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Dirac *R*-matrix with pseudo-states

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Abstract

We describe the development of the Dirac *R*-matrix with pseudo-states (DRMPS) method for electron and photon collisions with arbitrary atoms and ions. An *N*-electron atom is represented by an anti-symmetrized product of single-particle spinors comprising the usual four-component Dirac spinors as well as paired two-component Laguerre spinors (L-spinors). The convergent L-spinor basis forms a discretization of the electron and positron continua. This representation has been implemented quite generally within the general relativistic atomic structure package (GRASP) specifically GRASP^0. An $(N + 1)$th 'scattering' electron is represented by the exact same L-spinor basis plus the usual *R*-matrix box-state spinors which are chosen so as to form a combined complete finite linearly independent orthogonal basis. The (non-diagonal) Buttle correction is determined consistently. This representation has been implemented quite generally within the Dirac atomic *R*-matrix code (DARC). Results of some simple model problems are presented which demonstrate the correctness of the implementation.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The *R*-matrix approach to scattering (Burke and Robb 1975) is one of the most powerful and widespread. Its use of non-relativistic wavefunctions suffices up to about zinc and relativistic effects can be treated as a perturbation in the Hamiltonian if need be. This is encapsulated by the Breit–Pauli *R*-matrix (BPRM) method (Berrington *et al* 1995) and variants thereof such as the intermediate coupling frame transformation (Griffin *et al* 1998). Beyond zinc it becomes increasingly necessary to consider the use of relativistic wavefunctions. This is encapsulated by the use of the general relativistic atomic structure package (GRASP; Grant *et al* 1980) specifically the GRASP^0 code (Norrington 2004) and the Dirac atomic *R*-matrix code (DARC; Ait-Tahar *et al* 1996, Norrington 2004). We note that the theoretical foundations of the Dirac *R*-matrix method have been re-examined recently by Grant (2008) and found to be secure.

The *R*-matrix method is fundamentally a close-coupling one. The total wavefunction is formally expanded in terms of a complete basis of atomic states which includes the continuum. The traditional close-coupling method truncates this expansion to a small set of physical bound states thereby neglecting coupling to the continuum. It had long been known that such an effect was not necessarily negligible (Castillejo *et al* 1960). It was Bray and Stelbovics (1992) who showed that the continuum could be discretized by the use of Laguerre pseudo-states which form a quadrature for the continuum and that such a basis is convergent for practical purposes with relatively few terms. Their convergent close-coupling (CCC) method is implemented within the Lippmann–Schwinger representation which is not ideal for describing the resonances which so often dominate scattering processes.

The *R*-matrix method is ideally suited to describing resonances. Bartschat *et al* (1996) introduced the *R*-matrix with pseudo-states (RMPS) method. They encountered spurious poles in the *R*-matrix because of overcompleteness since their Laguerre basis was simply added to the usual box-state basis representation for the scattering electron. The problem was overcome by Gorczyca and Badnell (1997) and Badnell and Gorczyca (1997). They formed a new combined linearly independent basis and transformed the Buttle correction to the new representation. These works all took place within the non-relativistic wavefunction *R*-matrix suite of codes.

Accurate electron-impact excitation cross sections for heavy neutral atoms and low-charged ions are required for the spectral diagnosis of magnetic fusion (ITER Physics Basis 1999), technical (Smith 2004) and some astrophysical plasmas (Sterling *et al* 2007). Numerous studies with CCC and RMPS have demonstrated the large reduction over non-pseudo-state cross sections due to the ionization loss represented by

continuum coupling. A Dirac *R*-matrix with pseudo-states (DRMPS) treatment is clearly necessary. It is the purpose of this paper to describe such a development. We note that very recently Fursa and Bray (2008) have reported a similar development of their CCC approach.

2. Theory

It is deceptively simple to write 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. We discuss each in turn.

