R-matrix electron-impact excitation update

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Outline

- Breit–Pauli R-matrix intermediate coupling frame transformation approach (ICFT) applied along isoelectronic sequences, for astrophysics and magnetic fusion — Guiyun Liang (Strathclyde).

- Dirac R-matrix for heavy species (for ITER, laser plasmas): Dirac R-matrix with Pseudo-States (DRMPS) and excitation of neutral Gold — Connor Ballance (Auburn)

RM ICFT: along isoelectronic sequences

- Create a baseline database for electron-impact excitation which includes resonant enhancement: all ions of a sequence up to Zn (or Kr).
- Consider shell boundaries: H-, He-, Li- and F-, Ne-, Na-.
- Use (Perl) script to automate R-matrix calculation — requires reliable, robust codes.
- Works on serial or parallel machines.
- Uses AUTOSTRUCTURE (for structure and infinite energy limit points Bethe/Born) and ICFT R-matrix approach.
- End product: *adf04* file.
- R-matrix analysis package (RAP) has been developed by Mike Witthoeft (Python-based GUI) to validate the large amount of data.

- F-like sequence: see Witthoeft, Whiteford & Badnell J.Phys.B40, 2969 (2007).

- Na-like sequence:

  Outer-Shell: $(nl \rightarrow n'l')$ for $n, n' = 3-6$ — see Liang, Whiteford & Badnell Astron. Astrophys. 500, 1263 (2009)

  Inner-shell: 134CC $(2\mathrm{p}^6 3l, 2\mathrm{p}^5 3l3l',$ ex $3\mathrm{d}^2)$ allowing for Auger and radiation damping of resonances — Liang, Whiteford & Badnell J.Phys.B (At Press)

- Ne-like: 209CC $2\mathrm{s}^p 2\mathrm{p}^q nl\ (n = 2-5)$ and $2\mathrm{p}^2 2\mathrm{p}^5 n'l'(n' = 6, 7 \quad l' = 0-2)$ — Liang & Badnell (In progress)

- H-like and He-like sequences in ADAS — Witthoeft & Whiteford, methodology as per previously published for single ions (i.e. allows for radiation damping.)

- Li-like: simpler version of Na-like (TBD)

Fully relativistic (Dirac) scattering

It is deceptively simple to write down the scattering problem to be solved

$$\Psi = \mathcal{A} \sum\!\!\!\!\!\!\int_{\nu} \psi_\nu \phi \, . \tag{1}$$

The antisymmetric total wavefunction for the target-plus-colliding particle Ψ is expanded in terms of a known complete basis of target states ψ_ν. The expansion coefficients ϕ representing the colliding particle (projectile) are then to be freely determined. Complete solutions:

- DRMPS
- Relativistic convergent close-coupling (RCCC)
- Dirac B-spline R-matrix (DBSR)

All use relativistic analogues of the non-relativistic (orbital) approach.

Dirac R-matrix with pseudo-states (DRMPS)

L-spinors (Grant, 2007) are the relativistic analogue of the Sturmians.

Proto-type L-spinors are described by large and small components

$$\psi_{E\kappa m}(\boldsymbol{r}) = \frac{1}{r}\begin{bmatrix} P_{E\kappa}(r)\chi_{\kappa m}(\theta,\varphi) \\ iQ_{E\kappa}(r)\chi_{-\kappa m}(\theta,\varphi) \end{bmatrix}. \tag{2}$$

The $\chi_{\kappa m}(\theta,\varphi)$ denote the usual spin-angle 2-spinors while the radial parts satisfy

$$\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) P_{E\kappa} = \frac{\alpha}{2}\left[E + \frac{4z}{\lambda N_{nr\kappa} r} + \frac{2}{\alpha^2}\right] Q_{E\kappa} \tag{3}$$

and

$$\left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\kappa}{r}\right) Q_{E\kappa} = -\frac{\alpha}{2}\left(E + \frac{\lambda z N_{nr\kappa}}{r} - \frac{2}{\alpha^2}\right) P_{E\kappa} \tag{4}$$

for a point charge z.

The apparent principal quantum number $N_{nr\kappa}$ is given by

$$N_{nr\kappa}^2 = n^2 - 2n_r(|\kappa| - \gamma) \tag{5}$$

where $n_r = n - |\kappa|$, $\gamma^2 = \kappa^2 - z^2\alpha^2/4$ and n and κ are the principal and combined angular quantum numbers respectively. ($\kappa = l$ for $j = l - 1/2$ and $\kappa = -l - 1$ for $j = l + 1/2$ where l, j are the orbital and total angular momenta quantum numbers respectively.) E denotes the total energy and so the non–rest-mass energy ϵ is given by

$$\epsilon = E - 2/\alpha^2 = 2/\alpha^2 \left[\left(1 - \frac{\alpha^2\lambda^2 z^2}{4} \right)^{1/2} - 1 \right] . \tag{6}$$

Note: λ here corresponds to that used in the non-relativistic (NR) pseudo-states formulation — just expand the above for α small to obtain $\epsilon \approx -\lambda^2 z^2/4$ again. Following the non-relativistic approach, we will take $\lambda \approx 1$. Again, 'physical' relativistic Coulomb functions are recovered on setting $\lambda = 2/N$.

