OMEUPS : AN INTERACTIVE GRAPHICS PROGRAM FOR ANALYSING COLLISION DATA

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Résumé – Le but du programme OMEUPS, qui fonctionne sur des micro-ordinateurs, est de fournir un moyen simple pour analyser et compacter des données atomiques (forces de collision) pour l'excitation des ions positifs par choc électronique. Le programme est interactif et permet l'analyse graphique des données: il doit être d'un intérêt particulier aux astrophysiciennes et aux astrophysiciens aussi bien qu'aux spécialistes de la physique atomique. La méthode sur laquelle le programme est basé permet à l'utilisateur d'interpoler où d'extrapoler des données existantes en fonction de l'énergie et de la température; de stocker des données dans une forme compacte sans perdre de l'information significative; de faire des moyennes de Maxwell; de déceler des erreurs d'imprimerie et de calcul dans des données tabulées.

Abstract – The aim of the micro-computer program OMEUPS is to provide a simple means of critically assessing and compacting collision strength data for electron impact excitation of positive ions. The program is interactive and allows data to be analysed graphically: it should be of particular interest to astrophysicists as well as to those specialising in atomic physics. The method on which the program is based allows one to interpolate or extrapolate existing data in energy and temperature; store data in compact form without losing significant information; perform Maxwell averaging; detect printing and computational errors in tabulated data.

1 – OMEUPS

This is an interactive program written by one of us (A.B.) which is based on a new method for analysing atomic collision data. It is easy to use even by non-specialists in atomic physics. The program is in BBC BASIC and is designed to run on ACORN microcomputers: BBC models B, B+, Master and Archimedes. With a suitable emulator⁽¹⁾ it also runs on the Macintosh and IBM micros (or clones) that have graphics. The present program grew out of an earlier version which was developed by A. Burgess, J. Lang and J. Payne for use on a Hewlett Packard System 45 at the Rutherford-Appleton Laboratory.

⁽¹⁾Available from Human Computer Interface Ltd., 25 City Road, Cambridge CB1 1DP, U.K. for the Macintosh and from M-Tec Computer Services, The Market Place, Reepham, Norfolk NR10 4JJ, U.K. for IBM micros.

OMEUPS has two branches labelled OMEGA and UPSILON. As the names suggest these are for analysing energy-dependent collision strengths $\Omega(E)$ and thermally averaged collision strengths $\Upsilon(T)$. The method is designed to analyse data for the following 4 types of transition in positive ions.

1. Electric dipole (optically allowed).
2. Electric multipole other than dipole (optically forbidden).
3. Exchange (spin change, i.e. intersystem or intercombination).
4. Electric dipole with abnormally small oscillator strength.

The originality of the method arises from the use of scaling techniques which (i) remove the main energy or temperature dependence from the data and (ii) map the entire range of E or T onto the interval $[0,1]$. The appropriately scaled or reduced variables are denoted by (E_{red}, Ω_{red}) and $(T_{red}, \Upsilon_{red})$.

Let $x \equiv E_{red}$ and $y \equiv \Omega_{red}$ be the reduced variables used in OMEGA. They are defined as follows for the 4 types of transition:

$$\text{Type 1: } x = 1 - \ln(C)/\ln(E_j/E_{ij} + C), \quad y = \Omega_{ij}/\ln(E_j/E_{ij} + e), \quad (C > 1); \quad (1)$$

$$\text{Type 2: } x = (E_j/E_{ij})/(E_j/E_{ij} + C), \quad y = \Omega_{ij}, \quad (C > 0); \quad (2)$$

$$\text{Type 3: } x = \text{as for type 2}, \quad y = (E_j/E_{ij} + 1)^2 \Omega_{ij}, \quad (C > 0); \quad (3)$$

$$\text{Type 4: } x = \text{as for type 1}, \quad y = \Omega_{ij}/\ln(E_j/E_{ij} + C), \quad (C > 1). \quad (4)$$

The indices i and j label the lower and upper energy levels. E_j is the energy of the colliding electron *after* excitation and E_{ij} is the transition energy. The parameter C depends on the ion and transition in question; its value can be chosen to optimise the plot of y versus x . e is the base of Napier's logarithm.

