple. At low electron densities, every excitation to the two metastable levels $^2D^o_{(5/2,3/2)}$ is followed by a spontaneous decay back to the ground level $^4S^o_{3/2}$ since the collisional mixing rate among the two excited levels is negligible. In that case the line ratio in principle must be equal to the ratio of the excitation rate coefficients

$$\lim_{N_e\to 0}\frac{I(3729)}{I(3726)}=\frac{q\left(^4S^o_{3/2}–^2D^o_{5/2}\right)}{q\left(^4S^o_{3/2}–^2D^o_{3/2}\right)}, \tag{1}$$

where the excitation rate coefficient q_{ij} is

$$q_{ij}(T)=\frac{8.63\times10^{-6}\ \exp(-E_{ij}/kT)}{g_i\sqrt{T}}\Upsilon_{ij}(T)\ \mathrm{cm^3\ s^{-1}}; \tag{2}$$

here g_i is the statistical weight of the initial level and the quantity Υ_{ij} is the Maxwellian averaged collision strength:

$$\Upsilon_{ij}(T)=\int_{E_j}^{\infty}\Omega_{ij}(E)\exp(-E/kT)\,\mathrm{d}(E/kT). \tag{3}$$

If relativistic effects are negligible then the collision strengths may be calculated in *LS* coupling, and an algebraic transformation may be employed to obtain the fine-structure collision strengths. This was the procedure employed by P76. The ratio of fine-structure *LSJ* to *LS* collision strength is especially simple when the lower level has either L or $S = 0$, such as for O II and S II, i.e.

$$\frac{\Omega(SLJ-S'L'J')}{\Omega(SL-S'L')}=\frac{2J'+1}{(2S'+1)(2L'+1)}. \tag{4}$$

If the excited levels are so closely spaced that the excitation rates have virtually the same temperature dependence, the line ratio is then equal to the ratio of the statistical weights $(2J'+1)$ of the upper levels $^2D^o_{5/2,3/2}$, i.e. 6/4. If, however, relativistic mixing is significant then the line ratio will depart from the *LS* coupling value. That was the contention of MB98 and K99.

Therefore we carry out the present calculations including relativistic effects and with a suitably large target wavefunction expansion. In the present calculations we employ a 16-level target: $1s^22s^2[2p^3(^4S^o_{3/2},\ ^2D^o_{5/2,3/2},\ ^2P^o_{3/2,1/2});\ 2s2p^4(^4P_{5/2,3/2,1/2},\ ^2D_{5/2,3/2}),\ 2p^23s(^4P_{1/2,3/2,5/2},\ ^2P_{1/2,3/2}),\ 2s2p^4(^4S_{1/2})]$. All resonance structures up to the highest target threshold energy $E(2s2p^4(^4S_{1/2})) = 1.7829$ Ryd (Rydbergs) are resolved. The last threshold lies sufficiently high to ensure that resonance and coupling effects in the collision strengths are fully accounted for in the excitation of the first five levels considered in the collisional–radiative model to compute the line ratios. Collision strengths at energies 1 Ryd higher than the highest of the first five levels $[E(^2P^o_{1/2}) = 0.369$ Ryd] contribute negligibly to the rate coefficients; at $T =$ 20 000 K the Maxwellian factor $\exp(-E/kT)\approx e^{-8}$, and decreasing accordingly for $E > 1$ Ryd in equation (3).

The present close coupling expansion is more than sufficient to obtain accurate collision strengths for the first five levels. The BPRM calculations are described in detail in another paper (Montenegro et al. 2005). We find that deviations from *LS* coupling are not significant. The BPRM collision strengths for all forbidden transitions among the first five levels are in accord with those obtained from *LS* coupling values through a purely algebraic transformation from *LS* to *LSJ*. For example, in addition to the collision strengths for transitions from the ground level, those for the four transitions $^2D^o_{5/2,3/2}$–$^2P^o_{3/2,1/2}$ also divide according to the algebraic ratios given in P76. It follows that the differences from MB98 must lie in electron correlation effects. However, since MB98 do not give details of the full configuration–interaction expansion used to obtain the target eigenfunction, it is difficult to ascertain the precise nature of these differences. One possible cause is the different methods of target optimization. In the present calculations, we employ a set of target configurations that optimizes over all terms dominated by the three configurations listed above. Therefore the number of target levels *per se* is not the deciding factor in accuracy. For instance, including only the first five levels, but with the same configuration–interaction expansion, yields essentially the same results as the 16-level target (also clear from the agreement with P76). The only difference is the additional resonance structures owing to higher targets in the 16-level calculation. However, resonance effects also do not play a decisive role in the rate coefficients and line ratios. The reason for not including all 21 levels, as in MB98, is that a significantly larger wavefunction expansion is needed to optimize over some of the higher lying terms dominated by the even-parity $2s2p^4$ and $2s^22p^23s$ configurations, but again this is not of consequence for the forbidden transitions among the first five levels (although it will be in subsequent work on allowed transitions among levels of the odd-parity ground configuration $2s^22p^3$ and the higher even-parity configurations in O II).