2.1. Target basis

The RMPS and CCC approaches approximate the sum over high Rydberg states and the integration over continuum states by a quadrature over Laguerre (Sturmian) states. The choice of the Dirac spinor analogue of the non-relativistic Laguerre states is not straightforward and it is discussed in detail by Grant and Quiney (2000) for the one-electron problem. This is our starting point. The reader is also referred to the excellent reference work by Grant (2007) for any of the usual details which we omit to mention. The main point to note is that the use of so-called L-spinors is fundamental to avoiding pathologies such as 'finite-basis disease' and 'variational collapse'.

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

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

$\chi_{\kappa m}(\theta,\varphi)$ denote the usual spin-angle 2-spinors while the radial parts satisfy[1]

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

and

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

for a point charge z. The apparent principal quantum number $N_{n_r\kappa}$ is given by

$$N^2_{n_r\kappa} = n^2 - 2n_r(|\kappa|-\gamma), \tag{5}$$

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

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

We note that the λ used here corresponds to that used in our non-relativistic Laguerre pseudo-states formulation (Badnell and Gorczyca 1997). If we expand (6) for α small then we obtain $\epsilon \approx -\lambda^2 z^2/4$. This is not the λ used by Grant and Quiney (2000). The two are related via $\lambda = 2\lambda_{\mathrm{GQ}}/z$, where λ_{GQ} denotes Grant and Quiney's. The reason for this choice is to factor-out the 'z-dependence' and make $\lambda \approx 1$ the usual choice. 'Physical' relativistic Coulomb functions are recovered on setting $\lambda = 2/N_{n_r\kappa}$.

Analytic solutions $f^{\pm}_{n_r\kappa}$ can be written in terms of Laguerre polynomials L^n_m:

$$f^{\pm}_{n_r\kappa}(x) = \mathcal{N}_{n_r\kappa} x^\gamma \mathrm{e}^{-x/2} \times\left[-(1-\delta_{n_r 0})L^{2\gamma}_{n_r-1}(x) \pm \frac{N_{n_r\kappa}-\kappa}{n_r+2\gamma}L^{2\gamma}_{n_r}(x)\right], \tag{7}$$

where $x = \lambda z r$ and $\mathcal{N}_{n_r\kappa}$ is a normalization constant. If $\mathcal{N}_{n_r\kappa}$ is chosen such that $f^{\pm}_{n_r\kappa}$ are both normalized to unity on r then taking

$$\begin{aligned} P_{E\kappa}(r) &= \left(1+\frac{\alpha^2 E}{2}\right)^{1/2} f^{+}_{n_r\kappa}(\lambda z r) \\ Q_{E\kappa}(r) &= \left(1-\frac{\alpha^2 E}{2}\right)^{1/2} f^{-}_{n_r\kappa}(\lambda z r) \end{aligned} \tag{8}$$

satisfies[2] the small-r relative normalization condition of the Dirac equation, namely,

$$\left.\frac{Q_{E\kappa}(r)}{P_{E\kappa}(r)}\right|_{r=0} = \frac{\lambda N_{n_r\kappa}(\kappa+\gamma)}{\alpha z}. \tag{9}$$

We note that these large and small components are kinetically matched:

$$f^{-}_{n_r\kappa}(x) \underset{c\to\infty}{\sim} C\left(\frac{\mathrm{d}}{\mathrm{d}x}+\frac{\kappa}{x}\right)f^{+}_{n_r\kappa}(x), \tag{10}$$

and so the large component f^+ satisfies the Schrödinger equation in the non-relativistic limit. This is a key property which we will require next.

Consider the Rayleigh quotient

$$E(\phi) = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle}. \tag{11}$$

A Ritz variational leads to

$$\delta E = 0 \iff (H-E)\phi = 0, \tag{12}$$

and so stationary values of E correspond to eigenstates of H. If H is the non-relativistic Schrödinger Hamiltonian then the stationary value is a minimum and the eigenstates form an electron representation. If H is the relativistic Dirac Hamiltonian then the eigenstates can represent electrons or positrons. In normal atomic structure calculations, it is

[1] We use Rydberg atomic units: the speed of light is related to the fine-structure constant by $c = 1/\alpha$ and the unit of energy is $e^2/(2a_0)$.

