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A discrete procedure for solving asymptotic equations

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Abstract. A method is described for solving the close-coupling equations that arise in non-relativistic scattering theory in the asymptotic region where the scattered particle is far removed from the residual atom or ion. Typical results are presented that indicate the convergence and accuracy of the method.

1. Introduction

In performing scattering calculations a considerable part of the computational effort arises from evaluating solutions in the asymptotic region defined as that region wherein only the long-range r^{-n} coupling between the scattering channels is significant. A variety of methods for generating solutions have been used (Norcross 1969, Crees 1981, Croskery *et al* 1982, Baluja *et al* 1982). In particular, Rudge (1985) developed a variational procedure that facilitates this task. This method works very well for scattering by neutral species, and a computer code that implements it has been written (Rudge 1984). Later, a discrete procedure was developed for solving coupled integrodifferential equations (Rudge 1989) which can be used in scattering calculations to describe the inner scattering region. The purpose of this paper is to indicate that a very similar technique can be used to solve the asymptotic equations and that this new method applies equally well to the scattering by neutral or charged species.

2. The scattering equations

We consider non-relativistic scattering in an N-channel representation. Let

$$D_q=\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k_q^2+2Zr^{-1}-l_q(l_q+1)r^{-2} \tag{1}$$

and define the operator matrix

$$\mathscr{L}_0=\mathrm{diag}(D_q)\,. \tag{2}$$

The asymptotic equations to be solved are

$$\mathscr{L}_0\mathbf{F}_j+V\mathbf{F}_j=\mathbf{0} \tag{3}$$

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where

$$V=\sum_{\lambda=2}^{N_\lambda} r^{-\lambda}v_\lambda. \tag{4}$$

In (4) the v_λ are $N\times N$ matrices that represent the coupling between the channels and in (3) the $\mathbf{F}_j$ are solution matrices that are specified by their form in the region of large r.

On defining

$$\eta_j=Zk_j^{-1} \tag{5}$$

and

$$\theta_j=k_jr-l_j\pi/2+\eta_j\ln(2k_jr)+\arg\Gamma(l_j+1-i\eta_j) \tag{6}$$

the asymptotic forms are

$$[\mathbf{F}_2+i\mathbf{F}_1]_{jk}\underset{r\to\infty}{\sim}\delta_{jk}[k_j^{-1/2}\exp(i\theta_j)] \tag{7}$$

for $1\leqslant j\leqslant N$ and $1\leqslant k\leqslant N_o$, where N_o is the number of open channels (for which $k_j^2>0$). Let $N_c=N-N_o$ be the number of closed channels ($k_j^2<0$). Then we can also obtain N_c solution vectors specified by

$$[\mathbf{F}_3]_{jk}\underset{r\to\infty}{\sim}\delta_{jk}\{\exp[-k_jr+\eta_j\ln(r)]\} \tag{8}$$

for $1\leqslant j\leqslant N$ and $1\leqslant k\leqslant N_c$ where $k_j=|k_j^2|^{1/2}$. There are thus $2N_o+N_c$ solution vectors

$$\mathbf{F}=[\mathbf{F}_1\mathbf{F}_2\mathbf{F}_3] \tag{9}$$

that satisfy

$$\mathbf{F}''+[V_0+V]\mathbf{F}=0 \tag{10}$$

where

$$V_0=\mathrm{diag}[k_q^2+2Zr^{-1}-l_q(l_q+1)r^{-2}]. \tag{11}$$

Since the matrices V_0 and V are symmetric, it follows that

$$\bar{\mathbf{F}}''+\bar{\mathbf{F}}[V_0+V]=0. \tag{12}$$

From (10) and (12) and the boundary conditions (7) and (8) it follows that the Wronskian matrix is

$$W=\bar{\mathbf{F}}\mathbf{F}'-\bar{\mathbf{F}}'\mathbf{F}=\begin{bmatrix}\mathbf{0}&\mathbf{I}&\mathbf{0}\\-\mathbf{I}&\mathbf{0}&\mathbf{0}\\\mathbf{0}&\mathbf{0}&\mathbf{0}\end{bmatrix}. \tag{13}$$

In (13) the first two rows and column blocks contain N_o rows or columns, and the third row and third column are of length N_c.

Let $\mathscr{F}$ be an $N\times N$ matrix of solutions in the range $0\leqslant r\leqslant R_1$ that satisfies $\mathscr{F}(0)=\mathbf{0}$. Then there are $N\times N_o$ matrices C and K such that

$$\mathscr{F}C=\mathbf{F}_1+[\mathbf{F}_2\mathbf{F}_3]K \tag{14}$$

and

$$\mathscr{F}'C=\mathbf{F}_1'+[\mathbf{F}_2\mathbf{F}_3]'K. \tag{15}$$

Hence the matrix $\boldsymbol{K}$, from which all the scattering parameters may be calculated, is given by