In the calculation of [O II] line ratios we employ the transition probabilities from Zeippen (1982). Eissner & Zeippen (1981) computed the *A*-coefficients for [O II] transitions taking full account of the magnetic dipole M1 operator, and they showed that in the high-density limit the line ratio

$$\lim_{N_e\to\infty}\frac{I(3729)}{I(3726)}=\frac{6}{4}\frac{A\left(^2D^o_{5/2}–^4S^o_{3/2}\right)}{A\left(^2D^o_{3/2}–^4S^o_{3/2}\right)}=0.35. \tag{5}$$

3 RESULTS AND DISCUSSION

Fig. 1 shows the fine-structure BPRM collision strengths $\Omega(^4S^o_{3/2}–^2D^o_{5/2})$, $\Omega(^4S^o_{3/2}–^2D^o_{3/2})$ and $\Omega(^2D^o_{5/2}–^2D^o_{3/2})$. These figures appear to be the first clear presentation of the resonances in these collision strengths. P76 did not present detailed resonance structures except in the near-threshold region of $\Omega(^2D^o_{5/2}–^2D^o_{3/2})$. MB98 plotted these on an energy scale up to 30 Ryd, which is well above the resonance region up to ∼2 Ryd, but does not exhibit the resonances in detail to enable comparison. An interesting feature clear from Fig. 1 is that the resonances do not play a large role in $\Omega(^4S^o_{3/2}–^2D^o_{5/2})$ and $\Omega(^4S^o_{3/2}–^2D^o_{3/2})$ and hence the rate coefficients for these transitions. Although they are significant in $\Omega(^2D^o_{5/2}–^2D^o_{3/2})$, collisional mixing via this transition is not important in the low-density limit, which

