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COLLISION STRENGTHS FOR [O II] AND [S II]

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SUMMARY

Collision strengths and parameters $\Upsilon(i \rightarrow j)$ required for the calculation of collisional rate coefficients are calculated for the fine-structure transitions $^2D_{3/2}$–$^2D_{5/2}$, $^2P_{1/2}$–$^2P_{3/2}$, $^4S_{3/2}$–^2D_J, $^4S_{3/2}$–^2P_J and ^2D_J–$^2P_{J'}$ within the ground configuration of [O II]. The complicated resonance structure in the $^2D_{3/2}$–$^2D_{5/2}$ collision strength above the ^2D threshold is taken into account. The collision strengths are obtained from reactance matrices calculated by Pradhan using the close-coupling approximation.

Distorted-wave and close-coupling calculations are made for the forbidden transitions in the ground configuration of [S II]. The target is represented by the ground configuration, $3s^2 3p^3$, plus the quasi-degenerate configuration $3p^5$, which gives some correlation effect. The present close-coupling results confirm the essentially similar calculation of Conneely, Smith & Lipsky, and the present distorted-wave results are in good agreement with the close-coupling results but are not in agreement with the earlier distorted wave calculations of Czyzak & Krueger.

1. RATE COEFFICIENT PARAMETERS FOR [O II]

1.1 *Introduction*

The transitions between the fine-structure levels of the ground configuration of [O II] (particularly the $^2D_{5/2}$–$^2D_{3/2}$ transition) are of considerable importance in interpreting the observed line intensities in the spectra of gaseous nebulae (Seaton & Osterbrock 1957). Accurate reaction rates are therefore required for these transitions. In an earlier work (Pradhan 1976) we made accurate close-coupling calculations for electron impact excitation of the metastable levels of [O II]. Reactance matrices, **R**, were calculated in LS coupling for transitions between these levels. Using Racah algebra these **R** matrices may be transformed to **R** matrices in pair coupling and hence the fine-structure collision strengths may be calculated (Saraph 1972).

The collision strength for the $^2D_{5/2}$–$^2D_{3/2}$ transition contains a complicated resonance structure below the ^2P excitation threshold. For an accurate calculation of the rate coefficient one must therefore take this structure into account while integrating the collision strength over the Maxwellian distribution of incident electron velocities. Martins & Seaton (1969) formulated the problem and calculated the collision strength $\Omega(^2D_{5/2}$–$^2D_{3/2})$, along with the resonance structure, using reactance matrices obtained in a single configuration approximation. In the present work, the method described by Saraph (1972) for the calculation of fine-structure collision strengths from **R** matrices in LS coupling, is modified to incorporate the formulation of Martins & Seaton (1969) for the calculation of detailed resonance structures.

1.2 *Method*

In this section we briefly outline the procedure mentioned above. The **R** matrices obtained in the LS representation are transformed to the pair coupling representation $J_i lKJ$, where $J_i + l \rightarrow K$ and $K + s \rightarrow J$ (s is the spin of the colliding electron), using a program described by Saraph (1972). The expression relating the **R** matrix elements in the two representations is

$$\mathbf{R}^J(S_iL_iJ_ilK, S_i'L_i'J_i'l'K'; k_1^2) = \sum_{\mathrm{LS}} C(SLJ, S_iL_iJ_ilK)\, \mathbf{R}^{SL}(S_iL_ils, S_i'L_i'l's, k_1^2)\, C(SLJ, S_i'L_i'J_i'l'K'). \quad (1)$$

From these new **R** matrices (in pair coupling) we calculate the matrices $\boldsymbol{\chi}$ defined by

$$\boldsymbol{\chi} = (i - \mathbf{R})(i + \mathbf{R})^{-1}. \quad (2)$$

For energies below the ^2P threshold, we transform to a representation where the submatrix $\boldsymbol{\chi}_{cc}$ is diagonal: $\boldsymbol{\chi}_{cc}$ contains the elements connecting the closed ^2P channels. Then we calculate the scattering matrix **S** in the region below threshold using

$$S_{\alpha\beta} = \chi_{\alpha\beta} - \sum_n \chi_{\alpha n}(\chi_{nn} - \exp\{-2\pi i\nu\})^{-1}\, \chi_{n\beta} \quad (3)$$

where the indices α, β refer to open channels and n, m to the closed channels. The fine-structure energy differences, which are small compared with energy differences between terms, are neglected and all closed channels are treated as degenerate with an effective quantum number such that the energy below the ^2P threshold is $k_3^2 = -1/\nu^2$ in Rydberg units.

