Computer Physics Communications 182 (2011) 1528–1535

Contents lists available at ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc

A Breit–Pauli distorted wave implementation for AUTOSTRUCTURE ☆

N.R. Badnell

Department of Physics, University of Strathclyde, Glasgow, G4 0NG, UK

ARTICLE INFO

Article history:
Received 11 November 2010
Received in revised form 18 March 2011
Accepted 22 March 2011
Available online 6 April 2011

Keywords:
Atomic collisions
Electron-impact excitation
Distorted wave method

ABSTRACT

We describe the Breit–Pauli distorted wave (BPDW) approach for the electron-impact excitation of atomic ions that we have implemented within the AUTOSTRUCTURE code.

Program summary

Program title: AUTOSTRUCTURE
Catalogue identifier: AEIV_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEIV_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 130 987
No. of bytes in distributed program, including test data, etc.: 1 031 584
Distribution format: tar.gz
Programming language: Fortran 77/95
Computer: General
Operating system: Unix
Has the code been vectorized or parallelized?: Yes, a parallel version, with MPI directives, is included in the distribution.
RAM: From several kbytes to several Gbytes
Classification: 2, 2.4
Nature of problem: Collision strengths for the electron-impact excitation of atomic ions are calculated using a Breit–Pauli distorted wave approach with the optional inclusion of two-body non-fine-structure and fine-structure interactions.
Solution method: General multi-configuration Breit–Pauli atomic structure. A *jK*-coupling partial wave expansion of the collision problem. Slater state angular algebra. Various model potential non-relativistic or kappa-averaged relativistic radial orbital solutions — the continuum distorted wave orbitals are not required to be orthogonal to the bound.
Additional comments: Documentation is provided in the distribution file along with the test-case.
Running time: From a few seconds to a few hours.

1. Introduction

An accurate description of the electron-impact excitation of atomic ions continues to challenge state-of-the-art methods such as convergent close-coupling [1], *R*-matrix close-coupling [2] and time-dependent close-coupling [3] on the largest of (parallel) computers. For 'simple' systems it may be due to the requirement of a complete description of all scattering parameters or just total cross sections in the case of highly-excited states. For 'complex' systems the number of scattering channels themselves can be overwhelming. Spectroscopic diagnostic modelling of astrophysical and laboratory plasmas has a large appetite for electron-impact excitation rate coefficients since they largely determine the emitting population distribution within a charge state. The close-coupling method can in principle provide excitation data between all target states included in its expansion. The nature of a plasma ion's population distribution favours an alternative

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

E-mail address: badnell@phys.strath.ac.uk.

0010-4655/$ – see front matter
doi:10.1016/j.cpc.2011.03.023

approach — distorted wave (DW) — which neglects coupling via any intermediate state for a transition between a given initial and final state. The bulk of an ion's population resides in a few low-lying metastable states while the population of the remaining excited states is small. The population of the diagnostically important excited states is largely driven by direct electron-impact excitation from these metastables followed by radiative decay. Transitions between excited states can be neglected or be described by a simpler method such as plane-wave Born (PWB). The DW method is an efficient computational reflection of the dominant physics. Such a picture describes most non-equilibrium astrophysical and magnetic fusion plasmas. This is not quite the full picture. Resonances in electron scattering are a manifestation of coupling and are automatically included within a close-coupling calculation. They can strongly enhance low temperature rate coefficients for weak transitions. It is up to the user whether or not they are included independently (perturbatively) in a DW calculation.

A number of codes have been developed over the years which are general both in the sense of the ion that they treat and the electron collision processes which they describe. These include the Hebrew University Lawrence Livermore Atomic Code (HULLAC) [4], the Flexible Atomic Code (FAC) [5] and the Los Alamos DW (LADW) code suite of Sampson and co-workers [6]. All three use fully relativistic wavefunctions and optionally include the Breit interaction besides the two-body Coulomb. They all make use of a hierarchical Racah algebra angular momentum coupling scheme which is factorized for efficiency. Cowan's structure code [7] is also in widespread use. It uses kappa-averaged relativistic wavefunctions while its treatment of electron-impact excitation is restricted to the plane-wave Born approximation — but that does make it highly efficient. The University College London DW code [8] has been used extensively in the past for electron-impact excitation but less so now perhaps. It uses non-relativistic wavefunctions and level-resolved cross sections are determined[1] by term-coupling LS-coupling scattering matrices using the JAJOM code [10]. It is notable in that it takes a completely different approach to the angular momentum problem. It uses the non-hierarchical uncoupled Slater state representation. It is here we make the connection with the present approach and the AUTOSTRUCTURE code [11].