[2] Strictly speaking the equality is exact only for the Coulomb case $\lambda = 2/N_{n_r\kappa}$. Otherwise there are higher-order terms in α^{2m} contributing to the energy factor in (8). Their effect is small though. Our final solution explicitly determines the correct relative normalization and so it is actually irrelevant as far as the initial basis is concerned.

sufficient to start with an electron basis representation so as to ensure an electron eigenstate representation since there are no corresponding positron solutions for $-2c^2 < E < 0$. In a pseudo-state structure problem, we try to represent the electron continuum and we cannot help but describe the positron continuum at the same time. Indeed, we must treat electrons and positrons on an equal footing.

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

$$\psi_{E\kappa m}(\boldsymbol{r}) = \begin{bmatrix} \psi^{+}_{E\kappa m}(\boldsymbol{r}) \\ \mathrm{i}\psi^{-}_{E\kappa m}(\boldsymbol{r}) \end{bmatrix} = \frac{1}{r}\begin{bmatrix} \sum_{n_r=1}^{N} c^{+}_{n_r} f^{+}_{n_r\kappa}(r)\chi_{\kappa m}(\theta,\varphi) \\ \mathrm{i}\sum_{n_r=1}^{N} c^{-}_{n_r} f^{-}_{n_r\kappa}(r)\chi_{-\kappa m}(\theta,\varphi) \end{bmatrix}. \quad (13)$$

For N basis functions we seek $2N$ solutions—N-electron and N-positron.

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

$$c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m_{\mathrm{e}}c^2 + U(r) \quad (14)$$

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

$$\begin{bmatrix} (c^2 - E/2)\mathbf{S}^{++} + \mathbf{U}^{++} & c\boldsymbol{\Pi}^{+-} \\ c\boldsymbol{\Pi}^{-+} & -(c^2 + E/2)\mathbf{S}^{--} + \mathbf{U}^{--} \end{bmatrix} \begin{bmatrix} \mathbf{c}^{+} \\ \mathbf{c}^{-} \end{bmatrix} = 0. \quad (15)$$

The Gram overlap terms are given by

$$S^{\pm\pm}_{mn} = \int_0^\infty f^{\pm}_m(r) f^{\pm}_n(r)\,\mathrm{d}r. \quad (16)$$

The potential terms are given by

$$U^{\pm\pm}_{mn} = \int_0^\infty f^{\pm}_m(r) f^{\pm}_n(r) U(r)\,\mathrm{d}r. \quad (17)$$

The kinetic terms are given by

$$\Pi^{\pm\mp}_{mn} = \mp\int_0^\infty f^{\pm}_m(r)\left(\frac{\mathrm{d}}{\mathrm{d}r} \mp \frac{\kappa}{r}\right) f^{\mp}_n(r)\,\mathrm{d}r. \quad (18)$$

We note that $S^{\pm\pm}_{mn}$ and $U^{\pm\pm}_{mn}$ are symmetric whilst $\Pi^{-+}_{mn} = \Pi^{+-}_{nm}$.

The preceding formulation ensures that $\psi^{+}_{E\kappa m}(\boldsymbol{r})$ satisfies the Schrödinger equation in the non-relativistic limit (Grant 2007). Consider equation (15) in the limit $c \to \infty$. Eliminating $\mathbf{c}^{-}$ leads to the kinetic operator acting on $\mathbf{c}^{+}$ being of the form

$$\mathbf{T}^{++} = \boldsymbol{\Pi}^{+-}(\mathbf{S}^{--})^{-1}\boldsymbol{\Pi}^{-+}. \quad (19)$$

Since each basis function is kinetically matched $\boldsymbol{\Pi}^{-+} = \mathbf{S}^{--}$ and so

$$\mathbf{T}^{++} = \mathbf{S}^{--}. \quad (20)$$

It follows readily that $\mathbf{S}^{--} = \mathbf{p^2}$ and so $\psi^{+}_{E\kappa m}(\boldsymbol{r})$ does indeed satisfy the Schrödinger equation in the limit.

