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1989 J. Phys. A: Math. Gen. 22 4339

(http://iopscience.iop.org/0305-4470/22/20/013)

J. Phys. A: Math. Gen. **22** (1989) 4339-4345. Printed in the UK

A discrete procedure for solving integro-differential equations

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Received 6 April 1989

Abstract. A discrete procedure is described for solving coupled integro-differential equations. In particular, the method is applied to the close coupling equations that arise in scattering theory. It is found that the method converges rapidly provided that the number of linearly independent solutions does not exceed the number of equations. Typical results are shown as a function of the basis size.

1. Introduction

Various numerical techniques have been used to solve the close coupling equations that arise in scattering theory. A review of these has been presented by Burke and Seaton (1971) in which three main techniques are described for solving this set of coupled integro-differential equations. They are:

(i) step by step methods using finite difference formulae;

(ii) using finite difference formulae to reduce the equations to algebraic equations;

(iii) expanding the solution in terms of a set of basis states and solving for the coefficients—the R-matrix method.

The alternative procedure described here is a type of collocation method in which the solutions are represented by an expansion and the equations are satisfied identically over a discrete set of points. This is equivalent to replacing a homogeneous set of equations by an inhomogeneous set in which one attempts to ensure that the right-hand side is small. The technique is similar to (iii) in that an expansion is used and similar to (ii) in that the problem reduces to solving linear equations. It has the advantage that, although it is necessary to evaluate the effect of the operator on the basis functions, it is not necessary to perform further analytic or numerical work other than solve linear equations. As is the case with the R-matrix method, one calculation suffices to obtain results over a range of energies.

2. The close coupling equations

The close coupling equations for e^--H scattering have been described by Percival and Seaton (1957). Subsequently Norcross (1969) modified the formulation to include orthogonality conditions designed to overcome numerical instability. A variety of different orthogonality schemes are discussed in the review by Burke and Seaton (1971). The aim of these procedures is to define the scattering functions uniquely, and to this end inhomogeneous Lagrange terms are introduced. The equations are rederived here

0305-4470/89/204339+07$02.50

from a slightly different viewpoint to show how the trivial solutions for the wavefunction have been eliminated by modifying the exchange kernel. The convergence of the method used was found to be adversely affected if these solutions are not eliminated.

In the usual way let the wavefunction Ψ for the e^--H system be represented as

$$\Psi(r_1, r_2) = (r_1 r_2)^{-1}(1+(-1)^S P_{12}) \sum_{\bar{n}\bar{l}_1\bar{l}_2 L} \mathcal{Y}(\bar{l}_1\bar{l}_2 L|\hat{r}_1\hat{r}_2) P_{\bar{n}\bar{l}_1}(r_1) F_{\bar{n}\bar{l}_1\bar{l}_2}(r_2) \tag{1}$$

where S is the total electronic spin and the dependence of F on L and S is suppressed: $\mathcal{Y}$ denotes coupled spherical harmonics, the $P_{\bar{n}\bar{l}_1}(r_1)$ are the radial hydrogen eigenfunctions, and the $F_{\bar{n}\bar{l}_1\bar{l}_2}(r_2)$ are the scattering functions that must be determined. Let $\mathcal{H}$ be the Hamiltonian and E the total energy. If we impose the condition that

$$\langle \mathcal{Y}^*(l_1 l_2 L|\hat{r}_1\hat{r}_2) r_1^{-1} P_{nl_1}(r_1)[\mathcal{H}-E]\Psi\rangle_{r_1\hat{r}_2} = 0 \tag{2}$$

then we obtain coupled integro-differential equations of the form

$$F''_{nl_1l_2}(r_2) + \sum_{\bar{n}\bar{l}_1\bar{l}_2} V^{\bar{n}\bar{l}_1\bar{l}_2}_{nl_1l_2} F_{\bar{n}\bar{l}_1\bar{l}_2}(r_2) + \langle W^{\bar{n}\bar{l}_1\bar{l}_2}_{nl_1l_2}(r_2, r_1) F_{\bar{n}\bar{l}_1\bar{l}_2}(r_2)\rangle_{r_1} = 0. \tag{3}$$

