Improved collision strengths and line ratios for forbidden [O III] far-infrared and optical lines

Ethan Palay,1 Sultana N. Nahar,1 Anil K. Pradhan1* and Werner Eissner2

1Department of Astronomy, The Ohio State University, Columbus, OH 43210, USA
2Institut für Theoretische Physik, Universität, 70599 Stuttgart, Germany

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ABSTRACT
Far-infrared and optical [O III] lines are useful temperature–density diagnostics of nebular as well as dust obscured astrophysical sources. Fine-structure transitions among the ground state levels 1s22s22p3 P0,1,2, 1D2, 1S0 levels yield the well-known optical lines λλ4363, 4959 and 5007 Å. These lines are excited primarily by electron impact excitation. However, despite their importance in nebular diagnostics collision strengths for the associated fine-structure transitions have not been computed taking full account of relativistic effects. We present Breit–Pauli R-matrix calculations for the collision strengths with highly resolved resonance structures. We find significant differences of up to 20 per cent in the Maxwellian averaged rate coefficients from previous works. We also tabulate these to lower temperatures down to 100 K to enable determination of physical conditions in cold dusty environments such photodissociation regions and ultraluminous infrared galaxies observed with the Herschel Space Observatory. We also examine the effect of improved collision strengths on temperature- and density-sensitive line ratios.

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

1 INTRODUCTION
[O III] optical lines have long been standard nebular temperature diagnostics with wavelengths almost in the middle of the optical spectrum at λλ4363, 4959, 5007 (see e.g. Aller 1956; Dopita & Sutherland 2003; Pradhan & Nahar 2011). In recent years, owing to the advent of far-infrared (FIR) space observatories and instruments such as the Infrared Space Observatory Long Wavelength Spectrograph (ISO-LWS), the Spitzer Infrared Spectrograph and the Herschel Photodetector Array Camera and Spectrometer (PACS), the [O III] FIR lines have proven to have great potential in providing diagnostics of physical conditions in a variety of astrophysical objects that are generally obscured by dust extinction at optical or shorter wavelengths. These range from Galactic H II regions (Martín-Hernandez et al. 2002; Morisset et al. 2002) to star-forming galaxies at intermediate redshift (Liu et al. 2005) and ultraluminous infrared galaxies (ULIRGs). For example, the [O III] FIR lines at λλ88 and 52 μm are observed from dusty ULIRGs, which are copious IR emitters and become more prominent with increasing redshift (Nagao et al. 2011). They may be valuable indicators of the metalliclicity evolution from otherwise inaccessible star-forming regions buried deep within the galaxies (Houck et al. 2004, 2005).

The forbidden FIR lines arise from very low energy excitations within the fine-structure levels of the ground state of atomic ions, such as the [O III] 3P0,1,2 transition at 88.36 μm and the 3P1,2 transition at 51.81 μm. As such, they can be excited by electron impact at low temperatures, even at T_e ~ 1000 K or less. That also accounts for their utility since the FIR lines can be formed in (and therefore probe) not only H II regions but also photodissociation regions where the temperature–density gradients are large (Nagao et al. 2011).

However, excitation of levels lying very close to each other implies that the associated cross-sections need to be computed with great accuracy at very low energies in order to yield reliable rate coefficients. The Maxwellian electron distribution at low-temperatures samples only the near-threshold energies above the small excitation energy of the fine-structure transition. Relativistic fine-structure separations therefore assume special importance even for low-Z atomic ions in determining not only the energy separation but also the interaction of the incident electron with the target levels. Owing to its prominence in astrophysical spectra, a large number of previous studies have been carried out on electron impact excitation of O III (namely compilation of evaluated data by Pradhan & Zhang 2001). Among the recent ones, whose collision strengths are employed in astrophysical models, are Burke, Lennon & Seaton (1989),

*E-mail: pradhan.1@osu.edu

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Aggarwal & Keenan (1999), and Crawford et al. (2000). However, these calculations are basically in LS coupling (Burke et al. 1989), or with intermediate coupling effects introduced perturbatively via an algebraic transformation from the LS to LSI scheme (Aggarwal & Keenan 1999). Although the earlier calculations employed the coupled channel R-matrix method which takes account of the extensive resonance structures; the fine-structure separations are not considered. In this report we take account of both the resonances and fine structure in an ab initio manner.

Another recent development in relativistic R-matrix codes is the inclusion of the two-body (fine-structure) Breit interaction terms in the Breit–Pauli Hamiltonian (Nahar et al. 2011; Eissner & Chen, in preparation). A relativistic calculation of collision strengths can therefore be carried out, including fine structure explicitly and more accurately than in previous works. Relativistic effects are likely to be insignificant for optical transitions compared to the FIR transitions since the former involve relatively larger energy separations and relativistic corrections are small. Nevertheless, we consider all 10 forbidden transitions among the levels dominated by the ground configuration of O iv.