Since the $\boldsymbol{\chi}$ matrices vary slowly with energy, the $\boldsymbol{\chi}$ matrices used in (3) are calculated only at a few points below the ^2P threshold. The variation in the **S** matrix is then mainly due to the term $\exp(-2\pi i\nu)$ in (3).

The fine-structure collision strengths are given by the expression

$$\Omega(S_iL_iJ_i, S_i'L_i'J_i') = \tfrac{1}{2}\sum_{ll'KK'J}(2J+1)\left|S^J(S_iL_iJ_ilK, S_i'L_i'J_i'l'K')\right|^2. \quad (4)$$

Using (3) and (4) the collision strengths are calculated as a function of the effective quantum number ν. The collision strengths thus obtained are integrated over a Maxwellian distribution of electron velocities to give the parameters $\Upsilon(i \rightarrow j)$ where,

$$\Upsilon(i \rightarrow j) = \int_0^\infty \Omega(i,j) \exp(-\epsilon_i/kT_e)\, d(\epsilon_i/kT_e). \quad (5)$$

$\epsilon_i = \frac{1}{2}mv_i^2$ is the kinetic energy of the colliding electron when the target is in state i, and T_e is the electron temperature. Also,

$$\frac{\frac{1}{2}mv_i^2}{kT_e} = \frac{157\,890\, k_i^2}{T_e} \quad (6)$$

with k_i^2 in Rydberg units. The collisional rate coefficients (i.e. the probability per unit time that an ion in level i undergoes a collisional transition to level j) are given by

$$q(i \rightarrow j) = \frac{8{\cdot}63 \times 10^{-6}}{\omega_i} \frac{N_e}{T_e^{1/2}} \Upsilon(i \rightarrow j)\ \mathrm{s}^{-1} \quad (7)$$

with N_e in cm^{-3} and T_e in K.

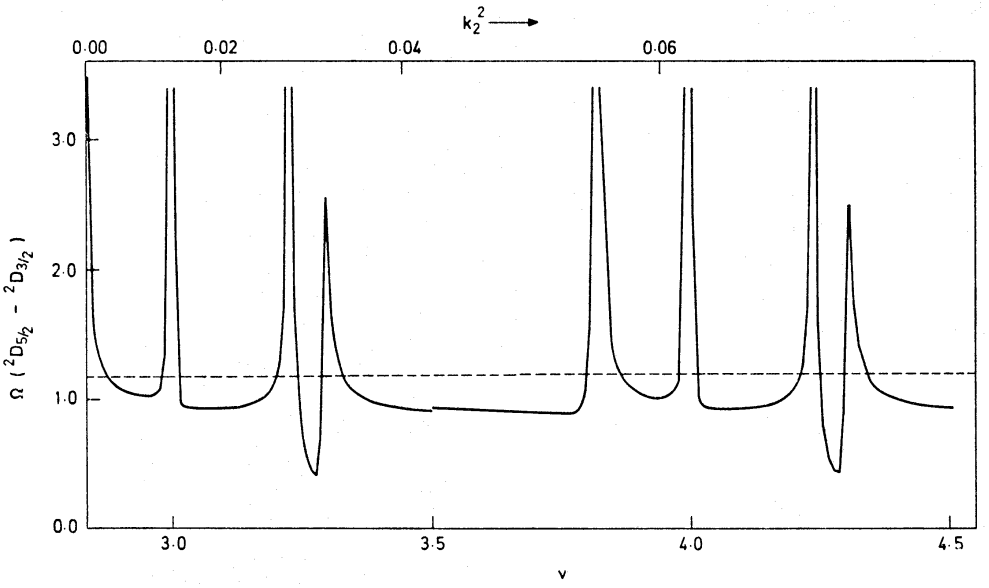

FIG. 1. *The total collision strength* $\Omega(^2D_{5/2}–^2D_{3/2})$, *as a function of the effective quantum number* ν, *at energies just above the* ^2D *threshold. The averaged collision strength is indicated by the dashed line.*