In (2) and (3), $\langle\,\rangle$ denotes integration over the entire physical range of the variables which are denoted by subscripts. The infinite set of coupled integro-differential equations (3) must be truncated to say N equations and the $F_{nl_1l_2}(r_2)$ can be taken to be the elements of an N-dimensional vector $\boldsymbol{f}$. This vector satisfies the boundary condition $\boldsymbol{f}(0) = \mathbf{0}$ and the truncated equations (3) can be written in matrix form as

$$\boldsymbol{f}'' + \mathbf{V}\boldsymbol{f} + \langle \mathbf{W}(r_2, r_1)\boldsymbol{f}(r_1)\rangle_{r_1} = \mathbf{0}. \tag{4}$$

These are the equations derived by Percival and Seaton (1957), who give expressions for the potential $\mathbf{V}$ and the kernel $\mathbf{W}$ which satisfy the symmetry conditions

$$\tilde{\mathbf{V}} = \mathbf{V} \qquad \tilde{\mathbf{W}}(r_2, r_1) = \mathbf{W}(r_1, r_2) \tag{5}$$

where the tilde denotes transposition.

If there were no integral terms in (4) then there would exist N linearly independent solution vectors $\boldsymbol{f}$. However, (4) contains additional unwanted solutions that correspond to a trivial solution for Ψ. These solutions must be eliminated and to see how they arise the expansion (1) can be rewritten

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = (r_1 r_2)^{-1} \sum_{\bar{n}\bar{l}_1\bar{l}_2 L} \mathcal{Y}(\bar{l}_1\bar{l}_2 L|\hat{r}_1\hat{r}_2)[P_{\bar{n}\bar{l}_1}(r_1) F_{\bar{n}\bar{l}_1\bar{l}_2}(r_2) + (-1)^\sigma P_{\bar{n}\bar{l}_2}(r_2) F_{\bar{n}\bar{l}_2\bar{l}_1}(r_1)] \tag{6}$$

where

$$\sigma = L + S + \bar{l}_1 + \bar{l}_2.$$

Following Norcross (1969), it follows from (6) that the linear combination

$$F_{\bar{n}\bar{l}_1\bar{l}_2}(r_2) = \sum_{n'} \alpha^{n'}_{\bar{n}\bar{l}_1} P_{n'\bar{l}_2}(r_2) \tag{7}$$

gives a trivial solution for Ψ if

$$\sum_{\bar{n}n'} [\alpha^{n'}_{\bar{n}\bar{l}_1} P_{\bar{n}\bar{l}_1}(r_1) P_{n'\bar{l}_2}(r_2) + (-1)^\sigma \alpha^{n'}_{\bar{n}\bar{l}_2} P_{n'\bar{l}_1}(r_1) P_{\bar{n}\bar{l}_2}(r_2)] = 0.$$

This is the case if

$$\alpha^{n'}_{\bar{n}\bar{l}_1} + (-1)^\sigma \alpha^{\bar{n}}_{n'\bar{l}_2} = 0. \tag{8}$$

Let $T^{(j)}(r)$ denote all the solution vectors that correspond in this way to a trivial solution. For example, in a two-state expansion in which $L=0$, $S=1$ and $n=1$ or 2 there are three such vectors:

$$\boldsymbol{T}^{(1)}=\begin{bmatrix}P_{10}\\0\end{bmatrix}\qquad \boldsymbol{T}^{(2)}=\begin{bmatrix}0\\P_{20}\end{bmatrix}\qquad \boldsymbol{T}^{(3)}=\frac{1}{\sqrt{2}}\begin{bmatrix}P_{20}\\P_{10}\end{bmatrix}. \tag{9}$$

Each of the $\boldsymbol{T}^{(j)}$ satisfies (4) because it corresponds to the solution $\Psi(r_1, r_2)=0$, and they are orthogonal.