In UPSILON the reduced variables are $x \equiv T_{red}$ and $y \equiv \Upsilon_{red}$. These are defined as follows:

$$\text{Type 1: } x = 1 - \ln(C)/\ln(kT/E_{ij} + C), \quad y = \Upsilon_{ij}/\ln(kT/E_{ij} + e), \quad (C > 1); \quad (5)$$

$$\text{Type 2: } x = (kT/E_{ij})/(kT/E_{ij} + C), \quad y = \Upsilon_{ij}, \quad (C > 0); \quad (6)$$

$$\text{Type 3: } x = \text{as for type 2}, \quad y = (kT/E_{ij} + 1) \times \Upsilon_{ij}, \quad (C > 0); \quad (7)$$

$$\text{Type 4: } x = \text{as for type 1}, \quad y = \Upsilon_{ij}/\ln(kT/E_{ij} + C), \quad (C > 1). \quad (8)$$

After introducing data to the OMEGA branch of the program and providing an initial estimate for C , Ω_{ij} is transformed to Ω_{red} and displayed as a function of E_{red} . It may be desirable to replot with a different value for C , the effect of increasing (decreasing) C being to move the data points towards the left (right) hand side of the graph as well as modifying the separation between adjacent points. The program then calculates a least-squares spline fit to the data and draws the corresponding curve on the screen. The values of Ω_{red} at the 5 equally distributed knots (i.e. $E_{red} = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1$) are displayed on the right hand side of the screen. There exists an option for printing the contents of the screen. The root mean square (r.m.s.) error of the fit is typically less than 1%. The original data can be interpolated or extrapolated to good accuracy by means of the spline function. A short program for doing this is given in /1/.

If Ω_{ij} shows complicated resonance structure then it cannot be treated by OMEUPS. However the thermally averaged collision strength Υ_{ij} will in general be a smoothly varying function of temperature T , and can be processed in the UPSILON branch of the program. The five-point spline procedure described

above is used to fit the reduced thermally averaged collision strength Υ_{red} . In this way the original data is conveniently interpolated and extrapolated.

2 -- Maxwell averaging

The OMEGA menu has an option for evaluating $\Upsilon_{ij}(T)$ by performing the Maxwell average of Ω_{ij} , i.e.

$$\Upsilon_{ij}(T) = \int_0^\infty \Omega_{ij} \exp(-E_j/kT) d(E_j/kT). \quad (9)$$

An N-point Gauss-Laguerre approximation is used to calculate this integral. The program offers a choice of N (viz. 5, 10, 15, 20). The appropriate values of Ω_{ij} for use in the quadrature formula are obtained from the interpolating spline. The number of temperatures for which Υ_{ij} is to be calculated is set by the user. The temperatures are then selected automatically in order to divide the entire range of T_{red} into approximately equal intervals. The data so obtained can then be reduced and splined in the UPSILON branch of OMEUPS.

The line excitation rate coefficient $q(i \rightarrow j)$ is given in terms of Υ_{ij} by the following relationship

$$q(i \rightarrow j) = 2\pi^{\frac{1}{2}} a_0 \hbar m^{-1} (I_\infty/kT)^{\frac{1}{2}} \exp(-E_{ij}/kT) \Upsilon_{ij}/g_i \quad (10)$$

where $2\pi^{\frac{1}{2}} a_0 \hbar m^{-1} = 2.1716 \times 10^{-18} \text{ cm}^3 \text{ s}^{-1}$, I_∞ is the rydberg energy (13.6058 eV) and g_i is the statistical weight of level i . The rate coefficient $q(j \rightarrow i)$ for collisionally de-exciting a line is given by

$$q(j \rightarrow i) = (g_i/g_j) \exp(E_{ij}/kT) q(i \rightarrow j). \quad (11)$$