AUTOSTRUCTURE is a general code [11] for the description of free-bound electron and photon collision processes [12]. It also describes a wide variety of bound-state problems since it incorporates the SUPERSTRUCTURE atomic structure code [13]. It makes use of non-relativistic or kappa-averaged relativistic wavefunctions and the full Breit interaction in the Pauli approximation. It is particularly noted-for and efficient-in its description of dielectronic recombination (DR) which takes place through large numbers of highly-excited states. DR can be viewed as the complement of resonant-excitation. In this (DR) connection it has been intimately involved in defining standards for the Atomic Data and Analysis Structure (ADAS) [14] collisional–radiative modelling of magnetic fusion plasmas. Light elements have historically dominated magnetic fusion devices such as JET [15] and the R-matrix method has been able to supply the key excitation data. The prospect of the larger (hotter) ITER device [16] means that extensive studies are now underway for the diagnostic modelling of heavy species such as Kr, Xe, W, etc., which likely will be in use. The R-matrix approach will be more limited in its practical application here and so we seek to extend AUTOSTRUCTURE to provide direct non-resonant DW excitation data efficiently and tailored to the needs of magnetic fusion. It is also equally applicable to astrophysical data needs such as the excitation of highly excited states.

The historical emphasis of the DW approach for electron-impact excitation was to mimic the close-coupling method as closely as possible [8,17]. It is questionable whether the ultimate result of the most accurate DW calculation possible — an exact treatment of all (diagonal) distorting potentials and full unitarization — is worth the cost compared to an R-matrix calculation. Our philosophy is to seek a CPU time and memory efficient solution at a judgemental cost of a slightly less accurate final DW result but one for which uncertainties in atomic structure and the effect of resonances are likely to be more important. We are also more concerned with Maxwell-averaged effective collision strengths at temperatures of broad ionic abundance than the underlying ordinary collision strengths at all energies equally.

The focus of this paper is to describe such a Breit–Pauli distorted wave approach for the electron-impact excitation of atomic ions[2] that we have implemented within AUTOSTRUCTURE. We also highlight related relevant aspects of its atomic structure determination and representation. We do not repeat details of the theory which are common to the SUPERSTRUCTURE [13] and/or UCL-DW [8] codes nor do we discuss bound-free processes which were the basis of the original implementation [12] of AUTOSTRUCTURE.

2. Target representation

Eissner et al. [13] describe the theory behind the full Breit–Pauli atomic structure. (The two-body non-fine-structure operators were not actually incorporated into SUPERSTRUCTURE at the time but only into AUTOSTRUCTURE some time later [18].) It is instructive to look at aspects of the Slater state approach to the angular momentum problem. (All quantities are assumed to be for fixed total spin and orbital magnetic quantum numbers $M_S M_L$.)

A Slater state $|u\rangle$ is defined by

$$|u\rangle = \prod_{q=1}^{N} |n_q l_q \mu_q m_q\rangle \tag{1}$$

where $n_q l_q \mu_q m_q$ represent the one-electron quantum numbers $nlm_s m_l$ for the q-th electronic state of an N-electron wavefunction and they are subject to

$$M_S = \sum_{q=1}^{N} \mu_q \quad \text{and} \quad M_L = \sum_{q=1}^{N} m_q. \tag{2}$$

Antisymmetrization is imposed by permuting the sets $(n_q l_q \mu_q m_q)$. Slater determinants are never explicitly used.

The interaction of any required operator O is first determined in the uncoupled representation

$$\langle u' | O | u \rangle. \tag{3}$$

[1] Jones [9] proposed a Breit–Pauli version of the UCL-DW code but it was never implemented.

[2] The code also works for neutral atoms but the accuracy of the DW method is likely not high then.

Eissner et al. [13] give explicit expressions for all Breit–Pauli operators evaluated in the uncoupled representation. The uncoupled representation is then transformed to a coupled representation labelled by $t = C\beta SL$ via

$$|t\rangle = |u\rangle\langle u|t\rangle \tag{4}$$

so as to efficiently sum over all of the one-electron magnetic quantum numbers. The final result is independent of the particular choice of $M_S M_L$. The N-electron vector-coupling coefficients $\langle u|t\rangle$ are defined by Eissner and Nussbaumer [19]. The t-representation is labelled by (nl) configuration C and total spin (S) and orbital (L) angular momentum quantum numbers and a degeneracy label β which reflects the fact that the same total SL-values can occur many times in a complex configuration. We note that we have no parentage or grandparentage, etc., just a simple configuration and βSL to fully label each term.

The historic implementation of Slater state algebra within the UCL suite of codes was an efficient balance of CPU time and memory for the size of problems that could be tackled on the computers of the day. Three non-trivial changes produce scalability to modern computers. The first is to note that β does not occur in Eq. (3) but only in Eq. (4) via $\langle u|t\rangle$. β was small historically and additional memory is required to store the uncoupled interaction. Memory is relatively more plentiful on modern machines and β is large for the complex configurations that can now be tackled. Up to a factor of ~ 30 speed-up was obtained [20] on re-organizing the angular algebra to take account of this before it became too tedious to run the old method. This approach carries-over to the scattering representation.