The integrals in (16) and (18) can be evaluated analytically as can (17) for $U(r) = -z/r$ and expressions have been given by Grant and Quiney (2000).[3] The matrix equation (15) constitutes a generalized eigenvalue problem which can be solved using standard numerical packages such as LAPACK. This completes the solution of the one-electron problem, and sample results have been presented and discussed by Grant and Quiney (2000). We have implemented this exact same procedure as a standalone code so as to be able to benchmark the general approach which we discuss next.

2.1.1. Multi-electron atoms. We require a solution for an arbitrary multi-electron atom and one which can be incorporated readily into an existing general multi-configuration relativistic structure code such as GRASP^0. We discuss our implementation and the additional constraints imposed on the problem by this approach.

The main point to our advantage is that general codes such as GRASP^0 build-up a trial multi-electron wavefunction as an anti-symmetrized product of one-electron wavefunctions. The whole machinery developed for the one-electron problem is readily applicable to the multi-electron one.

We start by generating a trial basis of one-electron wavefunctions as defined by equation (13). The component basis $f^{\pm}_{n_r\kappa}$ is tabulated on a radial grid by evaluating the analytic expression (7). The radial integrals (16)–(18) are then evaluated numerically. This enables us to include an arbitrary effective central potential in (17) if we so desire rather than just the pure λ-scaled Coulomb one. In the non-relativistic case we have only used the scaled-Coulomb to-date but relativistic heavy atoms contain a much larger number of electrons and it will be of future interest to see if the use of a central potential improves basis convergence. It is also possible to mix-in ordinary four-component spinors which represent low-lying electron states. Ultimately we require numerically tabulated radial functions so as to be able to determine the two-electron integrals etc that arise when evaluating the multi-electron Hamiltonian and so using the analytic approach of Grant and Quiney (2000) gains us little here. The solution of the Galerkin equation provides us with N-eigenenergies and N-eigenvectors each for both electron and positron states. We have no further use for the positron solutions currently other than to check that all absolute energies lie below $-2c^2$ Ryd. This provides us with the initial one-electron basis required for the solution of the multi-electron problem.

The main restriction we encounter with a general code such as GRASP^0 is that our one-electron basis orbitals must be orthogonal with unit weight. The underlying Laguerre polynomials form a linearly independent orthogonal basis with non-unit weight. This means that we can carry-out a simple Schmidt orthogonalization procedure to produce a linearly independent basis that is orthogonal on unit weight. The components of our one-electron basis satisfied the kinetic matching condition prior to the application of this procedure. We show now that this is still the case following orthogonalization. This is necessary since kinetic matching is central to avoiding the pathologies noted previously.

We start with our kinetically matched basis $\{f^{\pm}_i\}$ (the radial part of $\psi^{\pm}_{E\kappa m}$)

$$f^{-}_i \underset{c\to\infty}{\sim} C\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) f^{+}_i \quad (21)$$

[3] The last term in line 2 of Grant and Quiney's (2000) equation (42) should be prefaced by a plus sign and not a minus. They do not appear to define G_{nm}. It can be defined by $G_{nm}(a) = (n+a)G_n(a-1)\delta_{nm}$ in terms of quantities which are given by them.

and note that the normalization constant C is independent of i for fixed κ in this limit. Consider an arbitrary step in the Schmidt orthogonalization procedure at which all basis functions are kinetically matched up to this point. Then form

$$\overline{f}_j^{\pm} = f_j^{\pm} - \beta_{ij} f_i^{\pm}, \tag{22}$$

where

$$\beta_{ij} = \int_0^\infty \left(f_i^+ f_j^+ + f_i^- f_j^-\right) \mathrm{d}r. \tag{23}$$

Then

$$\overline{f}_j^- \underset{c\to\infty}{\sim} C\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) f_j^+ - \beta_{ij} C\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) f_i^+ \tag{24}$$

$$= C\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) \overline{f}_j^+ \tag{25}$$

is also kinetically matched and the subsequent (overall) renormalization step does not alter the relative normalization.