Analytic solutions $f_{nr\kappa}^{\pm}$ (with unit normalization) can be written in terms of the Laguerre polynomials $L_{nr}^{2\gamma}$ and $L_{nr-1}^{2\gamma}$, then $\{P, Q\} = (1 \pm \alpha^2/2E)^{1/2} f_{nr\kappa}^{\pm}$ satisfy the Dirac small-r relative normalization.

Crucial difference from NR case

Consider the Rayleigh quotient

$$E(\phi) = \frac{< \phi | H | \phi >}{< \phi | \phi >} \,. \tag{7}$$

A Ritz variational leads to

$$\delta E = 0 \iff (H - E)\phi = 0 \tag{8}$$

and so stationary values of E correspond to eigenstates of H.

In the case of the Schrödinger Hamiltonian the stationary value is a minimum and the eigenstates form an electron representation.

In the case of the Dirac Hamiltonian the eigenstates can represent electrons or positrons.

Normal atomic structure calculations start with an electron basis representation so as to ensure an electron eigenstate representation (there are no positron solutions for $-2c^2 < E < 0$.)

Now, we must treat electrons and positrons on an equal footing otherwise one obtains spurious solutions: 'variational collapse'.

Trial wavefunctions are taken to be linear combinations of paired two-component basis sets

$$\psi_{E\kappa m}(\boldsymbol{r}) = \left[\begin{array}{c} \psi^{+}_{E\kappa m}(\boldsymbol{r}) \\ i\psi^{-}_{E\kappa m}(\boldsymbol{r}) \end{array} \right] = \frac{1}{r} \left[\begin{array}{c} \sum_{n_r=1}^{N} c^{+}_{n_r} f^{+}_{n_r\kappa}(r)\chi_{\kappa m}(\theta,\varphi) \\ i\sum_{n_r=1}^{N} c^{-}_{n_r} f^{-}_{n_r\kappa(r)}\chi_{-\kappa m}(\theta,\varphi) \end{array} \right] . \quad (9)$$

So, for N basis functions we seek $2N$ solutions — N-electron and N-positron.

Application of the Rayleigh–Ritz method to the Dirac-Coulomb Hamiltonian

$$c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m_{\rm e}c^2 + U(r) \quad (10)$$

leads to the Galerkin equation for the $c_i^{\pm}$ which can be written in matrix form as

$$\left[\begin{array}{cc} \left(c^2 - E/2\right)\mathbf{S}^{++} + \mathbf{U}^{++} & c\mathbf{\Pi}^{+-} \\ c\mathbf{\Pi}^{-+} & -\left(c^2 + E/2\right)\mathbf{S}^{--} + \mathbf{U}^{--} \end{array} \right] \left[\begin{array}{c} \mathbf{c}^{+} \\ \mathbf{c}^{-} \end{array} \right] = 0 . \quad (11)$$

$S_{mn}^{\pm\pm}$ denote the Gram overlap terms, $U_{mn}^{\pm\pm}$ denote the potential terms and $\Pi_{mn}^{\pm\mp}$ denote the kinetic terms.

Solution of the Galerkin equation constitutes a generalized eigenvalue problem.

We retain the N-electron solutions but have no futher use for the N-positron solutions (currently).

The 'one-electron' approach is easily implemented for a multi-electron atom in, for example GRASP0, since multi-electron wavefunctions are built from one-electron wavefunctions.

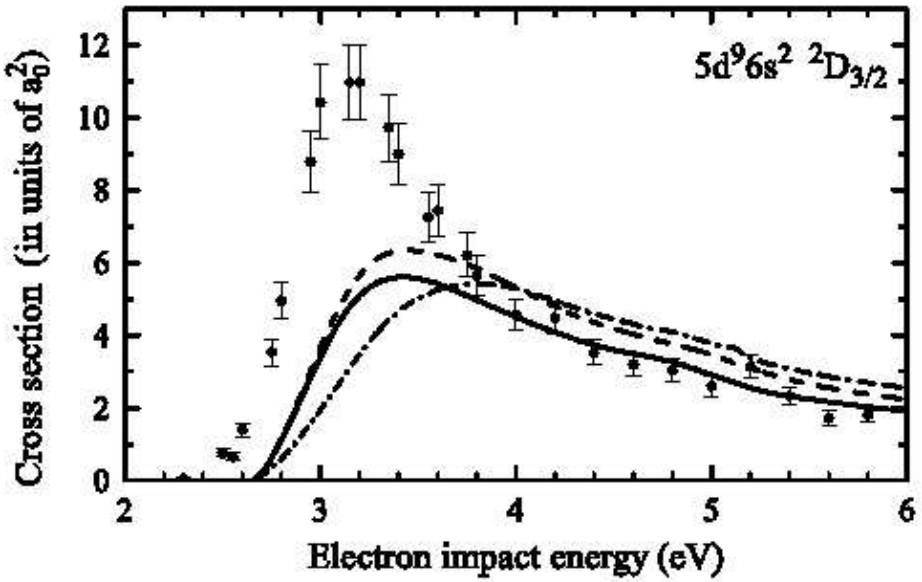
• Some R-matrix (DARC) niceties:

We first Schmidt orthogonalize the pseudo-state basis (it is initially linearly independent, but orthogonal on non-unit weight) and to any other target orbitals. Then we have two, separate, orthonormal bases: the pseudo-state (target) and the continuum. We form a linearly independent orthogonal continuum basis by a straightforward generalization, to two components, of the NR case. ((N+1)-electron target states are added to the total wavefunction in compensation.) Similarly, for the transformation of the (now, non-diagonal) Buttle correction back to a diagonal representation.

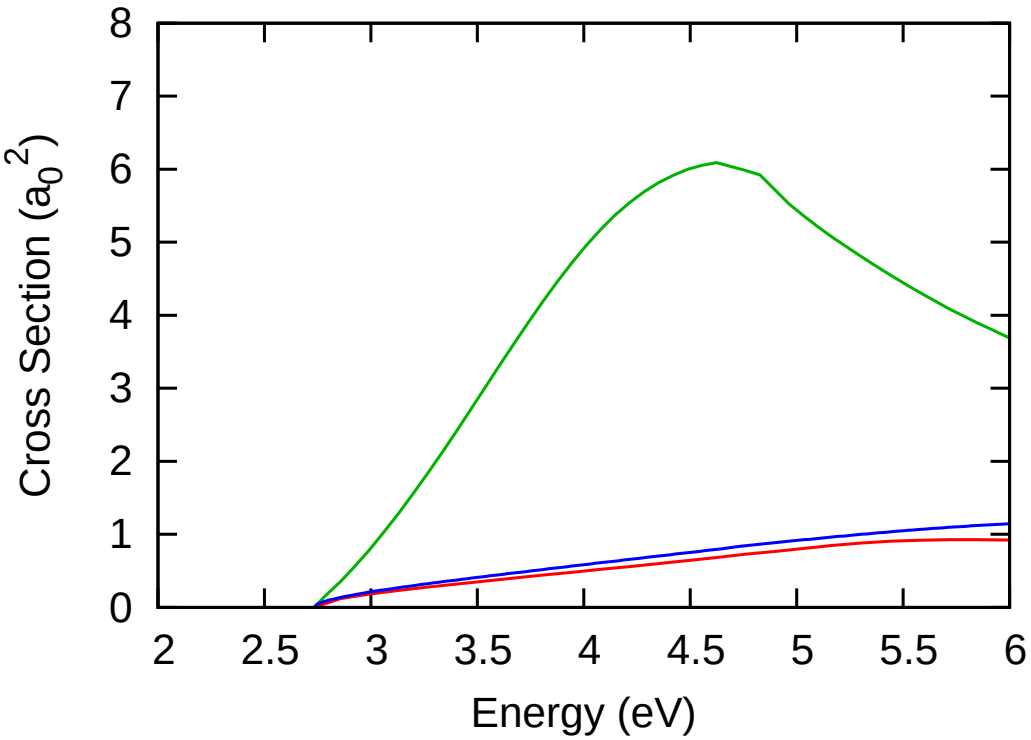
This approach has been implemented in GRASP0 and DARC by Badnell J.Phys.B v41 175202 (2008).

Electron-impact excitation of Gold

$$5d^{10}6s\,^2S_{1/2} \rightarrow 5d^9 6s^2\,^2D_{3/2} \tag{12}$$



Measurement by Maslov et al [Phys. Rev. A78, 042713 (2008)] compared with results of non-orthogonal DBSR calculations carried-out by Zatsarinny & Bartschat (Ibid.) with large configuration interaction but small close-coupling expansions (10,15,32CC).



Large-scale CI orthogonal orbital calculations with DARC:

Green curve: 6CC with only (N+1)-e^- target configurations required by orthogonality
Blue curve: 6CC with all possible (N+1)-e^- target configurations, i.e. large correlation
Red curve: 100CC with all possible (N+1)-e^- target configurations

A work in progress...

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