A second historic issue was the simultaneous diagonalization of the L^2 and S^2 matrices for each configuration so as to determine the allowed terms and vector-coupling coefficients $\langle u|t\rangle$. Such an approach does not scale well when there are thousands of terms in a configuration and it is numerically ill-conditioned due to the large degree of degeneracy (β) of eigenvalues. Nussbaumer and Storey [21] showed the way to an efficient solution. They split complex configurations into two groups: one of common (open-shell) parents and the other of the remaining daughters. The parents' and daughters' L^2 and S^2 matrices were simultaneously diagonalized separately and their (inequivalent) parts vector-coupled together. We have implemented a more efficient approach. We treat each configuration separately and within a configuration diagonalize each equivalent electron subshell (nl^q) in turn and then vector-couple it to the previous one. The worst case scenario for this new diagonalization procedure is a half-open h-shell and it takes less than a second to determine its allowed terms and transformation vector-coupling coefficients.

The third and final scalability improvement concerns the transformation vector-coupling coefficients themselves. If all possible values are stored then they can be stored in a way that allows any one to be recovered at random without any additional mapping array. This includes zeroes. It turns out that the 'matrix' of coefficients is quite sparse for large scale problems involving tens of thousands of terms. It is efficient then to store only the non-zero coefficients and to array-index their location. A significant reduction in memory is still achieved as well as a corresponding speed-up in their access. The original indexing then no longer approaches the limit for INTEGER*4 representation.

Now we consider the fine-structure operators. Only the total angular momentum (J) and its associated magnetic (M) quantum numbers are conserved now. We can work with the Slater states $|u\rangle$ still because we have no explicit j-dependence in our wavefunctions — we work with nl-configurations and not nlj-subconfigurations. We do need to consider that more than one $M_S M_L$ pair can contribute to our chosen M. This is reflected in the transformation from the t-representation to an $i = C\beta SLJ$ representation

$$|iM\rangle = |tM_S M_L\rangle\langle tM_S M_L|iM\rangle. \tag{5}$$

The vector-coupling coefficient is simply

$$\langle tM_S M_L|iM\rangle = (-1)^{L-S-M}(2J+1)^{1/2}\begin{pmatrix} S & L & J \\ M_S & M_L & -M \end{pmatrix} \tag{6}$$

where $(\cdots)$ is a Wigner $3j$-symbol [22].

The angular algebra is combined with the associated radial integrals in exactly the same manner as described by Eissner et al. [13] so as to form the Hamiltonians resolved by $SL\pi$ or $J\pi$ where π is the parity label. The t- and i-representations do not in general give rise to diagonal representations of the LS-coupling and Breit–Pauli Hamiltonians. They are transformed to diagonal $\bar{t}$- and $\bar{i}$-representations via

$$|\bar{t}\rangle = |t\rangle\langle t|\bar{t}\rangle \quad \text{and} \quad |\bar{i}\rangle = |i\rangle\langle i|\bar{i}\rangle \tag{7}$$

where $\langle\,|\,\rangle$ are eigenvectors of the appropriate Hamiltonian.

The differences between AUTOSTRUCTURE and SUPERSTRUCTURE on the radial side are more about functionality than efficiency. Alternative model potentials are available in addition to the original Thomas–Fermi–Dirac–Amaldi [13]. These include the Slater-Type-Orbital potential of Burgess [23] and the self-consistent configuration average potential of Cowan [7]. These potentials either deliver an orthogonal set of bound radial orbitals or else this is imposed via a Schmidt orthogonalization procedure. It is possible to relax the orthogonality requirement along the lines described by Cowan [7] and assume all overlaps are still zero or unity. The sensitivity to the neglect of the overlaps can be assessed by introducing the explicit overlaps which were originally taken to be unity.

We have already mentioned the optional use of the $\kappa = -1$ average of $j = l \pm 1/2$ (i.e. $\kappa = -l-1, l$) relativistic wavefunctions of Cowan and Griffin [24] which can also include an approximation for the small component. Sensitivity to higher-order relativistic effects can be assessed by the use of a non-zero energy for the transverse photon in the form of the real part of the Generalized Breit interaction. The QED vacuum polarization and electron self-energy contributions have also been incorporated along the lines of the GRASP0 code of Norrington — see Grant et al. [25]. A precise description of these effects requires a fully-relativistic approach but the present implementation is sufficient to assess their importance for any particular problem.