We now have a linearly independent orthogonal L-spinor basis which we can use in the construction of the Hamiltonian for an arbitrary multi-electron atom which is then diagonalized to form the final eigensolutions for use in subsequent applications. The user would normally only specify one L-spinor per electronic configuration. The usual (GRASP^0) strategy is to decide on some z-charged core representation and then couple-on a single electron pseudo-state to represent the continuum of the atom. The core orbitals are determined via a multi-configuration Dirac–Fock operation as usual and then 'fixed', and a configuration interaction (CI) calculation is carried-out with the additional electron (L-spinor) representation attached to this core. The user can specify different λ-values for each relativistic nlj orbital. The only time when this may be of interest is to try and ensure an even distribution of eigenenergies both above and below the ionization limit so as to minimize the need for projection when determining ionization cross sections by summing-over excitation cross sections to eigenstates above the limit.

2.1.2. Example. When there is only one electron then we should recover the original eigenenergies of the Galerkin equation since orthogonalization and re-diagonalization can have no effect on them in this instance. In table 1, we present s-state results for the case of $z = 50, \lambda = 2$ considered by Grant and Quiney (2000). The results labelled 'Galerkin' are from our standalone re-implementation of the 'analytic' solution of the one-electron problem of Grant and Quiney (2000). The default value of the speed of light used by GRASP^0 $c = 137.035\,999\,76$ au differs slightly from that used by Grant and Quiney (2000) $c = 137.035\,9895$ au. If we use their value then our 'Galerkin' results agree with theirs for s-, p-, d-state levels to all significant figures that they give (p- and d-states not shown). We see that the s-state results from the numerical implementation within GRASP^0 utilizing the general three-step strategy described above also agree to eight or more significant figures. We have also run some test calculations on multi-electron atoms so as to check that the algorithms implemented function correctly in such cases.

Table 1. S-state energies (au) for $z = 50, \lambda = 2$.

n	Galerkin	GRASP^0
1	−1.294 626 148(3)[a]	−1.294 626 148(3)
2	−3.264 948 039(2)	−3.264 948 039(2)
3	−1.438 293 524(2)	−1.438 293 524(2)
4	−7.957 309 342(1)	−7.957 309 327(1)
5	−3.513 916 636(1)	−3.513 916 674(1)
6	2.816 045 671(1)	2.816 045 799(1)
7	1.175 877 451(2)	1.175 877 440(2)
8	2.378 653 467(2)	2.378 653 502(2)
9	3.968 369 662(2)	3.968 369 639(2)
10	6.065 196 125(2)	6.065 196 202(2)
11	8.851 427 284(2)	8.851 427 238(2)
12	1.260 835 482(3)	1.260 835 500(3)
13	1.778 332 027(3)	1.778 332 019(3)
14	2.511 698 362(3)	2.511 698 410(3)
15	3.590 017 968(3)	3.590 017 954(3)
16	5.253 618 934(3)	5.253 619 093(3)
17	7.991 649 083(3)	7.991 649 058(3)
18	1.293 859 064(4)	1.293 859 143(4)
19	2.336 639 160(4)	2.336 639 152(4)
20	5.416 045 880(4)	5.416 047 074(4)

[a](m) denotes $\times 10^m$.

2.2. Projectile basis

We now discuss the extension of the work of Gorczyca and Badnell (1997) to forming a linearly independent R-matrix basis for relativistic wavefunctions and its implementation within DARC.