3 -- High energy and temperature limits

$\Omega_{red}(1)$ is the limit to which Ω_{red} tends as $E_j/E_{ij} \rightarrow \infty$; similarly $\Upsilon_{red}(1)$ is the limit to which Υ_{red} tends as $T \rightarrow \infty$. Numerical values for the limits can be obtained fairly easily except in the case of $\Upsilon_{red}(1)$ for a type 3 transition. They are extremely useful for our purposes but have rarely been used in past extrapolation procedures. The reduced variable definitions lead to the following expressions for the limits:

$$\text{Type 1: } \Omega_{red}(1) = \Upsilon_{red}(1) = 4g_i f_{ij}/E_{ij}, \quad (12)$$

$$\text{Type 2: } \Omega_{red}(1) = \Upsilon_{red}(1) = \lim\{\Omega_{ij}\}, \quad (13)$$

$$\text{Type 3: } \Omega_{red}(1) = \lim\{(E_j/E_{ij})^2 \Omega_{ij}\}, \quad \Upsilon_{red}(1) = \int_0^\infty \Omega_{ij} d(E_j/E_{ij}), \quad (14)$$

$$\text{Type 4: } \Omega_{red}(1) = \Upsilon_{red}(1) = 4g_i f_{ij}/E_{ij}. \quad (15)$$

Note that f_{ij} is the absorption oscillator strength and the energy unit is the rydberg (i.e. 13.6058 eV). The limiting value for a type 2 transition is given by the Born approximation, and that for a type 3 transition by the Ochkur approximation. If the appropriate limiting value is known then it can be input to the program and will be used in the least squares fitting procedure. However, if this data point is not available then the user may be required to estimate one or more of the knots before the spline can be drawn.

4 - Examples

The main impetus behind the development of the program was the need for a convenient means of representing collision data in compact form. This is illustrated in the first example which concerns the intersystem transition $2s^2 2p^2 \ ^2P^\circ \rightarrow 2s 2p^2 \ ^4P$ in boron-like oxygen. Hayes /2/ calculated Ω for many transitions in O^{+3} with a close-coupling approximation and then thermally averaged her results to obtain Υ at 15 temperatures in the range $1 \leq T/10^4 \leq 22$. Her data points for Υ_{red} are plotted in Fig. 1 which also shows the spline fit corresponding to a minimum r.m.s. error of 0.27% ($C = 0.75$). The 5 knot values which define the interpolating spline curve are listed alongside the graph. In the present case the value of $\Upsilon_{red}(1)$ was not available, for the integral in (14) had not been evaluated. Knowing the high temperature limit in advance enhances confidence in the fit since the program can then interpolate across the region from the last data point to $T = \infty$.

Our second example illustrates how the program can be used to evaluate Υ from Ω . Fig. 2 shows Ω_{red} for the type 1 transition $2s^2 2p^3 \ ^4S^\circ \rightarrow 2s 2p^4 \ ^4P$ in O^+ , the data points being generated from the analytic fit which Ho and Henry /3/ used to interpolate their 2-state close-coupling results. The figure includes the Bethe-Born limit $\Omega_{red}(1) = 3.304$ which is denoted by an asterisk. This was calculated in the program from the oscillator strength (0.233) and transition energy ($1.128I_\infty$) given in /3/. Ho and Henry's interpolation formula is unsuitable for extrapolating to impact energies beyond $6I_\infty$; this is clear from Fig. 2 since the data points do not tend towards the Bethe-Born limit. The figure also shows a spline curve which is an optimised least squares fit to Ho and Henry's data in the region $E_i \leq 6$ and the high energy limit point. The parameter C has the value 2.3 and the r.m.s. error is 0.01%. The program uses this fit in order to perform the Maxwell averaging with a 20 point Gauss-Laguerre formula. The resulting plot of $\Upsilon_{ij}(T)$ is given in Fig. 3 together with the interpolating curve which corresponds to the spline fit for $\Upsilon_{red}(T_{red})$.

Ω is obtained by summing partial collision strengths and sufficient of these should be included to ensure convergence. It is generally well known that distant encounters can make important contributions for type 1 transitions; fortunately these can be allowed for by using Burgess's /4/ sum rule. However for other types of transition many investigators truncate the expansion at an arbitrary value of L , which is independent of energy, and ignore the effect of higher partial waves. As an example we plot Ω_{red} in Fig. 4 for the $2p^2 \ ^1D \rightarrow 2p^2 \ ^1S$ transition in Mg^{+6} , corresponding to the collision strength which Aggarwal /5/ calculated with a 12-state close-coupling approximation. Aggarwal included partial waves up to $L = 12$ and consequently his high energy data points fall short of the Born limit $\Omega_{red}(1) = 0.1983$ which we calculated using the Born integral given in /6/ and mixing coefficients from /5/.