3. Scattering representation

We assume an antisymmetric total wavefunction Ψ for an atom described by an N-electron wavefunction ψ plus a colliding free electron described by a wavefunction ϕ of the form

$$\Psi = \mathcal{A}\psi\phi. \tag{8}$$

Several important assumptions are represented by Eq. (8). We do *not* assume the free-electron wavefunction to be orthogonal to those of the one-electron bound orbitals. This means that we do not require a compensating bound $(N+1)$-electron expansion. This means that in general we have one-body exchange operator overlap contributions present [26] when we come to evaluate the scattering interaction

$$\langle \Psi | H - E | \Psi' \rangle. \tag{9}$$

This does not lead to great complexity since we assume that the bound and continuum orbitals themselves each form an orthogonal set. (We neglect the spin–orbit contribution to the overlap and only include the mass-velocity plus Darwin contributions when using kappa-averaged wave functions, i.e. when they are likely non-negligible.) The UCL-DW code [8] *does* assume complete orthogonality and so low angular momentum scattering symmetries can have large bound $(N+1)$-electron expansions to compensate. The simplest strategy is to force the continuum orbitals to be orthogonal to the bound ones and then no such compensation is required. This is the approach taken in the HULLAC [4], FAC [5] and LADW [6] codes. It is not incompatible with ours.

Eq. (8) does not couple atomic states. It represents elastic scattering. If we introduce an atomic state label ν and consider scattering from an initial state ν to a final state ν' by an electron with corresponding wavenumbers and angular momenta kl and $k'l'$ then the use of Eq. (8) represents the distorted wave approximation. The total energy of the system E satisfies

$$E_\nu + k^2 = E = E_{\nu'} + k'^2 \tag{10}$$

where E_ν is the energy of the atomic state. The transmission matrix $T_{ii'}$ for $i = \nu kl$ satisfies [8]

$$|T_{ii'}| = 2|K_{ii'}| = \left|\langle \Psi_i | H - E | \Psi_{i'} \rangle\right| \tag{11}$$

for inelastic scattering ($\nu \neq \nu'$) in the non-unitarized approximation for the Kohn-corrected [9] reactance matrix $K_{ii'}$. (In practice we implement a unitarization of the 2×2 reactance matrix of the initial and final state.)

The above scattering description is in the uncoupled Slater state representation with labelling of the magnetic quantum numbers suppressed. The whole machinery of the structure problem carries-over into the collision one. We summarize the LS-coupling problem discussed in detail by Eissner [8] and then look at its extension to the Breit–Pauli one. We assume that the total angular momentum quantum numbers for the atomic target are now labelled by $L^a M_L^a$, etc. Slater states for the scattering problem are a simple product of the target $|u\rangle$ and a Slater state for the continuum electron $q = N+1$ — see Eq. (1). We now require only interactions involving the continuum electron pair with a pair of target states. The non-hierarchical nature of the uncoupled Slater state representation means that they are readily determined. Expressions for $\langle u'q'|O|uq\rangle$ are identical to those for an $(N+1)$-electron structure — compare those of Eissner et al. [13] with those of Eissner [8] for LS-coupling and Jones [9] for Breit–Pauli — with the trivial replacement of a bound radial orbital pair by a continuum one. The interactions are mostly two-body since the one-body only contribute to elastic scattering and/or any exchange overlap. We sum over magnetic quantum numbers by utilizing the target transformation to the t-representation and the conserved $(N+1)$-electron quantum numbers SLM_SM_L via

$$|tklSLM_SM_L\rangle = \left|tM_S^a M_L^a klm\mu\right\rangle \left\langle S^a \tfrac{1}{2} M_S^a \mu \middle| SM_S\right\rangle \left\langle L^a l M_L^a m \middle| LM_L\right\rangle \tag{12}$$

where $\langle\,|\,\rangle$ are the vector-coupling coefficients. We note the implied sum over all $M_S^a M_L^a \mu m$ which satisfy the usual triangle relations. The final result is again independent of the particular choice of M_SM_L. The angular algebra is then combined with the associated Slater and two-body non-fine-structure integrals to form the complete interaction matrix (9). If LS-coupling cross sections are required then a further transformation from the t- to $\bar{t}$ representation is made at this stage.

Two-body fine-structure interactions may be present in the Breit–Pauli case and SL, etc., are not conserved then. They are determined in the uncoupled representation in an analogous fashion to the target fine-structure and with the additional continuum Slater state as for the LS-coupling scattering just detailed above. The uncoupled interactions are then transformed to an LSJ-representation via

$$|tklSLJM\rangle = |tklSLM_SM_L\rangle \langle tklSLM_SM_L | tklSLJM\rangle \tag{13}$$

where we make use of Eq. (12) as an intermediate step and the vector-coupling coefficient $\langle\,|\,\rangle$ is given by the RHS of Eq. (6) with all angular momenta being the total. We note now the implied sum over M_SM_L. The result is independent of M. We note that we are still in the $t = C\beta S^a L^a$ representation for the target.

The total Breit–Pauli DW interaction matrix (11) is then the sum of the fine-structure and non-fine-structure contributions. The latter are trivially transformed by (13) being subject to $SL = S'L'$. The final step is to transform to a target level-resolved jK-coupling representation via [7]

$$\left|tJ^a lKLSJ\right\rangle = (-1)^{(J+1/2+l+J^a)} \left[\left(2J^a+1\right)(2K+1)(2L+1)(2S+1)\right]^{\frac{1}{2}} \begin{Bmatrix} S^a & L^a & J^a \\ l & K & L \end{Bmatrix} \begin{Bmatrix} S & L & J \\ K & 1/2 & S^a \end{Bmatrix} \tag{14}$$

and then to the diagonal Breit–Pauli target representation $\bar{i}$ using the second of Eqs. (7) since $i = tJ^a$. ($\{\cdots\}$ denotes the Wigner $6j$-symbol [22].) In the absence of electron exchange (and two-body collisional fine-structure operators) additionally $S^a = S^{a'}$. We can then make use of the orthogonality of the $6j$-symbols on summing over S to set $K = K'$.