In this paper we tabulate the parameters $\Upsilon(i \to j)$ at several values of the electron temperature T_e in the range 5000–20 000 K.

1.3 *Calculations*

The resonances lying between the ^2D and the ^2P levels correspond to several overlapping Rydberg series of states of the type $^2P\,ns$, $^2P\,np$ etc. Relative to the ^2P level the effective quantum number of the ^2D excitation threshold is $\nu_t = 2{\cdot}8352$ (we use experimental energy differences throughout). The **R** matrices calculated in LS coupling at a few points above the ^2P threshold, are fitted to an expression in energy and extrapolated below threshold to two points corresponding to $\nu = 3{\cdot}0$ and $\nu = 4{\cdot}0$. The validity of these extrapolations has been checked by solving the coupled equations at selected energies below the ^2P threshold. The $\boldsymbol{\chi}$ matrices calculated at $\nu = 3{\cdot}0$ are used to obtain collision strengths (as a function of ν) between $\nu = \nu_t$ and $\nu = 3{\cdot}5$; and $\boldsymbol{\chi}$ matrices at $\nu = 4{\cdot}0$ are used for collision strengths between the range $\nu = 3{\cdot}5$ and $\nu = 4{\cdot}5$. The interval in ν at which calculations are made is taken to be 0·01. The results for the collision strength $\Omega(^2D_{5/2}–^2D_{3/2})$ are shown in Fig. 1. The slight discontinuity in the graph at $\nu = 3{\cdot}5$ is the result of having used slightly different $\boldsymbol{\chi}$ matrices at either side of the discontinuity.

We assume that for $\nu > 4{\cdot}5$ we may average over the resonances and use the averaged collision strengths in calculating (5). The expression for the scattering matrix averaged over resonances is derived by Gailitis (1963) and may be expressed in terms of the $\boldsymbol{\chi}$ matrices as (Seaton 1969):

$$\langle |S_{\alpha\beta}|^2 \rangle = |\chi_{\alpha\beta}|^2 + \sum_{n,m} \frac{\chi_{\alpha m}\chi_{m\beta}\chi_{\alpha n}{}^*\chi_{n\beta}{}^*}{1 - \chi_{mm}\chi_{nn}{}^*}. \tag{8}$$

The averaged collision strength is then calculated as in (4).

Thus in calculating the quantities $\Upsilon(i \to j)$ we use the collision strengths

TABLE I

Rate coefficient parameters $\Upsilon(i \rightarrow j)$ *for* [O II]

T (K)	Υ $(^2D_{5/2} \rightarrow {}^2D_{3/2})$	Υ $(^2P_{3/2} \rightarrow {}^2P_{1/2})$	Υ $(^2D \rightarrow {}^4S)$	Υ $(^2P \rightarrow {}^4S)$	Υ $(^2P \rightarrow {}^2D)$
5000	1·220	0·280	1·325	0·398	1·677
6000	1·208	0·282	1·326	0·399	1·683
7000	1·197	0·283	1·328	0·401	1·689
8000	1·186	0·284	1·331	0·403	1·694
9000	1·177	0·286	1·333	0·404	1·700
10000	1·168	0·287	1·335	0·406	1·706
12000	1·152	0·290	1·340	0·409	1·718
14000	1·139	0·292	1·346	0·412	1·730
16000	1·128	0·295	1·351	0·415	1·741
18000	1·119	0·297	1·357	0·418	1·753
20000	1·112	0·300	1·363	0·421	1·765