We assume that we have an orthonormal target basis $\{P_i, Q_i\}$ which can be a mixture of 'physical' Dirac spinors and 'unphysical' L-spinors. We assume that we have an initial orthonormal 'continuum' basis for the projectile $\{F_i, G_i\}$ which normally consists of R-matrix box-state spinors. We require a linearly independent basis $\{V_i, W_i\}$ which consists of $\{P_i, Q_i\}$ plus that part of $\{F_i, G_i\}$ necessary for $\{V_i, W_i\}$ to be complete.

Define an overlap matrix $\mathbf{M}$ by

$$M_{ij} = \int_0^\infty (P_i F_j + Q_i G_j)\,\mathrm{d}r \approx \sum_k \omega_k (P_{ik} F_{kj} + Q_{ik} G_{kj}) \tag{26}$$

with quadrature weights ω_k and k such that $r_k = kh$ etc. Then absorb ω_k into $(P, Q)_{ik}$ etc and rewrite as

$$\mathbf{M} = \mathbf{P}\mathbf{F}^{\mathrm{T}} + \mathbf{Q}\mathbf{G}^{\mathrm{T}}. \tag{27}$$

We require $\{V_i, W_i\}$ such that

$$\mathbf{V}\mathbf{V}^{\mathrm{T}} + \mathbf{W}\mathbf{W}^{\mathrm{T}} = \mathbf{1}. \tag{28}$$

Let

$$\mathbf{V} = \begin{pmatrix} \mathbf{P} \\ \mathbf{a}\mathbf{P} + \mathbf{b}\mathbf{F} \end{pmatrix} \qquad \text{and} \qquad \mathbf{W} = \begin{pmatrix} \mathbf{Q} \\ \mathbf{a}\mathbf{Q} + \mathbf{b}\mathbf{G} \end{pmatrix}. \tag{29}$$

Then we require the off-diagonal block to satisfy

$$\mathbf{P}\mathbf{P}^{\mathrm{T}}\mathbf{a}^{\mathrm{T}} + \mathbf{P}\mathbf{F}^{\mathrm{T}}\mathbf{b}^{\mathrm{T}} + \mathbf{Q}\mathbf{Q}^{\mathrm{T}}\mathbf{a}^{\mathrm{T}} + \mathbf{Q}\mathbf{G}^{\mathrm{T}}\mathbf{b}^{\mathrm{T}} = \mathbf{0}, \tag{30}$$

i.e.,

$$\mathbf{a} = -\mathbf{b}\mathbf{M} \tag{31}$$

as in the non-relativistic RMPS case. We require the lower diagonal block to satisfy

$$\mathbf{b}(\mathbf{1} - \mathbf{M}\mathbf{M}^{\mathrm{T}})\mathbf{b}^{\mathrm{T}} = \mathbf{1}. \tag{32}$$

For numerical stability we form

$$\mathbf{O}^{\mathrm{T}}(\mathbf{1} - \mathbf{M}\mathbf{M}^{\mathrm{T}})\mathbf{O} = \mathbf{d}, \tag{33}$$

where $\mathbf{d}$ is diagonal. We then take

$$\mathbf{b} = \frac{\mathbf{1}}{\sqrt{\mathbf{d}}}\mathbf{O}^{\mathrm{T}} \tag{34}$$

which satisfies

$$\mathbf{V}\mathbf{V}^{\mathrm{T}} + \mathbf{W}\mathbf{W}^{\mathrm{T}} = \mathbf{1}. \tag{35}$$

Any linear dependence is eliminated by discarding the eigenvectors $\mathbf{b}_i$ corresponding to eigenvalues $d_{ii} < \delta$. We take $\delta = 10^{-3}$. We find that this value gives good numerical stability.