Let $\mathbf{W}_0$ be another kernel and let $\boldsymbol{g}$ be any column vector that satisfies the equations

$$\boldsymbol{g}''+\mathbf{V}\boldsymbol{g}+\langle\mathbf{W}_0(r_2, r_1)\boldsymbol{g}(r_1)\rangle_{r_1}=\mathbf{0}. \tag{10}$$

From (4)

$$\tilde{\boldsymbol{T}}''+\tilde{\boldsymbol{T}}\tilde{\mathbf{V}}+\langle\tilde{\boldsymbol{T}}(r_1)\tilde{\mathbf{W}}(r_2, r_1)\rangle_{r_1}=\mathbf{0} \tag{11}$$

where $\boldsymbol{T}$ is one of the vectors $\boldsymbol{T}^{(j)}$. Since $\tilde{\mathbf{V}}=\mathbf{V}$ and $\lim_{r\to\infty}\boldsymbol{T}(r)=\mathbf{0}$ it can be seen that

$$\langle\tilde{\boldsymbol{T}}(r_2)\mathbf{W}_0(r_2, r_1)\boldsymbol{g}(r_1)-\tilde{\boldsymbol{T}}(r_1)\tilde{\mathbf{W}}(r_2, r_1)\boldsymbol{g}(r_2)\rangle_{r_1r_2}=0$$

which can be written

$$\langle\tilde{\boldsymbol{T}}(r_2)[\mathbf{W}_0(r_2, r_1)-\mathbf{W}(r_2, r_1)]\boldsymbol{g}(r_1)\rangle_{r_1r_2}=0. \tag{12}$$

Now let us choose $\mathbf{W}_0$ so that

$$[\mathbf{W}_0(r_2, r_1)-\mathbf{W}(r_2, r_1)]_{kl}=\delta_{kl}\sum_{j'}\beta_{j'}T_k^{(j')}(r_1)T_l^{(j')}(r_2) \tag{13}$$

where the $T_k^{(j)}$ are the components of $\boldsymbol{T}^{(j)}$. If $\boldsymbol{T}=\boldsymbol{T}^{(j)}$ then (12) becomes

$$\sum_k\langle T_k^{(j)}(r)g_k(r)\rangle_r=0$$

or

$$\langle\tilde{\boldsymbol{T}}^{(j)}\boldsymbol{g}\rangle=0. \tag{14}$$

So the solution of (10) is orthogonal to the vectors $\boldsymbol{T}^{(j)}$ if $\mathbf{W}_0$ is chosen according to (13). What has been proved in effect is that removing from (4) any multiple of the terms that would be zero if f were orthogonal to the vectors $\boldsymbol{T}^{(j)}$ ensures that the resulting solutions are indeed orthogonal to them.

It can be shown using (14) that for large r_2 the non-exponential solutions of (4) and the solutions of (10) are the same. Equations (10) have only N linearly independent solutions which comprise a square matrix $\mathbf{F}$. The final equations to be solved are therefore

$$\mathbf{F}''+\mathbf{V}\mathbf{F}+\langle\mathbf{W}_0(r_2, r_1)\mathbf{F}(r_1)\rangle_{r_1}=0 \tag{15}$$

where

$$\mathbf{W}_0(r_2, r_1)=\mathbf{W}(r_2, r_1)+\sum_j\beta_j\Delta^{(j)} \tag{16}$$

the β_j are any constants and

$$(\Delta^{(j)})_{kl}=\delta_{kl}[\boldsymbol{T}^{(j)}(r_1)\tilde{\boldsymbol{T}}^{(j)}(r_2)]_{kl}. \tag{17}$$

The problem of trivial solutions for Ψ can thus be eliminated by redefining the exchange kernel $\mathbf{W}$.

