Fine structure effective collision strengths for the
electron impact excitation of the sulphur ion S\textsc{v}

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Abstract. We have performed a 14-state $R$-matrix calculation to determine effective collision strengths for fine structure transitions in S\textsc{v} ion. The target states were taken to be the 14 lowest $LS$ states, which involve configurations of the form - (2p$^6$)3s$^2$, 3s3p, 3p$^2$, 3s3d, 3s4s, 3p3d. These target states give rise to 26 fine structure levels and 325 possible transitions. The fine structure collision strengths were obtained by transforming to a $jj$-coupling scheme using the JAJOM program of Saraph and using a sufficiently fine energy mesh so that the resonance structure can be properly delineated. Effective collision strengths were calculated by averaging the electron collision strengths over a Maxwellian distribution of velocities. Comparisons are made with an earlier $R$-matrix calculation and with a distorted-wave approximation.

1. Introduction
S\textsc{v} emission lines have been observed in solar flares, solar upper atmospheres, quiet sun regions and broad band absorption line quasars. Particular lines are used as diagnostics for electron temperature and density. Accurate atomic data are needed to analyse the observations and to date, the best available calculations for this ion have not included contributions from resonances.

The most recent theoretical investigations providing collisional data for this ion are the $R$-matrix calculation of Dufton & Kingston \cite{1} and the distorted-wave approximation of Pradhan \cite{2} (using the collision strengths of Christensen \textit{et al} \cite{3}). Discrepancies have been noted between the earlier calculations and observed data. For example, Doschek \textit{et al} \cite{4} used the results of Pradhan \cite{2} and for the 786.48Å/1199.13Å ratio, i.e. $(3s^2 \, ^1S_0-3s3p \, ^1P_1)/(3s^2 \, ^1S_0-3s3p \, ^3P_1)$, they find that distorted-wave theory predicts an intensity ratio which is a factor of five larger than the observed ratio. The current work aims to resolve these discrepancies.

2. Calculation Method
Configuration Interaction (CI) wavefunctions for the 14 lowest $LS$ target states of S\textsc{v} have been calculated using the CIV3 code \cite{5}. Each state $\Psi$ is represented by a linear combination of single-configuration functions $\Phi_i$, all having the same total $LS\pi$ symmetry:

$$\Psi(LS) = \sum_{i=1}^{m} a_i \Phi_i(\alpha_i LS) \quad (1)$$

where the $a_i$ are eigenvector components of the Hamiltonian matrix with particular $LS\pi$ symmetry. The $\Phi_i$ are constructed from a set of one-electron orbitals, each consisting of a radial function $\frac{1}{r}P_{nl}(r)$, a spherical harmonic $Y_{l}^{m_i}(\theta, \phi)$ and a spin function $\chi_{m_s}(\sigma)$.
Table 1. Target state energy levels in Rydbergs relative to the ground state.

| LS state | NIST [6] | Current | Christensen et al [1] | Dufton & Kingston [3] | No. of J-levels | J values |
|----------|----------|---------|------------------------|------------------------|----------------|----------|
| 3s$^2$1$S^e$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 1 | 0 |
| 3s3p$^3$P$^o$ | 0.7634 | 0.7519 | 0.7567 | 0.7518 | 3 | 0,1,2 |
| 3s3p$^1$P$^o$ | 1.1587 | 1.1699 | 1.1709 | 1.1694 | 1 | 1 |
| 3p$^2$1$D^e$ | 1.7655 | 1.7468 | 1.7477 | 1.7518 | 1 | 2 |
| 3p$^2$3$P^e$ | 1.8294 | 1.8252 | 1.8197 | 1.8266 | 3 | 0,1,2 |
| 3s3d$^3$D$^e$ | 2.1410 | 2.1255 | 2.1361 | 2.1578 | 3 | 1,2,3 |
| 3p$^2$1$S^e$ | 2.1477 | 2.1552 | 2.1618 | 2.1562 | 1 | 0 |
| 3s3d$^1$D$^e$ | 2.4668 | 2.4791 | 2.4864 | 2.5632 | 1 | 2 |
| 3s4s$^3$S$^e$ | 2.8395 | 2.8135 | 2.8188 | 1 | 1 |
| 3s4s$^1$S$^e$ | 2.9170 | 2.8922 | 2.9127 | 1 | 0 |
| 3p3d$^3$F$^o$ | 2.9496 | 2.9183 | 3 | 2,3,4 |
| 3p3d$^1$D$^o$ | 2.9931 | 2.9677 | 1 | 2 |
| 3p3d$^3$P$^o$ | 3.1487 | 3.1307 | 3 | 0,1,2 |
| 3p3d$^3$D$^o$ | 3.1715 | 3.1568 | 3 | 1,2,3 |

These orbitals are chosen to be analytic, with the radial part being expressed as a sum of Slater-type orbitals:

$$ u_{nlm_{ms}}(r, \sigma) = \frac{1}{r} P_{nl}(r) Y_l^m(\theta, \phi) \chi_{m_s}(\sigma) $$  \hspace{1cm} (2)