The Buttle correction for a non-RMPS Dirac continuum basis $\{F_i, G_i\}$ is given by

$$R^{\mathrm{c}}(\mathcal{E}) = R^0(\mathcal{E}) - \mathbf{u}^{\mathrm{T}}(\boldsymbol{\epsilon} - \mathcal{E})^{-1}\mathbf{u} \tag{36}$$

where $\mathbf{u}$ is the vector of basis surface amplitudes and $\boldsymbol{\epsilon}$ are the corresponding eigenenergies. R^0 is the zero-order R-matrix determined at a non-pole energy $\mathcal{E}$. It is given by

$$R^0(\mathcal{E}) = u^0\left[\frac{2v^0}{\alpha} - \left(b + \frac{\kappa}{a}\right)u^0\right]^{-1}. \tag{37}$$

Here (u^0, v^0) are the corresponding surface amplitudes, b is an arbitrary constant (the surface logarithmic derivative of the F_i) and a is the R-matrix boundary radius. We note that $\boldsymbol{\epsilon}$ is diagonal in this basis.

The DRMPS Buttle correction for the basis $\{V_i, W_i\}$ is given by

$$R^{\mathrm{c}}(\mathcal{E}) = R^0(\mathcal{E}) - \mathbf{u}^{\mathrm{T}}\left[(\mathbf{V} \quad \mathbf{W})\mathcal{L}\begin{pmatrix}\mathbf{V}^{\mathrm{T}}\\ \mathbf{W}^{\mathrm{T}}\end{pmatrix} - \mathcal{E}\right]^{-1}\mathbf{u}, \tag{38}$$

where

$$\mathcal{L} = \begin{pmatrix}0 & -2c\\ 2c & 0\end{pmatrix}\frac{\mathrm{d}}{\mathrm{d}r} + \begin{pmatrix}-\mathcal{V}(r) & 2c\kappa/r\\ 2c\kappa/r & -\mathcal{V}(r) - 4c^2\end{pmatrix} \tag{39}$$

and so $\mathcal{L}$ no longer constitutes a diagonal representation. ($\mathcal{V}$ denotes the effective potential used for the generation of the R-matrix box-states.)

In practice we diagonalize the matrix representation of $\mathcal{L}$ and transform the Buttle correction back to a diagonal representation. This has the advantage of being able to work within the framework of the existing DARC. It also provides us with a check on our implementation since we should recover all of the original box-state eigenenergies and surface amplitudes as well as an additional contribution from the L-spinor basis. If we were to transform our new basis with this representation it would correspond to the opposite problem of fixing the box-state basis and retaining only that part of the original target basis necessary to make the box-state basis complete. In such a representation the target continuum is largely represented by box-states and gives rise to a dense pseudo-resonance spectrum as the target states no longer vanish on the R-matrix boundary. It has similarities with the intermediate energy R-matrix method in this respect and its drawbacks.

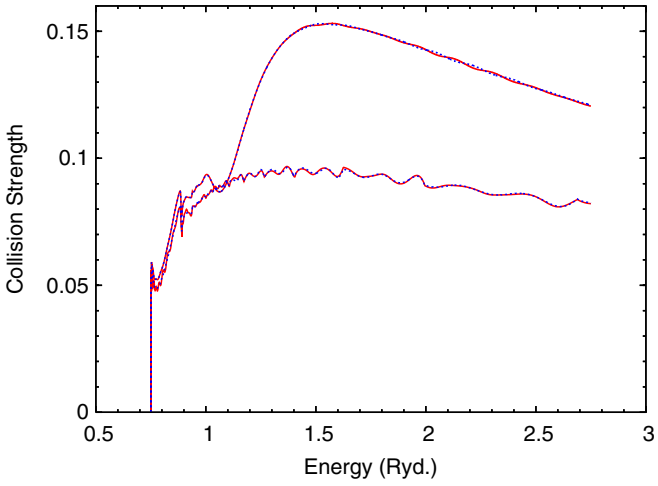

Figure 1. Electron-impact excitation of the 1s − 2s transition in H in the Poet–Temkin model. Solid (red) lines, DARC; dashed (blue) lines, BPRM. Upper pair, 5CC; lower pair, 20PS. See the text for details. All this work.