TABLE II

Ratios of $\Omega(SL_J\text{–}{}^2P_{J'})$ *to* $\Omega(SL\text{–}{}^2P)$

	SL_J		
^2P_J	$^2D_{3/2}$	$^2D_{5/2}$	$^4S_{3/2}$
$^2P_{1/2}$	0·161	0·173	0·333
$^2P_{3/2}$	0·239	0·428	0·666

containing the detailed resonance structure, up to $\nu = 4{\cdot}5$ ($k_1{}^2 = 0{\cdot}31938$) and collision strengths averaged over resonances from $\nu = 4{\cdot}5$ to $\nu = \infty$ (i.e. $k_1{}^2 = E(^2P) = 0{\cdot}368767$ Ryd). Above the ^2P threshold the fine-structure collision strengths fit well to a linear expression in energy and this is used to calculate $\Upsilon(i \rightarrow J)$ from $k_3{}^2 = 0$ to $k_3{}^2 = \infty$.

1.4 *Conclusion*

We give the total values of $\Upsilon(i \rightarrow j)$ in Table I: $\Upsilon(^2D \rightarrow {}^4S)$, $\Upsilon(^2P \rightarrow {}^4S)$ and $\Upsilon(^2P \rightarrow {}^2D)$ are calculated using collision strengths summed over the fine-structure levels belonging to the two terms, i.e. we use

$$\Omega(SL\text{–}S'L') = \sum_{J,J'} \Omega(SLJ\text{–}S'L'J') \qquad (9)$$

The ratios of $\Omega(SLJ\text{–}S'L'J')$ to $\Omega(SL\text{–}S'L')$ are given in Table II for the transitions from the ^2P_J levels to the ^2D_J and the ^4S_J levels. For the $(^2D_{5/2}\text{–}{}^4S_{3/2})$ and the $(^2D_{3/2}\text{–}{}^4S_{3/2})$ transitions, the ratios are 0·6 and 0·4 respectively.

One may use these ratios to obtain the parameters Υ for transitions between fine-structure levels belonging to different terms in the ground configuration of [O II].

2. COLLISION STRENGTHS FOR [S II]

2.1 *Introduction*

It has been noted by Saraph & Seaton (1970) that there is a considerable discrepancy, of a factor of about 2, between the values for electron densities in planetary nebulae obtained from calculated collision strengths for forbidden transitions in [O II] and [S II]. In their calculations for [S II] they used the collision strengths

calculated by Czyzak & Krueger (1967) (referred to as CK) in the distorted-wave (DW) approximation. However, on the basis of later calculations by Conneely, Smith & Lipsky (1970) (referred to as CSL), using the close-coupling (CC) approximation, Saraph & Seaton concluded that the DW collision strengths were a factor of 1·8 too small.

We have repeated the calculations for [S II] in both the DW and the CC approximations using the computer program package described by Eissner & Nussbaumer (1969), Eissner (1972) and Seaton (1974). The theoretical formulation of these approximations is discussed by Eissner & Seaton (1972).

2.2 *Calculations*

We carried out the DW calculations twice; first, with the target consisting of the ground configuration, $3s^2 3p^3$ only, and secondly, including in addition the quasi-degenerate configuration $3p^5$ which contributes significantly to the ^2P term of the ground configuration and hence to the collision strength $\Omega(^2D–^2P)$. For the CC calculations the target representation was also taken to be $(3s^2 3p^3 + 3p^5)$. The radial functions for the target orbitals were calculated in a scaled Thomas–Fermi–Dirac type statistical model potential $V(\lambda_l, r)$. The scaling parameters λ_l converge to values fairly close to unity (λ_s = 1·1038 and λ_p = 1·0565).