In this expression, the $I_{jnl}$ are kept fixed and the coefficients $C_{jnl}$ and exponents $\zeta_{jnl}$ are treated as variational parameters. In total 12 orthogonal orbitals are used in this calculation: 8 real orbitals (1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p) and 4 pseudo-orbitals ($4d$, $4f$, $5s$ and $5p$). The wavefunctions of the 14 LS target states are constructed from this orbital set using configurations generated by a two electron replacement on the 2p$^6$3s$^2$ basis configuration, with the 1s, 2s and 2p shells closed. The energies of the target states, relative to the ground state are compared with the values given by NIST [6] and the previous calculations in Table 1. The agreement between the present theory and the observed energies is generally very satisfactory. We are therefore confident that we are using accurate wavefunctions.

The ion-plus-electron ($N + 1$) system is described using the $R$-matrix method of Burke & Robb [7], using associated computer codes detailed by Berrington et al [8]. The $R$-matrix radius is calculated to be 11 atomic units and 20 continuum orbitals were included for each orbital angular momentum, ensuring convergence up to an incident electron energy of 16 Ryd. The LS-coupled Hamiltonian diagonal matrices are adjusted so that the calculated energy levels match those of experiment. This ensures the correct positioning of resonances relative to the thresholds included in the calculation. In forming the ($N + 1$)-electron symmetries, total angular momenta $L \leq 12$ for both even and odd parities, and for doublet and quartet multiplicities are included. Convergence of the collision strengths is thus fully achieved.

Configurations describing these ($N + 1$)-electron symmetries are obtained by the addition of one electron from the orbital set to those configurations previously generated. Having obtained
the scattering K-matrices in the LS-coupling scheme, the JAJOM program of Saraph [9] is used to transform to the LSJ-coupling scheme thus including fine-structure mixing of the target terms and so producing collision strengths, Ω, between the J-resolved levels. The cross-section \( \sigma_{if} (\text{cm}^2) \) between level \( i \) and level \( f \), is related to the collision strength \( \Omega_{if} \) by the expression

\[
\sigma_{if} = \frac{\Omega_{if} \pi a_0^2}{\omega_i k_i^2}
\]

where \( \omega_{if} \) is the statistical weight of the initial target level \( i \), \( k_i^2 \) the incident electron energy in Rydbergs and \( a_0 \) the Bohr radius. Applying a Maxwellian velocity distribution, the effective collision strength is then given by

\[
\Upsilon_{if}(T_e) = \int_0^\infty \Omega_{if}(E_f) \exp\left(-\frac{E_f}{kT_e}\right) d\frac{E_f}{kT_e}
\]

where \( T_e \) is the electron temperature (in Kelvin), \( E_f \) is the final free electron energy after excitation and \( k \) is Boltzmann’s constant.

3. Results and Discussion

A fine mesh of incident impact energies is used to properly delineate the resonances. Pseudoresonances above the highest target threshold energy (the 3p3d \(^3\)D\(^0\) level at 3.1715 Ryd) are smoothed out using a cubic spline fit, ensuring no distortion of results in the high energy region. For dipole-allowed transitions, it is necessary to consider the effect of partial waves with \( L > 12 \). The partial collision strengths are assumed to form a geometric series expansion with a geometric scaling factor given by the ratio of two adjacent terms. For this calculation effective collision strengths have been determined in the temperature range \( \log T_e(\text{K}) = 4.0-6.0 \).

Figure 1 shows that the collision strengths obtained from this method exhibit significant resonant character. The autoionizing resonances, which converge to the thresholds of the target states, can significantly enhance the effective collision strengths. The extent of this enhancement can be seen in Figure 2 where the current data is compared to previous calculations.

Collision strengths and effective collision strengths for the transitions considered by Doschek et al [4], i.e. the \( 3s^2 \, 1S_0 - 3p^2 \, 3P_1 \) and \( 3s^2 \, 1S_0 - 3s3p \, 3P_1^0 \) transitions observed at 786.48 Å and 1199.13 Å, are shown in Figures 3-6. The current data are significantly different from the Distorted Wave (DW) values and so our new evaluations should go some way in reducing the factor of five difference between observation and the theoretical previous predictions. Additional calculation details and results are noted in Hudson & Bell [10].
Figure 3. Collision strengths for the $3s^2 \, ^1S_0 - 3s3p \, ^3P^o_1$ fine structure transition.

Figure 4. Effective collision strengths for the $3s^2 \, ^1S_0 - 3s3p \, ^3P^o_1$ fine structure transition.

Figure 5. Collision strengths for the $3s^2 \, ^1S_0 - 3s3p \, ^3P^o_1$ fine structure transition.

Figure 6. Effective collision strengths for the $3s^2 \, ^1S_0 - 3s3p \, ^3P^o_1$ fine structure transition.

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