2 THEORY AND COMPUTATIONS

A brief theoretical description of the calculations is given. In particular, we describe relativistic effects and the representation of the (e + ion) system.

2.1 Relativistic fine structure

The relativistic Hamiltonian (Rydberg units) in the Breit–Pauli R-matrix (BPRM) approximation is given by

\[ H_{BPRM} = \sum_{i=1}^{N+1} \left( -\frac{1}{2} \frac{\hbar^2}{r_i} + \sum_{j=1}^{N+1} \frac{2}{r_{ij}} \right) + H_{\text{mass}} + H_{\text{Darwin}} + H_{\text{so}}, \]

where the last three terms are, respectively, the following relativistic corrections:

- the mass correction term, \[ H_{\text{mass}} = -\frac{\alpha^2}{4} \sum_i p_i^2, \]
- the Darwin term, \[ H_{\text{Darwin}} = \frac{Ze^2}{4} \sum_i \nabla^2 \left( \frac{1}{r_i} \right), \]
- the spin–orbit interaction term, \[ H_{\text{so}} = Ze^2 \sum_i \frac{1}{r_i} I_i \cdot s_i. \]

Equation (2) represents the one-body terms of the Breit interaction. In addition, another version of BPRM codes including the two-body terms of the Breit interaction (Nahar et al. 2011; Eissner & Chen, in preparation) has been developed, and is employed in the present work.

2.2 Effective collision strengths

Cross-sections or collision strengths at very low energies may be inordinately influenced by near-threshold resonances. Those, in turn, affect the effective collision strengths or rate coefficients computed by convolving the collision strengths over a Maxwellian function at a given electron temperature \( T_e \) as

\[ \gamma_{ij}(T_e) = \int_{0}^{\infty} \Omega_{ij}(\epsilon) \exp(-\epsilon/kT_e)N(\epsilon/kT_e), \]

where \( \Omega_{ij} \) is the energy difference and \( \Omega_{ij} \) is the collision strength for the transition \( \gamma_{ij} \). The exponentially decaying Maxwellian factor implies that at low temperatures only the very low energy \( \Omega_{ij}(\epsilon) \) would determine the \( \gamma(T_e) \).

2.3 Wavefunction representation and calculations

Based on the coupled channel approximation, the R-matrix method (Burke et al. 1971; Berrington et al. 1995) entails a wavefunction expansion of the (e + ion) system in terms of the eigenfunctions for the target ion. In the present case we are interested in low-lying O/FIR transitions of the ground configuration 2s2p2. Therefore, we confine ourselves to an accurate wavefunction representation for the first 19 levels dominated by the spectroscopic configurations [1s2]2s2p2, 2s2p3, 2s2p3s. A much larger set of correlations configurations is included for configuration interaction with the spectroscopic terms using the atomic structure code SUPERSTRUCTURE (Eissner et al. 1974; Nahar et al. 2003); [1s2]2p4, 2s2p3p, 2s2p3d, 2s2p3s, 2s2p2p, 2s2p2p, 2s2p3p, 2s2p3d, 2s2p3d, 2s2p3d, 2s2p3d, 2s2p3d, 2s2p3d, 2s2p3d, 2s2p3d, 2s2p3d. We note here that the crucial fine-structure separations between the ground state \( ^3\Pi_{0,1,2} \) levels reproduced theoretically agree with experimentally measured values to \( \pm 3 \) per cent (Nahar et al. 2011; see Paudel & Nahar 2011, for a general description of atomic processes and calculations). The observed energies were substituted for theoretical ones in order to reproduce the threshold energies more accurately. This is of particular importance for excitation at low temperatures dominated by near-threshold resonances. Even though the observed and experimental values are close, a small difference in resonance positions relative to threshold can introduce a significant uncertainty in the effective collision strengths.

The collision strengths were computed employing the extended BPRM codes (Eissner & Chen 2012). Particular care is taken to test and ensure convergence of collision strengths with respect to partial waves and energy resolution. Total (e + ion) symmetries up to (LSJ)/\( \pi \) with \( J \leq 19,5 \) and even/odd parities \( \pi \) were included in the calculations, though it was found that the collision strengths for all forbidden transitions converged for \( J \leq 9,5 \). An energy mesh of \( \Delta \epsilon < 10^{-4} \) Rydberg was used to resolve the near-threshold resonances. The resonances were delineated in detail prior to averaging over the Maxwellian distribution.

3 RESULTS AND DISCUSSION

We describe the two main sets of results for the FIR and the optical transitions, as well as diagnostic fine ratios.