3. The numerical procedure

For large values of r, $r > R_0$ say, there are a number of techniques whereby the equations (15) can be solved. The method to be used in these calculations is that of Rudge (1984, 1985). The problem is therefore to solve (15) in the range $0 \leq r \leq R_0$ subject to the boundary condition

$$\mathbf{F}(0) = \mathbf{0}. \tag{18}$$

As a consequence of this it follows that

$$[\tilde{\mathbf{F}}(\mathbf{F}')^{-1}]_{r=R_0} = [\tilde{\mathbf{F}}(\mathbf{F}')^{-1}]^{\mathrm{T}}_{r=R_0} \tag{19}$$

where the superscript T denotes transposition.

In practice it is inconvenient to apply the boundary condition (18) at $r = 0$. This is because N linearly independent sets of derivatives are needed to generate the N linearly independent solutions and some or all of these derivatives can vanish at $r = 0$ also. If the boundary condition is shifted to $r = \varepsilon$, say, then (19) is guaranteed if

$$\tilde{\mathbf{F}}\mathbf{F}'|_{\varepsilon} = \tilde{\mathbf{F}}'\mathbf{F}|_{\varepsilon}. \tag{20}$$

It is then possible to choose for example

$$\mathbf{F}(\varepsilon) = \varepsilon \mathbf{I} \qquad \mathbf{F}'(\varepsilon) = \mathbf{I} \tag{21}$$

and for small enough ε (21) implies that $\mathbf{F}(0) \approx 0$. However, it is possible, especially if there are closed channels, for the condition (21) to generate solutions in which one component of the solution vector is much larger than the others. In order to avoid this it is preferable to first solve the equations as a two-point boundary value problem

$$\mathbf{F}(\varepsilon) = \varepsilon \mathbf{I} \qquad \mathbf{F}(R_0) = \mathbf{I} \tag{22}$$

which ensures that all the solutions are of a similar size at $r = R_0$, but does not imply the necesary condition (19). From the solution $\mathbf{F}_{\mathrm{calc}}$ with the boundary condition (22) we can evaluate $\mathbf{F}'_{\mathrm{calc}}(\varepsilon)$. The calculation can then be repeated with the one-point boundary condition

$$\mathbf{F}(\varepsilon) = \varepsilon \mathbf{I} \qquad \mathbf{F}'(\varepsilon) = \tfrac{1}{2}[\mathbf{F}'_{\mathrm{calc}}(\varepsilon) + \tilde{\mathbf{F}}'_{\mathrm{calc}}(\varepsilon)]. \tag{23}$$

For significant l_2 values a better choice of $\mathbf{F}(\varepsilon)$ is

$$[\mathbf{F}(\varepsilon)]_{ij} = \delta_{ij}\varepsilon^{l_j+1} \tag{24}$$

where l_j is the l_2 value for channel j, and the appropriate choice of $\mathbf{F}'(\varepsilon)$ is

$$\mathbf{F}'(\varepsilon) = \tfrac{1}{2}[\mathbf{F}'_{\mathrm{calc}} + (\mathbf{F}^{-1})^{\mathrm{T}}(\mathbf{F}'_{\mathrm{calc}})^{\mathrm{T}}\mathbf{F}]_{\varepsilon}. \tag{25}$$

Now let $\{\phi_m\}$ $(1 \leq m \leq M)$ be any linearly independent set of basis functions, and let $\mathbf{\Phi}_m = \phi_m \mathbf{I}$ where $\mathbf{I}$ is the $N \times N$ unit matrix. We represent $\mathbf{F}$ in the form

$$\mathbf{F} = \sum_{m=1}^{M} \mathbf{\Phi}_m \mathbf{A}_m. \tag{26}$$

In order to do this we choose the $\mathbf{A}_m$ in such a way that the equations (15) are satisfied identically at a discrete set of points. Let $\{r_m\}$ $(1 \leq m \leq M)$ be this set of points where $r_1 = \varepsilon$, $r_M = R_0$.