We make some observations. The mixing coefficients are the eigenvectors of the Breit–Pauli target Hamiltonians and they both LS-configuration and fine-structure mix the interaction Hamiltonian. They do not correspond to the term coupling coefficients used by the UCL-DW and JAJOM codes [8,10] to fine-structure mix the (open–open part of) the LS-mixed reactance matrix. We always have the full expansion of *all* channels at our disposal (both 'open' and 'closed') since we work with the interaction Hamiltonian. (We only construct and hold a single $J^a J'^a \pi$ sub-block in memory at any one time.) This is in contrast to working with the (physical) reactance matrix where only the open–open components are to hand. (Working with the unphysical reactance matrix is an alternative solution which was developed by Griffin et al. [27].) Our approach to re-coupling and mixing is essentially the same as that employed to set-up the $(N+1)$-electron inner-region Hamiltonian in the Breit–Pauli R-matrix method [28].

4. Radial details

The continuum distorted waves satisfy the same basic radial equation as the bound orbitals but utilize an $(N+1)$-electron model potential of the same functional form as that specified by the user for the target. They need not be orthogonal to bound orbitals of the same angular momentum.

It is convenient to calculate the collision strengths at the same set of final scattered energies for all transitions. Then zero gives every threshold collision strength for example. Only a small set is required since they vary slowly with energy. The conservation of energy Eq. (10) in principle still gives an impractical and unnecessarily large number of initial energy continuum distorted waves for all but the smallest of problems. We supplement the final state energies by a small number of additional energies so as to form a continuum interpolation basis. All of the scattering integrals are calculated at all interpolation energies which can possibly contribute to each final scattered energy. It is then straightforward to interpolate them at the appropriate initial energy for each transition and for each final scattered energy. The order of the (Lagrange) interpolation formula and the distribution of interpolation energies can be controlled by the user or left to the program's default. The default is to use final scattered energies at: 0, $E_x/3$, E_x, $3E_x$ and possibly $8E_x$ where E_x is the maximum of the highest target excitation energy and the (estimated) ionization potential. Additional interpolation energies are given by Eq. (10) on assuming two logarithmically spaced characteristic values for the excitation energies in addition to zero. A two-point interpolation formula is used by default due to the coarse energy spacing.

The defaults likely give reasonable effective collision strengths. The largest source of inaccuracy lies with the continuum interpolation. *It is highly recommended that the user satisfy themselves that the interpolation is sufficiently accurate for their requirements*. This is especially true if the interest lies in the underlying ordinary collision strengths as opposed to the Maxwell-averaged effective collision strengths. Several interpolation strategies have been implemented — see the distribution write-up. The most efficient one in many cases is the use of a small number of characteristic excitation energies which span those for the transitions of interest. It is relatively easy for a user to look at the distribution of target energies and deduce such a set. It is much harder to implement this as an automatic algorithm which is why the default one is simple.

It is well known that (direct) Slater integrands have a long-range nature viz. $\sim 1/r^{\lambda+1}$ where $\lambda = 1$ for dipole transitions, etc.[3] We use the JWKB approach of Burgess and Sheorey [29] for their efficient computation. (Use of this method for the special case of $k'^2 = 0$ has long been a part of AUTOSTRUCTURE due to its approximation of high Rydberg states by a zero-energy continuum orbital.)

All continuum distorted waves and associated radial integrals are calculated on-the-fly as they are needed and currently they can be held in memory without resort to disc storage.

5. Collision strengths

The fully-resolved partial collision strength is related to its corresponding T-matrix element by

$$\Omega_{\nu\gamma,\nu'\gamma'} = \omega_\gamma |T_{\nu\gamma,\nu'\gamma'}|^2 \tag{15}$$

where ν is a target state label, γ is the set of all other quantum numbers which define the scattering and ω_γ $(= \omega_{\gamma'})$ is the total statistical weight of the scattering symmetry viz. $(2J+1)$ for Breit–Pauli jK-coupling or $(2S+1)(2L+1)$ for LS-coupling.

Partial collision strengths are calculated for each total J (or L) by default. This is not necessary. The user can specify a factor by which the preceding J (or L) is multiplied so as to determine the next one. (Subject to safeguards implemented by the code.) The sum over J (or L) is then converted to an integral and evaluated by quadrature using Simpson's rule. This option is available only in the serial version of the code.