3.1 Far-infrared transitions

The BPRM collision strengths for the two FIR fine-structure transitions 88, 52 \( \mu \)m are shown in Figs 1a and b. Although the resonance structures look similar, the magnitude and energy variations are not the same. The Maxwellian averaged effective collision strengths \( \gamma(T_e) \) are quite different, as shown in Fig. 2. While \( \gamma(T_e;2\Pi_{0,1} \rightarrow \Pi_{1}) \) for the 88-\( \mu \)m transition is relatively constant over three orders of magnitude in temperature, the \( \gamma(T_e;2\Pi_{0,1} \rightarrow \Pi_{2}) \) for the 52-\( \mu \)m transition varies by about a factor of 1.5 from the low-temperature limit of 100 K to temperatures \( T_e > 10,000 \) K. A comparison with the earlier work by Aggarwal & Keenan (1999) is shown as dashed lines, which range down to their lowest.
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Figure 1. Collision strengths for the [O iii] IR fine-structure transitions $2\pi^2(\Pi_2^0-\Pi_2^1, \Pi_2^1-\Pi_2^2)$ at (a) 88 $\mu$m and (b) 52 $\mu$m, respectively. High resolution at near-threshold energies is necessary for accuracy in rate coefficients at low temperatures. The top panel shows an expanded view in the region $E \leq 1$ Rydberg; both transitions have similar resonance structures.

Figure 2. Maxwelian averaged effective collision strengths $\gamma(T_c)$ (equation 1) for the transitions $\Pi_2^0-\Pi_2^1$ at 88 $\mu$m and $\Pi_2^1-\Pi_2^2$ at 52 $\mu$m (solid lines; cf. Fig. 1). Previous results without relativistic effects (Aggarwal & Keenan 1999) are also shown (dashed lines) in the temperature range available $T_c \geq 2500$K.

Figure 3. The density and temperature dependence of the 5288 $\mu$m line ratios; (a) the solid curves are present results at 2500 and 30000 K and the dashed lines are using the Aggarwal & Keenan (1999) effective collision strengths; (b) 5288 ratio at temperatures $100 \leq T(K) \leq 10000$.

The line ratio decreases rapidly for $T < 1000$K to almost flat at 100 K. The low-temperature regime $100 \leq T(K) \leq 1000$ is therefore indicated by the curves shown in Fig. 3b, as well as the limit where the 5288 ratio is temperature invariant. Therefore, the 5288 ratio is excellent density diagnostics in the typical density range $N_e \sim 3 \times 10^4$ for $T_c > 1000$K without much dependence on temperature (Fig. 3a). However, at lower temperatures the ratio may differ by up to a factor of 10 (Fig. 3b). Whereas the primary variations are owing to the exponential factors in $\gamma(T_c)$ (equation 3), we emphasize the role of relativistic fine-structure splitting between the $\Pi_{0,1,2}$ levels and near-threshold resonances lying in between.

3.2 Forbidden optical transitions

Fig. 4 shows the collision strengths for the optical transitions $^{3}\Pi_{1} \rightarrow {^{1}\Sigma_{2}}, {^{3}\Pi_{2} \rightarrow {^{1}\Sigma_{2}}, {^{3}\Pi_{2} \rightarrow {^{1}\Pi_{2}}}$ at $\lambda\lambda 4959$, 5007, 4363, respectively. The effective collision strengths for the [O iii] optical lines are shown in Fig. 5. These also differ significantly from previously available ones by up to 15 per cent. The new results are also obtained down to 100 K; their limiting values at low temperatures tend to 0.40.6x1.0. Since $\lambda\lambda 4959$, 5007 are often blended, it is common to plot the blended line ratio (4959+5007)/4363 shown in Fig. 6. This ratio

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3.3 Maxwellian averaged collision strengths

In Table 1 we present the effective collision strengths (equation 3) for the 10 transitions among the ground configuration levels and their wavelengths. The tabulation is carried out at a range of temperatures typical of nebular environments, including the low-temperature range \( T_e \leq 1000 \text{K} \) not heretofore considered.

3.4 Conclusion

Improved collision strengths including fine structure with relativistic effects are computed. Owing to the diagnostic importance of the \([\text{O} \text{ii}]\) forbidden FIR and optical lines, the relatively small but significant differences of up to 20 per cent should provide more accurate line ratios. Particular attention is paid to the resolution of resonances in the very small energy region above threshold(s), enabling the study of low-temperature behaviour.