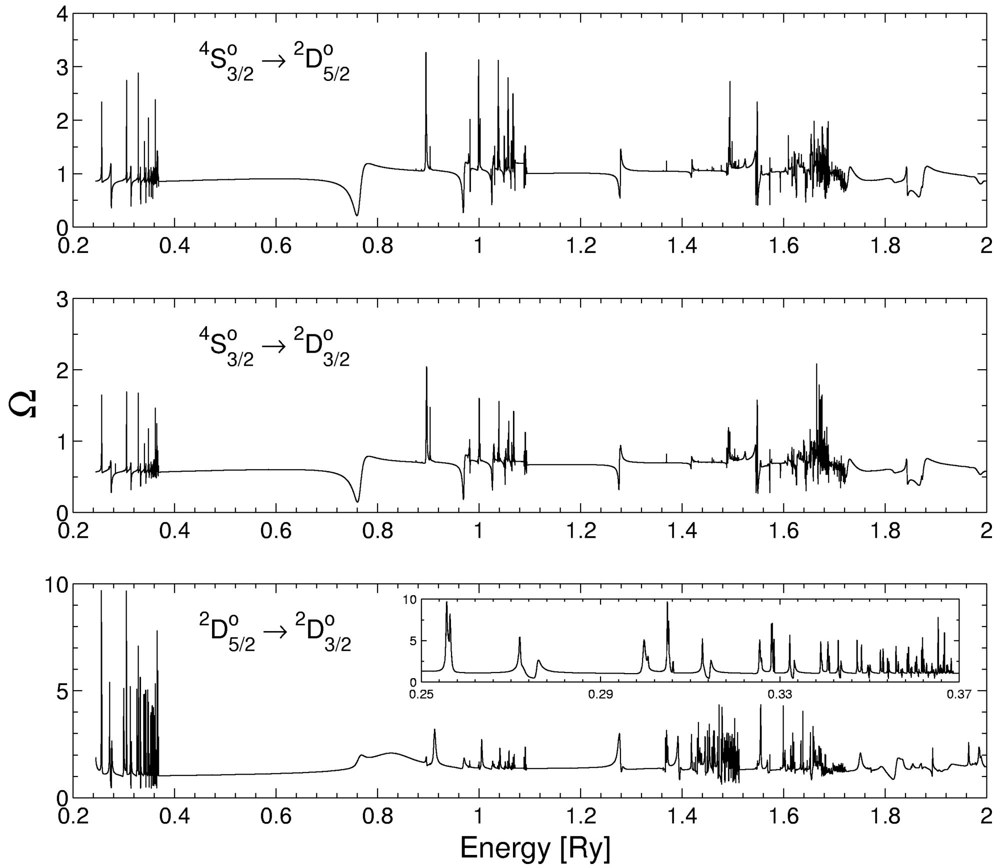

Figure 1. Collision strengths for the fine-structure transitions associated with the [O II] line ratio 3729 Å/3726 Å. Note that $\Omega(^4S^o_{3/2}\text{–}^2D^o_{5/2})/\Omega(^4S^o_{3/2}\text{–}^2D^o_{3/2}) = 1.5$ throughout. There is significant resonance enhancement in the collisional mixing transition $^2D^o_{5/2}\text{–}^2D^o_{3/2}$; the inset shows the near-threshold resonances on an expanded scale.

therefore depends only on the ratio of the transitions from the ground state $^4S^o_{3/2}$ to the $^2D^o_{5/2,\,3/2}$ levels. We find that this ratio is constant at 6/4 throughout the energy range under consideration, resonant or non-resonant values. Therefore we do not find any significant evidence of relativistic effects, which would manifest themselves in a departure from this ratio. Remarkably, the present total sum $\sum_{J=5/2,3/2} \Omega(^4S^o_{3/2} -{}^2 D^o_J) = 1.42$, compared to the *LS* coupling P76 value of 1.31, and an even earlier value of 1.36 obtained by Saraph, Seaton & Shemming (1969).

Table 1 gives the Maxwellian averaged collision strengths $\Upsilon(T)$ for the five-level [O II] model. At 10 000 K we obtain $\Upsilon(^4S^o_{3/2}\text{–}^2D^o_{3/2}) = 0.585$, in good agreement with the earlier P76 value of 0.534, about 9 per cent lower, but considerably higher than the M98 value of 0.422 (quoted in K99) which is 28 per cent lower than the new value. More importantly, our results disagree with MB98 for the ratio discussed above. It is this ratio that is responsible for the K99 line ratio $I(3729)/I(3726)$ being about 30 per cent higher ($\sim$2.0) than the expected low-density limit of 1.5, as shown in Fig. 2.

Comparing the present relativistic BPRM results for effective collision strengths with the *LS* coupling results of P76 we find good agreement, mostly within a few per cent, with the notable exception of $\Upsilon(^2D^o_{5/2}\text{–}^2D^o_{3/2})$. Owing to the more extensive delineation of

Table 1. Effective Maxwellian averaged collision strengths.

Transition	Υ(1000 K)	Υ(5000 K)	Υ(10 000 K)	Υ(15 000 K)	Υ(20 000 K)	Υ(25 000 K)
$^4S^o_{3/2}\text{–}^2D^o_{5/2}$	0.864	0.885	0.883	0.884	0.885	0.888
$^4S^o_{3/2}\text{–}^2D^o_{3/2}$	0.590	0.587	0.585	0.585	0.585	0.588
$^2D^o_{5/2}\text{–}^2D^o_{3/2}$	1.618	1.518	1.426	1.365	1.324	1.320
$^4S^o_{3/2}\text{–}^2P^o_{3/2}$	0.299	0.307	0.313	0.318	0.322	0.327
$^2D^o_{5/2}\text{–}^2P^o_{3/2}$	0.912	0.928	0.946	0.971	1.000	1.030
$^2D^o_{3/2}\text{–}^2P^o_{3/2}$	0.571	0.589	0.605	0.624	0.644	0.664
$^4S^o_{3/2}\text{–}^2P^o_{1/2}$	0.148	0.151	0.152	0.154	0.156	0.158
$^2D^o_{5/2}\text{–}^2P^o_{1/2}$	0.383	0.392	0.402	0.414	0.428	0.441
$^2D^o_{3/2}\text{–}^2P^o_{1/2}$	0.376	0.386	0.397	0.409	0.423	0.437
$^2P^o_{3/2}\text{–}^2P^o_{1/2}$	0.277	0.284	0.291	0.300	0.310	0.321