The contribution from electron exchange is dropped for sufficiently high J (or L) and the problem simplifies because the sum over S in the recoupling can be carried-out analytically. The direct Slater and non-fine-structure angular algebra also satisfy simple recurrence relations for L [8] and these are used for sufficiently high J (or L).

It is well known that the sum of partial collision strengths over the continuum orbital angular momentum is slow to converge for allowed transitions. This is especially true for the dipole case. We use the same methods and code that we implemented in the R-matrix outer-region code STGF. 'Top-up' for dipole transitions makes use of the Burgess sum rule [30] while that for higher multipoles assumes a geometric series in energy in combination with the degenerate energy limit following Burgess et al. [31]. Top-up is applied by default. The user can specify the maximum total angular momentum. It defaults to 30[4] and is likely consistent with the default maximum scattered energy of $3E_x$. If the user increases this maximum total angular momentum then the default maximum scattered energy is $8E_x$.

The total (sum over γ, γ') collision strengths for each transition as a function of final scattered energy are written to a (type-5) *adf04* file as defined by ADAS [14]. This file also contains energy levels, E_k and M_k radiative rates, and infinite energy PWB collision strengths which are passed-through from the structure run which initiates the scattering calculation. It can be converted to the more familiar Maxwell-averaged effective collision strength (type-3) *adf04* file using the program `adf04_om2ups.f` which is a standalone version of the ADAS809 code.

6. Metastables

We emphasized in the introduction the importance of metastables for diagnostic modelling and its corresponding requirements for electron-impact excitation data. If there are N target levels then the time to calculate excitation data between all possible levels scales as N^3. We identify a subset of M metastable levels. This subset can be specified by the user. The code defaults to all levels of the ground term elsewise. We have attempted to ensure that the time scales as MN^2 and especially as N^2 for $M \ll N$. This is not such a straightforward problem since the metastable eigenstates are a mixture of the full set of N target levels which are of the same $J^a\pi$.

[3] This behaviour is modified to $\sim 1/r^{\lambda+1/2}$ for $k^2 = 0 = k'^2$.

[4] 59/2, etc., for half-integer.

It is facilitated by the user specifying target levels or indeed whole configurations as 'correlation'. No excitation data is computed then to such levels and mixing between such levels is neglected. (We note that the UCL-DW [8] and JAJOM [10] codes both implement exclusion parameters of one kind or another.)

7. Parallelization

A simple parallel strategy has been implemented which distributes the $J\pi$ symmetries over the available processors. If there are more symmetries than processors then the $J\pi$ are grouped for efficient re-use of the angular algebra and radial integrals. Each processor calculates all of the data that it needs. This does mean that it is likely that the same data is being computed by several different processors. The communication and handshake overhead does not make it seem worthwhile to eliminate this duplication of effort at this point in time.

8. Testing

The collision angular algebra has been implemented completely separately from the target angular algebra. The collision algebra has been verified against its corresponding determination from an $(N+1)$-electron structure calculation utilizing inequivalent bound orbitals of the same angular momentum.

Selected reactance matrix elements and partial collision strengths for the excitation of He^+ have been reproduced from the tables of Burgess et al. [31]. (The structure is exactly the same for hydrogenic ions.)

Consistency of the high energy collision strengths with their infinite energy limit has been studied for many varied cases. This tests the veracity of the implementation of the various recoupling and mixing transformations.

We have started as a matter of course to make comparisons with R-matrix background collision strengths as new R-matrix calculations are undertaken.

9. Fortran code

The AUTOSTRUCTURE code has a Fortran77 heritage. Fortran95 constructs have been implemented in key places for memory efficiency but a complete implementation of the standard is still a work in progress and subject to funding. In this sense the code would be viewed as incomplete and/or still under development from the computer science perspective. It is complete and finished from the computational physics perspective. The most up-to-date version of the code can be downloaded from `http://amdpp.phys.strath.ac.uk/autos/` and there is information on installation, 'recent' updates, a reasonably comprehensive write-up so as to get the user started, and a comprehensive test-suite covering all atomic processes described by AUTOSTRUCTURE. There are also supporting utility codes such as `adf04_om2ups.f` (standalone ADAS809). The CPC snapshot distribution contains the files on installation, write-up and the (following) test-case.

10. Test-case

A simple test-case is provided in the CPC distribution which describes excitation within and from the ground and first excited level to the rest of the levels of the $n=2$ complex in Be-like Fe^{22+}. The objective is to provide a single self-contained file of atomic data suitable for simple population modelling within the ionization stage. This requires energy levels, radiative rates and (ultimately) collisional excitation rate coefficients.