Let $\mathbf{X}$ denote a matrix that contains $M \times M$ blocks of $N \times N$ matrices $\mathbf{X}^{PQ}$. Then

$$(\mathbf{X})_{rs} = (\mathbf{X}^{PQ})_{pq} \tag{27}$$

where

$$r=(P-1)N+p \qquad 1\leqslant P\leqslant M$$
$$s=(Q-1)N+q \qquad 1\leqslant Q\leqslant M. \tag{28}$$

Writing equation (15) as

$$\mathscr{L}\mathbf{F}=\mathbf{0}$$

we define

$$\mathbf{X}^{PQ}=\mathscr{L}\boldsymbol{\Phi}_Q(r_{P-1}) \qquad 3\leqslant P\leqslant M \tag{29}$$
$$\mathbf{X}^{1Q}=\boldsymbol{\Phi}_Q(r_1) \tag{30}$$
$$\mathbf{X}^{2Q}=\boldsymbol{\Phi}'_Q(r_1) \qquad \text{or} \qquad \boldsymbol{\Phi}_Q(R_0) \tag{31}$$

where in (31) the first choice occurs for the boundary condition (21) and the second for the boundary condition (22).

If $\mathbf{A}$ is the matrix with

$$\mathbf{A}^{P1}=\mathbf{A}_P \tag{32}$$

then the equations to be solved are

$$\mathbf{XA}=\mathbf{Z} \tag{33}$$

where

$$\begin{aligned}&\mathbf{Z}^{11}=\mathbf{F}(\varepsilon)\\ &\mathbf{Z}^{21}=\mathbf{F}'(\varepsilon) \quad \text{(boundary condition (21))}\\ &\qquad \mathbf{F}(\mathbf{R}_0) \quad \text{(boundary condition (22))}\end{aligned} \tag{34}$$

and all other blocks are zero.

The potential matrix $\mathbf{V}$ and the exchange kernel $\mathbf{W}$ can be written

$$\mathbf{V}=\mathbf{V}_0+2E\mathbf{I} \qquad \mathbf{W}=\mathbf{W}_0+2E\mathbf{W}_1 \tag{35}$$

and so correspondingly

$$\begin{aligned}\mathbf{X}&=\mathbf{X}_0+2E\mathbf{X}_1\\ &=\mathbf{X}_0(\mathbf{I}+2E\mathbf{SDS}^{-1})\end{aligned} \tag{36}$$

where

$$\mathbf{SDS}^{-1}=\mathbf{X}_0^{-1}\mathbf{X}_1.$$

It follows that

$$\mathbf{A}=\mathbf{S}(\mathbf{I}+2E\mathbf{D})^{-1}(\mathbf{X}_0\mathbf{S})^{-1}\mathbf{Z} \tag{37}$$

and so by diagonalising $\mathbf{X}_0^{-1}\mathbf{X}_1$ the $\mathbf{A}$ matrix can be found for a range of values E.

4. Calculations

Test runs have been carried out using a basis of Chebyshev polynomials

$$\phi_m=T_{m-1}(x) \qquad 1\leqslant m\leqslant M \tag{38}$$

where $x = (2r - R_0)/R_0$ and where the r_m $(2 \leq m \leq M-1)$ are the zeros of T_{M-2}. The equations (15) are thus replaced by the equations

$$\mathscr{L}\mathbf{F} = \mathbf{A}(r)\,T_{M-2}(x) \tag{39}$$

where $\mathbf{A}(r)$ is an amplitude function that can be computed. The solutions are accurate if $\mathbf{A}(r)$ is small.

Table 1. Computed one-channel phase shifts $\eta(S)$; $R_0 = 20.0$.