The above procedure has been implemented within DARC. Specifically it is fully contained within the orbital generation module (STG1D_ORBS). It should be noted that we 'only' use the original DARC to set-up the $(N + 1)$-electron Hamiltonian and any corresponding dipole matrices. Thereafter (Badnell *et al* 2004) we use our common suite of serial and parallel diagonalization (Mitnik *et al* 2003) and dipole transformation (Ballance and Griffin 2004) routines that also feed-off LS-coupling and Breit–Pauli R-matrix set-ups. This completes the solution in the R-matrix inner region. The outer-region solution is non-relativistic (Norrington and Grant 1987). It uses the efficient suite of routines originally written by Mike Seaton (see Berrington *et al* (1987) for some details). These routines (STGB, STGF, STGBB, STGBF, STGFF and their damped versions, Robicheaux *et al* 1995) describe a wide range of electron and photon collision processes.

2.2.1. Examples. We consider s-wave scattering of s-states in hydrogen—the so-called Poet–Temkin model. We have carried-out both RMPS (using the BPRM code) and DRMPS (using DARC) calculations including pseudo-states up to $n = 20$ (20PS). We also carried-out standard non-RMPS calculations including spectroscopic 1s through 5s states (5CC). All calculations utilized 80 box-state basis orbitals. In figure 1, we compare the results of the four sets of calculations for the 1s–2s transition. In both cases (non-pseudo-state and pseudo-state) the DARC results are in very close agreement with those from BPRM. It is particularly gratifying that the DRMPS results map-out the exact same pseudo-resonance structure as the RMPS results. It should be noted that this example tests the correctness of the implementation for both the large and small components even though $z = 1$. The reason for this is that the way the Dirac Hamiltonian problem is formulated means that the small component contributes explicitly to order $cQ \sim P$ at various points.

The Poet–Temkin model can also be applied to electron-impact ionization. We simply sum-over the collision strengths

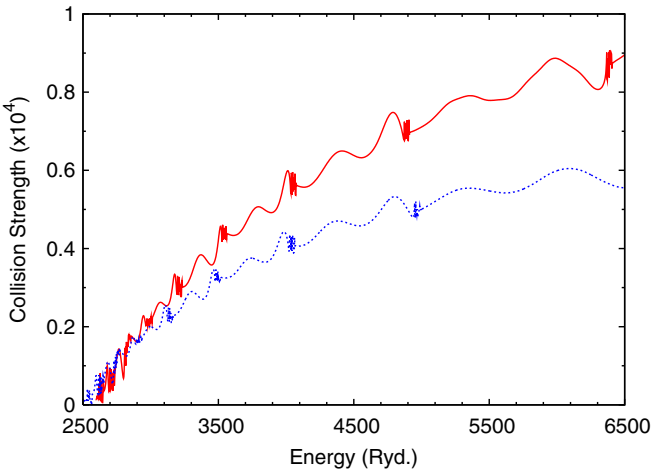

Figure 2. Electron-impact ionization of a $z - 1 = 49$ hydrogenic ion in the Poet–Temkin model. Solid (red) line, DRMPS; dashed (blue) line, RMPS. See the text for details. All this work.

to positive energy pseudo-states. We do not attempt any projection of positive energy pseudo-states back onto the true bound nor negative energy pseudo-states onto the continuum. We consider only the $z = 50$ pseudo-state target of section 2.1.2. (Our RMPS and DRMPS results for $z = 1$ are indistinguishable again.) In figure 2, we compare our RMPS and DRMPS results for $z = 50$. The DRMPS results become increasingly larger than the RMPS with increasing energy. This is typical of highly relativistic systems. The pseudo-resonance structure is more pronounced than for $z = 1$ because of the high charge state. This is typical of the pseudo-state approach.

3. Summary

We have described the development of the Dirac *R*-matrix with pseudo-states method and its general implementation within GRASP^0 and DARC. Together with previous developments (Badnell *et al* 2004) this opens-up the Dirac *R*-matrix procedure to the full range of electron and photon collision processes for heavy atoms which include coupling to the continuum.

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