The (user) input is:

```
A.S. Be-like Fe DW (BP)
 &SALGEB RUN='DE' CUP='IC' NMETAJ=2
         MXVORB=2 MXCONF=3 KCOR1=1 KCOR2=1 &END
2 0 2 1
 2   0
 1   1
 0   2
 &SMINIM NZION=26 MAXE=500 &END
 &SRADCON &END
```

It is all free-formatted and NAMELISTed *except* for the first four characters of the first line which would normally always be `A.S.` (Other values support historic input formats.) The rest of the first line is for user comments. The write-up within the distribution details all of the above input variables plus many additional optional ones. (All of the 'usual' atomic structure options can be used in conjunction with a DW calculation.) The test-case is an example of almost minimal input. The `RUN` variable specifies the atomic process — here it is Direct Excitation `'DE'`. ('DW' is too generic — all continuum processes described by AUTOSTRUCTURE use distorted waves viz. autoionization and photoionization.) The coupling scheme is specified as (target) intermediate coupling via `CUP='IC'`. `NMETAJ=2` metastable levels (including the ground) are specified (the default is levels of the ground term). The `MXCONF=3` configurations are then specified in terms of `MXVORB=2` *nl*-orbital occupation numbers (see the distribution write-up) and a $1s^2$ closed-shell range (`KCOR1, KCOR2`) based-on 'standard order' (1s, 2s, 2p, ..., correspond to orbital numbers 1, 2, 3, ...). Next follow the `NZION=26` nuclear charge and the (optional) maximum scattering energy (`MAXE=500` Rydbergs) which is used to ensure a satisfactory radial mesh for continuum orbital tabulation. The NAMELIST `&SRADCON` can be used to specify non-default final scattered energies as well as additional interpolation energies. This operation is described in detail in the distribution write-up. The defaults are quite 'coarse' and intended for Maxwell-averaged effective

collision strength final deliverables. The user should satisfy themselves that the ordinary collision strengths are of adequate accuracy for their intended purpose.

The above input gives the following results for the type-5 *adf04* output file:

```
FE+22        26        23         0.0000(0Y)
    1 2S2                (1)0( 0.0)              0.0000
    2 2S1 2P1            (3)1( 0.0)         346591.8865
    3 2S1 2P1            (3)1( 1.0)         377594.2160
    4 2S1 2P1            (3)1( 2.0)         465094.6993
    5 2S1 2P1            (1)1( 1.0)         753288.0279
    6 2P2                (3)1( 0.0)         949317.4436
    7 2P2                (3)1( 1.0)        1015719.5816
    8 2P2                (3)1( 2.0)        1063669.8032
    9 2P2                (1)2( 2.0)        1195220.0707
   10 2P2                (1)0( 0.0)        1412609.9561
   -1
23.00    5       0.00+00 4.65+01 1.40+02 4.19+02
   2   1 1.00-30 1.45-03 9.62-04 4.87-04 1.25-04 0.00+00
   3   1 4.70+07 1.07-02 1.16-02 1.17-02 1.39-02-1.72-03
   3   2 5.24+02 1.60-02 9.43-03 4.42-03 1.11-03 0.00+00
   4   1 1.00-30 6.95-03 4.60-03 2.33-03 5.96-04 0.00+00
   4   2 6.06-01 1.05-02 8.75-03 8.00-03 8.14-03 8.14-03
   5   1 2.02+10 2.96-01 3.77-01 4.41-01 6.04-01-9.33-02
   5   2 2.74+04 3.75-03 2.17-03 9.78-04 2.36-04 0.00+00
   6   1 1.00-30 1.17-04 8.52-05 6.24-05 4.96-05 4.44-05
   6   2 1.00-30 9.71-04 6.34-04 3.17-04 8.17-05 0.00+00
   7   1 1.04+04 1.84-04 9.90-05 3.97-05 8.48-06 0.00+00
   7   2 6.50+09 1.41-01 1.80-01 2.11-01 2.87-01-4.28-02
   8   1 1.72+03 4.39-04 3.85-04 3.66-04 3.87-04 3.96-04
   8   2 1.00-30 2.53-03 1.66-03 8.34-04 2.08-04 0.00+00
   9   1 7.67+03 6.21-04 7.06-04 8.13-04 9.45-04 9.87-04
   9   2 1.00-30 5.82-04 3.82-04 1.92-04 4.82-05 0.00+00
  10   1 1.00-30 3.92-04 3.71-04 3.52-04 3.35-04 3.18-04
  10   2 1.00-30 8.83-05 5.41-05 2.53-05 6.77-06 0.00+00
  -1
  -1  -1
...
```

plus comment lines.

This output file contains energy level information, transition radiative rates and collision strengths as a function of final scattered energy, and infinite energy collision strength information. Specifically (the actual line numbers pertain to this example only):

- Line 1: details the ion (along with dummy information for ADAS).
- Lines 2–11: contain the energy levels (in cm^{-1}) relative to the ground along with their configuration and term/level specification.
- Line 12: is a terminator.
- Line 13: specifies the final scattered energies (in Ryd) preceded by the ion-charge plus 1 and a type-5 label.
- Lines 14–30: contain the total collision strength for each indexed transition listed 'row-wise' with each entry under the column of relevant scattered energy. The 'first' and 'final' fixed format columns have no scattered energy in the header (line 13) since they contain the total radiative rate (s^{-1}) for the transition and information on the infinite energy collision strength limit respectively. In the latter case a negative value flags it as $-4S/3$ where S is the line strength, i.e. a dipole transition; a positive value flags it as the Born limit for an allowed transition; zero flags a forbidden transition which scales as $\sim 1/E^2$. (The infinite energy limits/behaviour are/should be used when convoluting the collision strengths with a Maxwellian distribution.)
- Lines 31–32: contain ADAS terminators.
- Lines 33 ...: contain comments (not shown).