	$M=12$		$M=14$		$M=16$		$M=18$		$M=20$	
k^2	$\eta^{(0)}$	$\eta^{(1)}$	$\eta^{(0)}$	$\eta^{(1)}$	$\eta^{(0)}$	$\eta^{(1)}$	$\eta^{(0)}$	$\eta^{(1)}$	$\eta^{(0)}$	$\eta^{(1)}$
0.1	1.488	2.453	1.460	2.423	1.460	2.427	1.460	2.427	1.460	2.427
0.3	0.933	1.977	0.944	1.985	0.945	1.985	0.946	1.985	0.946	1.985
0.5	0.685	1.727	0.734	1.735	0.736	1.734	0.736	1.734	0.736	1.734
0.7	0.683	1.635	0.626	1.570	0.619	1.563	0.620	1.563	0.620	1.563
0.9	0.627	0.893	0.582	1.366	0.561	1.438	0.560	1.440	0.560	1.440

Table 2. K-matrix elements 1s, 2s expansion.

		$M=14$		$M=16$		$M=18$		$M=20$	
k^2	Elements	$S=0$	$S=1$	$S=0$	$S=1$	$S=0$	$S=1$	$S=0$	$S=1$
0.5	K_{11}	0.967	−5.15	0.934	−5.26	0.957	−5.25	0.957	−5.23
1.0	K_{11}	0.478	3.43	0.583	5.38	0.589	−5.61	0.540	5.62
	K_{12}	0.379	0.105	0.450	0.156	0.454	0.162	0.454	0.162
	K_{22}	−0.807	0.041	−0.798	0.043	−0.798	0.043	−0.798	0.043
1.25	K_{11}	−0.0129	−5.25	0.386	4.25	0.421	3.35	0.422	3.32
	K_{12}	0.795	−0.299	0.591	0.225	0.566	0.180	0.565	0.179
	K_{22}	−0.945	−0.609	−1.16	−0.589	−1.19	−0.591	−1.19	−0.591

Table 3. K-matrix elements 1s, 2s,2p expansion.

		$M=16$		$M=18$		$M=20$	
k^2	Elements	$S=0$	$S=1$	$S=0$	$S=1$	$S=0$	$S=1$
0.81	K_{11}	0.791	5.98	0.822	6.81	0.824	6.60
	K_{12}	−0.256	2.96	−0.253	3.98	−0.253	3.89
	K_{13}	0.591	−1.67	0.585	−2.24	0.584	−2.19
	K_{22}	−1.049	14.6	−1.05	15.4	−1.051	15.4
	K_{23}	1.033	−9.00	1.04	−9.41	1.04	−9.45
	K_{33}	0.596	5.42	0.584	5.70	0.584	5.67
1.21	K_{11}	0.137	0.934	0.148	3.63	0.143	3.78
	K_{12}	0.275	0.212	0.467	0.447	0.506	0.523
	K_{13}	0.879	−0.081	1.505	−0.166	1.63	−0.194
	K_{22}	0.125	1.03	0.148	1.04	0.153	1.05
	K_{23}	−0.615	−1.49	−0.551	−1.49	−0.534	−1.49
	K_{33}	−6.18	0.705	−5.97	0.708	−5.91	0.709

In table 1 the computed phase shifts are shown for a one-channel expansion as a function of M. In tables 2 and 3 results are shown respectively for a two-state and a three-state calculation. In each case acceptable accuracy is attained at the energies shown with quite a small basis size.

5. Conclusions

A collocation procedure has been applied to the solution of a complicated set of coupled integro-differential equations that arise in scattering theory. This procedure in which the equations are satisfied identically over a discrete set of points has been shown to be simple and accurate. A Chebyshev basis was used, calculations using a Legendre basis were found to have very similar convergence properties. At higher energies than those examined here the solutions oscillate more rapidly and a different basis would then be appropriate. An attractive feature of the method is that it only requires the effect of the operator on the basis functions over a discrete set of points while variational methods, for example, require the more difficult evaluation of inner products.

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