Errors are occasionally introduced during the preparation of tables or they may arise from other causes; the present method provides a handy means of checking tabulated data. Fig. 5 shows Υ data from /7/ in reduced form for the transition $2p^5 \ ^2P^\circ \rightarrow 2p^4 3s \ ^2D$ in fluorine-like S^{+7} . The figure illustrates very clearly how much easier it is to spot errors on a graph than in a table. It also underlines the importance of knowing the f value for a type 1 transition. Unfortunately Mohan *et al.* /7/ did not include their oscillator strengths but these were kindly supplied to us recently by Dr. Mohan. Using $gf = 0.402$ and $E_{ij} = 14.8323$ we obtain the high temperature limit point in Fig. 5 which is depicted by an asterisk. From the plot we see that the first two data points are consistent with the Bethe-Born limit and this suggests

that the remaining 18 are incorrect, being apparently underestimated by a factor 10. It is interesting to note that after correction we were able to make a satisfactory spline fit to the data (r.m.s. error = 0.57%, $C = 1.12$) by treating this as a type 4 transition rather than a type 1.

We conclude with some examples for magnesium-like Si^{+2} . Dufton and Kingston /8/ have warned astronomers against using the atomic data for this ion tabulated by Baluja *et al.* /9/. The reason why some of the 1981 results are wrong was traced to a programming error in the collision code; this was corrected and P. L. Dufton then redid the 12-state close-coupling calculation. Instead of tabulating his results for $\Upsilon(T)$, Dufton felt it was more convenient to fit them to polynomials in $\log(T)$. These, however, are only valid in the interval $3.8 \leq \log(T) \leq 5.2$. The fitting parameters are given in /8/. It is instructive to compare results from /8/ and /9/ using OMEUPS in order to test the potential of our method for showing up errors arising from a faulty calculation.

In Fig. 6 we plot data from /8/ and /9/ for the type 2 transition $3s^2 \ ^1S \rightarrow 3s3d \ ^1D$. The asterisk denotes the high temperature limit point (1.646) which we calculated by means of the Born approximation. Without this point one would be hard put to it to know which of the two data sets is the correct one. Curve D (data from /8/) tends towards the Born limit whereas curve B (data from /9/) does not.

The $3s3d \ ^1D$ and $3p^2 \ ^1D$ terms of Mg-like ions interact strongly; for example, in Si^{+2} the mixing coefficients are (0.7650, -0.5445) for the $3s3d$ term and (-0.7970, -0.5917) for the $3p^2$ term. These values are for the wave functions defined in /10/. It is therefore of particular interest to make a comparison, similar to the one in Fig. 6, for the $3s^2 \ ^1S \rightarrow 3p^2 \ ^1D$ transition in Si^{+2} . This is done in Fig. 7, where we have the surprising result that curve B appears to be the correct one since it tends towards the Born limit (2.277) which we have calculated. We can make two pertinent comments on this strange state of affairs. Firstly, the curve B is actually veering away from the Born limit at the highest temperatures. This may be a real effect or it may be due to lack of convergence in the partial wave expansion. Secondly, the collision strength for this transition, which is stored in the atomic data bank at The Queen's University of Belfast, is in fact an increasing function of energy for $E_i \geq 2.0$ and tends towards our calculated Born limit. There is however one proviso, namely that one must include the contribution to Ω from all partial waves with $L > 12$. Like Baluja *et al.* /9/ it appears that Dufton and Kingston /8/ did not. Clearly a more thorough examination of this curious case is called for. It is unfortunate that the parametric fit reported in /8/ does not allow us to estimate Υ at temperatures above 16×10^4 K.

Fig. 8(a) is a plot of the Si^{+2} data from /9/ for the transition labelled 3-4, i.e. $3s3p \ ^1P^\circ \rightarrow 3p^2 \ ^1D$. The high temperature limit, which is denoted by an asterisk, was calculated in the program using the gf value 0.1242 from /10/. There is a striking discrepancy since the data points do not tend towards the asterisk. It should be noted that Baluja *et al.* /9/ only allowed for partial waves up to $L = 12$ and this presumably explains why Υ_{red} begins to fall off as T_{red} approaches 1. A plot of the data from /9/ for the transition labelled 3-10 (namely $3s3p \ ^1P^\circ \rightarrow 3s3d \ ^1D$) shows a similar discrepancy. From this it appears that the Υ values for these two $^1P^\circ \rightarrow ^1D$ transitions may have been interchanged during preparation of the tables in /9/. Fig. 8(b) is presented in order to test this hypothesis. Here we plot the data from /9/ for the transition labelled 3-4 assuming that it is in fact the transition 3-10. Our hypothesis seems plausible, although of course the programming error referred to above may be the true cause of this 'mixup'.