In Tables III, IV and V we give the present results along with the DW results of CK. The kinetic energy of the incident electron, when the ion is in the level ^2p, is k_3^2 which is taken to be 0·0005 Ryd for all the collision strengths given. In the CC calculations we have included the partial waves up to $l, l' \leq 3$ and summed over all the contributing total spin angular momenta, orbital angular momenta and parity ($SL\pi$) states. In the DW calculations we included $l, l' \leq 4$ for $\Omega(^4S–^2D)$ and $\Omega(^4S–^2P)$, and $l, l' \leq 5$ for the collision strength $\Omega(^2D–^2P)$ where we have long-range quadrupole interactions.

TABLE III

Partial-wave contributions to $\Omega(^4S–^2D)$ *at* k_3^2 = 0·0005 *Ryd for* [S II]

	l'	DW (CK)	DW SC(P)	DW SCC(P)	CC SCC(P)
1	1	0·232	1·4364	1·4476	1·3650
2	2	2·753	3·8631	3·7793	4·7790
3	3	0·006	0·0135	0·0087	0·0126
4	4	0·000	0·0000	0·0000	(0·0000)
2	0	0·070	0·3940	0·4194	0·4591
0	2				
3	1	0·000	0·0141	0·0103	0·0186
1	3				
4	2	0·004	0·0122	0·0062	(0·0062)
2	4				
Total		3·065	5·7333	5·6715	6·6405

Notes

DW (CK)—Distorted wave (Czyzak & Krueger).
DW SC(P)—Distorted wave single configuration (Present).
DW SCC(P)—Distorted wave single configuration + correlation (Present).
CC SCC(P)—Close-coupling single configuration + correlation (Present).
Numbers in brackets are distorted-wave values (DW SCC).

TABLE IV

Partial-wave contributions to $\Omega(^4S\text{–}^2P)$ *at* $k_3^2 = 0{\cdot}0005$ *Ryd*

l	l'	DW (CK)	DW SC(P)	DW SCC(P)	CC SCC(P)
1	1	0·037	0·4125	0·4290	0·3432
2	2	1·240	2·1350	2·1243	2·3860
3	3	0·001	0·0027	0·0023	0·0023
2	0	0·000	0·0000	0·0000	—
0	2				
3	1	0·000	0·0000	0·0000	—
1	3				
Total		1·278	2·5502	2·5556	2·7315

Notes

Abbreviations as in Table III.

TABLE V

Partial-wave contributions to $\Omega(^2D\text{–}^2P)$ *at* $k_3^2 = 0{\cdot}0005$ *Ryd*

l	l'	DW (CK)	DW SC(P)	DW SCC(P)	CC SCC(P)
1	1	0·268	0·8501	0·9330	0·9873
2	2	2·700	4·4586	7·1590	8·9687
3	3	0·569	0·7673	0·9626	0·8750
4	4	0·086	0·1263	0·1944	(0·1944)
5	5	0·011	0·0177	0·0371	(0·0371)
2	0	1·198	1·2548	0·6876	0·9214
0	2				
3	1	0·893	0·9690	0·6457	0·6192
1	3				
4	2	0·182	0·1007	0·0081	(0·0081)
2	4				
5	3	0·311	0·3660	0·1571	(0·1571)
3	5				
Total		6·218	8·9005	10·8046	12·7683

Abbreviations as in Table III.

In Table VI we give our results, along with the results of CK and CSL, for total collision strengths some way above the excitation threshold, at the energy $k_3^2 = 0{\cdot}1762$ Ryd.

2.3 *Discussion of results*

From Tables III, IV and V it is seen that the present DW results are in good agreement with the present CC results. However, when compared with the present DW values, the calculated DW values of Czyzak & Krueger are smaller by about a factor $\frac{1}{2}$ for total $\Omega(^4S\text{–}^2D)$ and $\Omega(^4S\text{–}^2P)$ and by about a factor $\frac{1}{3}$ for total $\Omega(^2D\text{–}^2P)$. Considering the partial collision strengths, it is seen that the largest disparities are for *pp* and *dd* contributions where the earlier DW values of Czyzak & Krueger are considerably lower than either the present DW or the CC results.