The full *adf04* specification is detailed by Summers [32]. This type-5 file can be converted to a Maxwell-averaged effective collision strength (type-3) *adf04* file using the (ADAS809) program[5] `adf04_om2ups.f`. The user may prefer to convolute and format according to their own requirements instead.

11. Summary

We have described the Breit–Pauli distorted wave method for the electron-impact excitation of atomic ions that we have implemented within the AUTOSTRUCTURE code. This has been done with a view to describe problems that are impractical or impossible for more sophisticated methods. Heavy species for magnetic fusion and highly excited states for astrophysics are such examples.

[5] Available from http://amdpp.phys.strath.ac.uk/autos/ver/misc.

Acknowledgements

The development of AUTOSTRUCTURE would not have been possible without the efforts of W. Eissner, M. Jones, H. Nussbaumer and P.J. Storey who developed the original SUPERSTRUCTURE code while the DW development reported-on here was much inspired by W. Eissner's UCL-DW code. I would also like to thank Alan Burgess for first introducing me to the DW method [33].

References

[1] I. Bray, A.T. Stelbovics, Phys. Rev. Lett. 69 (1992) 53.
[2] P.G. Burke, W.D. Robb, Adv. At. Mol. Phys. 11 (1975) 143.
[3] M.S. Pindzola, F. Robicheaux, S.D. Loch, et al., J. Phys. B 40 (2007) R39.
[4] A. Bar-Shalom, M. Klapisch, J. Oreg, Phys. Rev. A 38 (1988) 1773.
[5] M.F. Gu, Can. J. Phys. 86 (2008) 675.
[6] D.H. Sampson, H.L. Zhang, C.J. Fontes, Physics Reports 477 (2009) 111.
[7] R.D. Cowan, Theory of Atomic Structure and Spectra, University of California Press, Berkeley, 1981.
[8] W. Eissner, Comput. Phys. Commun. 114 (1998) 295.
[9] M. Jones, Phil. Trans. R. Soc. Lond. A 277 (1975) 587.
[10] H. Saraph, Comput. Phys. Commun. 15 (1978) 247.
[11] http://amdpp.phys.strath.ac.uk/autos/.
[12] N.R. Badnell, J. Phys. B 19 (1986) 3827.
[13] W. Eissner, M. Jones, H. Nussbaumer, Comput. Phys. Commun. 8 (1974) 270.
[14] H.P. Summers, The ADAS User manual v2.6, http://www.adas.ac.uk/, 2006.
[15] http://www.jet.efda.org/.
[16] http://www.iter.org/.
[17] N.R. Badnell, J. Phys. B 16 (1983) 3263.
[18] N.R. Badnell, J. Phys. B 30 (1997) 1.
[19] W. Eissner, H. Nussbaumer, J. Phys. B 2 (1969) 1028.
[20] N.R. Badnell, M.J. Seaton, J. Phys. B 36 (2003) 4367.
[21] H. Nussbaumer, P.J. Storey, Astron. Astrophys. 193 (1988) 327.
[22] A.R. Edmonds, Angular Momentum in Quantum Mechanics, Princeton University Press, Princeton, 1974.
[23] A. Burgess, H.E. Mason, J.A. Tully, Astron. Astrophys. 217 (1989) 319.
[24] R.D. Cowan, D.C. Griffin, J. Opt. Soc. Am. 66 (1976) 1010.
[25] I.P. Grant, B.J. McKenzie, P.H. Norrington, D.F. Mayers, N.C. Pyper, Comput. Phys. Commun. 21 (1980) 207.
[26] I.C. Percival, M.J. Seaton, Proc. Cam. Phil. Soc. 53 (1957) 654.
[27] D.C. Griffin, N.R. Badnell, M.S. Pindzola, J. Phys. B 31 (1998) 3713.
[28] N.S. Scott, P.G. Burke, J. Phys. B 13 (1980) 4299.
[29] A. Burgess, V.B. Sheorey, J. Phys. B 7 (1974) 2403.
[30] A. Burgess, J. Phys. B 7 (1974) L364.
[31] A. Burgess, D.G. Hummer, J.A. Tully, Phil. Trans. R. Soc. Lond. A 266 (1970) 225.
[32] H.P. Summers, The ADAS User manual v2.6, http://www.adas.ac.uk/man/appxa-04.pdf, 2006.
[33] N.R. Badnell, Ph.D. dissertation, University of Cambridge, 1984.