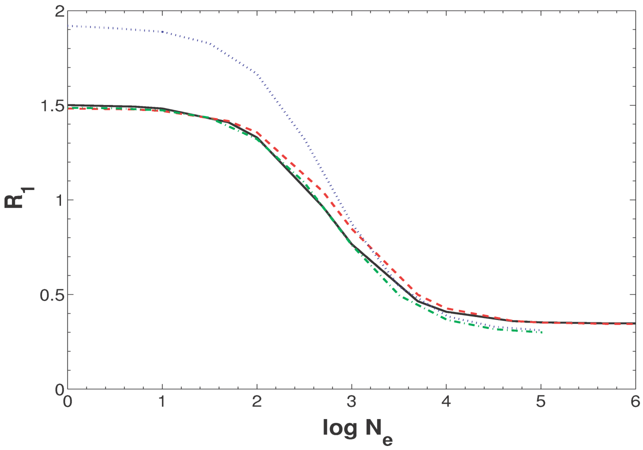

Figure 2. [O II] line ratio $I(3729)/I(3726)$ versus electron density N_e: present results, solid line; Pradhan (1976), dot–dashed line (nearly indistinguishable from the solid line); McLaughlin & Bell (1998), dotted line, at $T = 10\,000$ K. The dashed line is the line ratio at $T = 20\,000$ K.

resonance structures in the present calculations (Fig. 1), the Υ value is much higher. For example, at $T = 10,000$ K the P76 value is 1.168 compared with the present value of 1.426 in Table 1. On the other hand, the present $\Upsilon(^2P^o_{3/2}–^2P^o_{1/2}) = 0.291$ agrees well with the P76 value of 0.287 at $T = 10\,000$ K.

Fig. 2 shows that the present collision strengths yield the line ratio $R_1 = I(3729)/I(3726)$, which approaches the low- and high-density limits exactly. The difference is not discernible when we use the P76 values. On the other hand, the difference with MB98 is quite pronounced and approaches ∼30 per cent in the low-density limit. The temperature variation between $T = 10\,000$ K (solid line) and $T = 20\,000$ K (dashed line) is also small, demonstrating the efficacy of this ratio as an excellent density diagnostic.

4 CONCLUSION

We have carried out new relativistic Breit–Pauli **R**-matrix calculations for the [O II] transitions responsible for the important density diagnostic line intensity ratio of 3729 Å/3726 Å. We find no evidence of any significant departure from the earlier *LS* coupling results of Pradhan (1976). The line ratios derived from the present results also agree with the canonical limits expected on physical grounds. The new results are in considerable disagreement with the calculations of McLaughlin & Bell (1998) and the line ratios of Keenan et al. (1999). We also reconfirm the observational analyses of Copetti & Writzel (2002) and Wang et al. (2004).

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REFERENCES

Aller L. H., Hyung S., 1995, MNRAS, 276, 1101
Aller L. H., Hyung S., Feibelman W. A., 1996, PASP, 108, 488
Berrington K. A., Eissner W., Norrington P. H., 1995, Comput. Phys. Commun., 92, 290
Burke P. G., Hibbert A., Robb W. D., 1971, J. Phys. B, 4, 153
Copetti M. V. F., Writzel B. C., 2002, A&A, 382, 282
Crees M. A., Seaton M. J., Wilson P. M. H., 1978, Comput. Phys. Commun., 15, 23
Dopita M. A., Sutherland R. S., 2003, Astrophysics of the Diffuse Universe. Springer-Verlag, Berlin
Eissner W., Seaton M. J., 1972, J. Phys. B, 5, 2187
Eissner W., Seaton M. J., 1974, J. Phys. B, 7, 2533
Eissner W., Zeippen C. J., 1981, J. Phys. B, 14, 2125
Hummer D. G., Berrington K. A., Eissner W., Pradhan A. K., Saraph H. E., Tully J. A., 1993, A&A, 279, 298
Keenan F. P., Aller L. H., Bell K. L., Crawford F. L., Feibelman W. A., Hyung S., McKenna F. C., McLaughlin B. M., 1999, MNRAS, 304, 27 (K99)
Keyes C. D., Aller L. H., Feibelman W. A., 1990, PASP, 102, 59
Kingsburgh R. L., English J., 1992, MNRAS, 259, 635
McLaughlin B. M., Bell K. L., 1998, J. Phys. B, 31, 4317 (MB98)
Montenegro M., Eissner W., Nahar S. N., Pradhan A. K. 2005, J. Phys. B, submitted
Osterbrock D. E., 1989, Astrophysics of Gaseous Nebulae and Active Galactic Nuclei. University Science Books, Mill Valley, California
Pradhan A. K., 1976, MNRAS, 177, 31 (P76)
Saraph H. E., Seaton M. J., Shemming J., 1969, Proc. R. Soc., 264, 77
Seaton M. J., Osterbrock D. E., 1957, ApJ, 125, 66
The Opacity Project Team, 1995, The Opacity Project, Vol. 1. Institute of Physics, London
Wang W., Liu X.-W., Zhang Y., Barlow M., 2004, A&A, 873, 886
Zeippen C. J., 1982, MNRAS, 198, 111

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