References

- /1/ Burgess, A., Mason, H. E. and Tully, J. A., *Astron. Astrophys.* **217** (1989) 319.
- /2/ Hayes, M. A., *J. Phys. B: At. Mol. Phys.* **16** (1983) 285.
- /3/ Ho, Y. K. and Henry, R. J. W., *Astrophys. J.* **264** (1983) 733.
- /4/ Burgess, A., *J. Phys. B: Atom. Molec. Phys.* **7** (1974) L364.
- /5/ Aggarwal, K. M., *Astrophys. J. Suppl. Ser.* **56** (1984) 303.
- /6/ Tully, J. A., 11^{ème} Colloque National: Physique des Collisions Atomiques et Electroniques, Metz 18-20 juin (1986).
- /7/ Mohan, M., Baluja, K. L. and Hibbert, A., *J. Phys. B: At. Mol. Phys.* **20** (1987) 2565.
- /8/ Dufton, P. L. and Kingston, A. E., *Mon. Not. R. Astr. Soc.* **241** (1989) 209.
- /9/ Baluja, K. L., Burke, P. G. and Kingston, A. E., *J. Phys. B: At. Mol. Phys.* **14** (1981) 1333.
- /10/ Baluja, K. L. and Hibbert, A., *J. Phys. B: Atom. Molec. Phys.* **13** (1980) L327.

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Figures

Fig. 1 - $O^{+3}(2s^2 2p^2 P^o \rightarrow 2s 2p^2 {}^4P)$. Optimized spline fit to data from /2/. $C = 0.75$, r.m.s. = 0.27%. Knot values of the spline are listed alongside the graph.

Fig. 2 - $O^+(2s^22p^3\ ^4S^\circ \rightarrow 2s2p^4\ ^4P)$. Optimized spline fit to the encircled data points from /3/. $C = 2.3$, r.m.s. = 0.01%. The high energy limit point is based on the f_L value given in /3/. The spline knot values are listed alongside the graph.

Fig. 3 - $O^+(2s^22p^3\ ^4S^\circ \rightarrow 2s2p^4\ ^4P)$. $\Upsilon(T)$ from Υ_{red} calculated using the spline in Fig. 2.

Fig. 4 - $Mg^{+6}(2p^2 \ ^1D \rightarrow 2p^2 \ ^1S)$. Data from /5/. The asterisk is the high energy Born limit. $C = 39$.

Fig. 5 - $S^{+7}(2p^5 \ ^2P^o \rightarrow 2p^4 3s \ ^2D)$. Data from /7/. The high temperature limit point corresponds to the f value from Mohan and Hibbert (Physica Scripta, to be published). $C = 1.1$.

Fig. 6 - $\text{Si}^{+2}(3s^2 \ ^1S \rightarrow 3s3d \ ^1D)$. Curve D, data from /8/; curve B, data from /9/. The high temperature limit point (denoted by an asterisk) is based on the Born approximation. $C = 0.2$.

Fig. 7 - $\text{Si}^{+2}(3s^2 \ ^1S \rightarrow 3p^2 \ ^1D)$. Curve D, data from /8/; curve B, data from /9/. The high temperature limit point (denoted by an asterisk) is based on the Born approximation. $C = 0.2$.

Fig. 8(a) - $\text{Si}^{+2}(3s3p\ ^1P^o \rightarrow 3p^2\ ^1D)$. Data from /9/ for the transition labelled 3-4. The high temperature limit point is based on the f value from /10/. $C = 1.4$.

Fig. 8(b) - $\text{Si}^{+2}(3s3p\ ^1P^o \rightarrow 3s3d\ ^1D)$. Data from /9/ for the transition labelled 3-4. The high temperature limit point is calculated using the f value from /10/. $C = 1.2$.