The line emissivities and ratios computed in this work demonstrate the temperature-density behaviour at low temperatures and at typical nebular temperatures. However, depending on the astrophysical sources, a complete model of fine emissivities may also need to take into consideration the Bowen fluorescence mechanism: the radiative excitation of \( 2^3 \text{P}_2 \rightarrow 2^3 \text{P}_1 \rightarrow 2^3 \text{S}_1 \) by \( \text{He}\text{II L}\gamma \) at 304 Å and cascades into the upper levels of the forbidden transitions considered herein (e.g., Sanaph & Seaton 1970; Pradhan 
& Nahar 2011). In addition, for higher temperatures \( T_e > 20,000 \text{K} \) proton impact excitation of the ground state fine-structure levels \( 2^3 \text{P}_1,2 \) needs to be taken into account; at lower temperatures the excitation rate coefficient due to electrons far exceeds that due to protons (Ryan et al., 1999). Finally, there may be some contribution from \((e + \text{ion})\) recombination from \([\text{O} \text{n}]\) to \([\text{O} \text{ii}]\), since recombination rate coefficients increase sharply towards lower temperatures, while collisional excitation rates decrease level-specific and total recombination rate coefficients may be obtained from S. N. Nahar’s data base Nahar-OSU-Radiative-Data (NORAD) at www.astronomy.ohio-state.edu/nahar). Recombination contribution depends on the \([\text{O} \text{n}]\)[\text{O} \text{ii}]\) ionization fraction, which at low temperatures would be small.

**ACKNOWLEDGMENTS**

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**Table 1.** Effective Maxwellian averaged collision strengths.

<table>
<thead>
<tr>
<th>Transition</th>
<th>( \lambda )</th>
<th>( \Upsilon(100) )</th>
<th>( \Upsilon(5000) )</th>
<th>( \Upsilon(10000) )</th>
<th>( \Upsilon(50000) )</th>
<th>( \Upsilon(100000) )</th>
<th>( \Upsilon(200000) )</th>
<th>( \Upsilon(300000) )</th>
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</thead>
<tbody>
<tr>
<td>( 2^3 \text{P}_1 \rightarrow 2^3 \text{P}_1 )</td>
<td>88 μm</td>
<td>5.814(−1)</td>
<td>5.005(−1)</td>
<td>4.866(−1)</td>
<td>5.240(−1)</td>
<td>5.648(−1)</td>
<td>6.007(−1)</td>
<td>6.116(−1)</td>
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<tr>
<td>( 2^3 \text{P}_2 \rightarrow 2^3 \text{P}_0 )</td>
<td>33 μm</td>
<td>2.142(−1)</td>
<td>2.153(−1)</td>
<td>2.234(−1)</td>
<td>2.469(−1)</td>
<td>2.766(−1)</td>
<td>3.106(−1)</td>
<td>3.263(−1)</td>
</tr>
<tr>
<td>( 2^3 \text{P}_2 \rightarrow 2^3 \text{P}_1 )</td>
<td>52 μm</td>
<td>1.036(0)</td>
<td>1.032(0)</td>
<td>1.072(0)</td>
<td>1.210(0)</td>
<td>1.330(0)</td>
<td>1.451(0)</td>
<td>1.499(0)</td>
</tr>
<tr>
<td>( 1^3 \text{D}_2 \rightarrow 2^3 \text{P}_0 )</td>
<td>4933 Å</td>
<td>1.959(−1)</td>
<td>2.088(−1)</td>
<td>2.154(−1)</td>
<td>2.347(−1)</td>
<td>2.693(−1)</td>
<td>3.094(−1)</td>
<td>3.258(−1)</td>
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<td>( 1^3 \text{D}_2 \rightarrow 2^3 \text{P}_1 )</td>
<td>4999 Å</td>
<td>5.903(−1)</td>
<td>6.287(−1)</td>
<td>6.483(−1)</td>
<td>7.067(−1)</td>
<td>8.108(−1)</td>
<td>9.313(−1)</td>
<td>9.802(−1)</td>
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<tr>
<td>( 1^3 \text{D}_2 \rightarrow 2^3 \text{P}_2 )</td>
<td>5007 Å</td>
<td>9.934(−1)</td>
<td>1.056(0)</td>
<td>1.089(0)</td>
<td>1.188(0)</td>
<td>1.365(0)</td>
<td>1.568(0)</td>
<td>1.645(0)</td>
</tr>
<tr>
<td>( 1^3 \text{S}_0 \rightarrow 1^3 \text{D}_2 )</td>
<td>4365 Å</td>
<td>3.900(−1)</td>
<td>3.898(−1)</td>
<td>3.890(−1)</td>
<td>4.543(−1)</td>
<td>5.661(−1)</td>
<td>6.230(−1)</td>
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<td>( 1^3 \text{S}_0 \rightarrow 1^3 \text{S}_1 )</td>
<td>2321 Å</td>
<td>1.756(−1)</td>
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<td>1.747(−1)</td>
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<td>2.421(−1)</td>
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<td>2317 Å</td>
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