In Table VI we can see that for $\Omega(^4S\text{–}^2D)$ and $\Omega(^4S\text{–}^2P)$ the present results agree closely with the results of CSL. The present CC calculations were made close to the ^2P threshold at $k_3^2 = 0{\cdot}0005$ Ryd: however, we do not expect the collision strengths at $k_3^2 = 0{\cdot}1762$ Ryd to be very different (see the present DW

TABLE VI

Total collision strengths in different approximations

Approximation	k_3^2	Ω (^4S–^2D)	Ω (^4S–^2P)	Ω (^2D–^2P)
DW (CK)	0·1762	3·63	2·00	9·45
DW SC(P)	0·1762	5·3239	2·8936	10·1588
DW SCC(P)	0·1762	5·4045	2·8662	12·0049
CC (CSL)	0·1762	5·65	2·56	9·84
CC SCC(P)	0·0005	6·6405	2·7315	12·7683

Notes

CC (CSL)—Close-coupling (Conneely, Smith & Lipsky). Otherwise as Table III. Note that the DW (CK) values are with experimental energy differences.

results at these two energies). For $\Omega(^2D$–$^2P)$ there is a large discrepancy between the present results, both DW SCC and the CC SCC, and the CC(CSL) value. This is most probably due to the fact that we have included the correlation configuration $3p^5$ which improves the representation for the ^2P term, whereas CSL included only the ground configuration in their target.

The DW values of CK given in Tables III, IV and V are obtained using calculated energy differences between ion terms, whereas their values in Table VI are with experimental energy differences (Krueger & Czyzak 1970). Their results for total $\Omega(^4S$–$^2P)$ and $\Omega(^2D$–$^2P)$ in Table VI are over 50 per cent greater than the results of Tables IV and V. This seems rather a large difference to be accounted for by changing from calculated to experimental energies. We have used calculated energies in the DW calculations (DW SC(P) and DW SCC(P)), and experimental energy differences in the CC calculations. As already pointed out, the results of all three approximations are in reasonable agreement with one another. The calculations of CSL were also carried out using experimental energy differences.

2.4 *Conclusion*

On the basis of the present calculations it may be concluded that the earlier DW calculations of CK seem to be in error and that for electron energies under consideration there is no large disagreement between collision strengths calculated in the DW approximation and the CC approximation. The present CC calculations

TABLE VII

Fine-structure collision strengths for [S II] (*DW SCC approximation*)

Transition	Ω ($k_3^2 = 0{\cdot}0005$)	Ω ($k_3^2 = 0{\cdot}1762$)
$^4S_{3/2}$–$^2D_{3/2}$	2·27	2·16
$^4S_{3/2}$–$^2D_{5/2}$	3·40	3·24
$^4S_{3/2}$–$^2P_{1/2}$	0·85	0·96
$^4S_{3/2}$–$^2P_{3/2}$	1·70	1·91
$^2D_{3/2}$–$^2D_{5/2}$	6·06	6·16
$^2D_{3/2}$–$^2P_{1/2}$	1·63	1·77
$^2D_{3/2}$–$^2P_{3/2}$	2·77	3·00
$^2D_{5/2}$–$^2P_{1/2}$	2·04	2·21
$^2D_{5/2}$–$^2P_{3/2}$	4·56	4·92
$^2P_{1/2}$–$^2P_{3/2}$	2·29	2·40

also confirm the results of CSL who had used a different method to solve the coupled integro–differential equations for the (e + ion) system.

More detailed CC calculations, including states belonging to excited configurations of the [S II] target, are in progress. These will take into account additional resonances in the excitation cross-sections for the forbidden transitions of interest. The present results should therefore be considered preliminary to the more accurate calculations in progress.

For many astrophysical applications one requires the collision strengths for the fine-structure transitions within the ground configuration of [S II]. We have calculated these collision strengths in the DW SCC approximation and the results are given in Table VII. These values are slightly more accurate than those given in Table VI as we have included partial waves up to $l, l' \leq 7$ and all the contributing $SL\pi$ states.

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