$$\boldsymbol{R}\mathbf{F}_1' - \mathbf{F}_1 = \{[\mathbf{F}_2\mathbf{F}_3] - \boldsymbol{R}[\mathbf{F}_2\mathbf{F}_3]'\}\boldsymbol{K} \tag{16}$$

where

$$\boldsymbol{R} = \mathscr{F}(\mathscr{F}')^{-1}. \tag{17}$$

3. The computational procedure

Let $\boldsymbol{F}$ be one of the solution vectors and let φ be a row of basis functions of length N_f. We write

$$\boldsymbol{F} = \begin{bmatrix} \varphi & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \varphi & \dots & \mathbf{0} \\ \vdots & & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \varphi \end{bmatrix} \begin{bmatrix} \boldsymbol{a}_1 \\ \vdots \\ \boldsymbol{a}_n \end{bmatrix} = \Phi\boldsymbol{a} \tag{18}$$

where the $\boldsymbol{a}_j$ are vectors that contain N_f coefficients. In order to obtain a solution we select in the range $R_1 \leqslant r \leqslant R_2$ a set of points r_j, $1 \leqslant j \leqslant N_p$, called the collocation points, and set

$$\mathscr{L}_0\boldsymbol{F}(r_j) + \boldsymbol{V}\boldsymbol{F}(r_j) = 0 \tag{19}$$

which implies the linear equations

$$[\mathscr{L}_0\Phi(r_j) + \boldsymbol{V}\Phi(r_j)]\boldsymbol{a} = 0. \tag{20}$$

In addition, there are boundary conditions

$$\Phi(R_2)\boldsymbol{a} = \boldsymbol{F}(R_2) \tag{21}$$

and

$$\Phi'(R_2)\boldsymbol{a} = \boldsymbol{F}'(R_2). \tag{22}$$

This gives $N \times (N_p + 2)$ equations for the $N \times N_f$ coefficients $\boldsymbol{a}$. Let A denote the matrix that contains the $2N_o + N_c$ solution vectors corresponding to the boundary conditions (7) and (8). Then we see that

$$\begin{bmatrix} \Phi(R_2) \\ \Phi'(R_2) \\ [\mathscr{L}_0\Phi(r_j) + V(r_j)\Phi(r_j)] \end{bmatrix} A = \begin{bmatrix} \mathbf{F}(R_2) \\ \mathbf{F}'(R_2) \\ \mathbf{0} \end{bmatrix}. \tag{23}$$

In general, the number of rows exceeds the number of columns, in which case we need to solve the first $2N$ equations exactly and the remainder using a least squares criterion.

On writing the first $2N$ rows of the left-hand side matrix in (23) by X_1 and the remainder by X_2, we find that we need to solve the equations

$$X \begin{bmatrix} \Lambda \\ A \end{bmatrix} = \begin{bmatrix} \mathbf{F}(R_2) \\ \mathbf{F}'(R_2) \\ 0 \end{bmatrix} \tag{24}$$

where

$$X=\begin{bmatrix} \mathbf{0} & X_1 \\ \tilde{X}_1 & \tilde{X}_2 X_2 \end{bmatrix} \tag{25}$$

and the elements of Λ are Lagrange multipliers. For some cases the solution of the linear equations (24) can proceed efficiently by Gauss elimination. For a problem that contains, say, 20 non-degenerate channels, the matrix in (24) can be about 4000×4000. The direct application of the method by simply computing the matrix and then using Gauss elimination can then impose a substantial computing burden both in terms of time and storage. However, we note that the problem is structured in such a way that, although the matrix X is not sparse, an iterative method can be used. In this method we require to multiply an arbitrary vector by X. Since X_2 contains blocks of the form $\Phi_j''|(V_0|\ V)\Phi_j$, where $\Phi_j=\Phi(r_j)$, we see that the essential products are of the type Φv and $\tilde{\Phi} w$ where v and w are arbitrary vectors of the appropriate dimension and Φ contains the blocks Φ_j. If the first $N \times N_f$ elements of v are written

$$v=\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix} \tag{26}$$

then

$$[\Phi v]_{(j-1)N+k}=\tilde{\varphi}_j v_k \tag{27}$$

where $\varphi_j=\varphi(r_j)$. On defining $l=(p-1)N_f+q$ it can be seen that

$$(\tilde{\Phi} w)_l=\sum_{j=1}^{N_p} \varphi_q(r_j) w_k \tag{28}$$

where $k=(j-1)N+p$. Hence in the iterative method the only arrays that need to be stored are those for φ_j, φ_j'' and V, and the matrix X need never be calculated explicitly. This considerably reduces the amount of storage required.

4. The choice of basis

Let

$$S_j=\int [k_j^2+2Zr^{-1}-l_j(l_j+1)r^{-2}]^{1/2}\,\mathrm{d}r \tag{29}$$

where the constant of integration is chosen so that

$$S_j \underset{r\to\infty}{\sim} \theta_j \tag{30}$$

(cf. Seaton and Peach 1962). Then, (7) can be written

$$[\mathbf{F}_2+\mathrm{i}\mathbf{F}_1]_{jk} \underset{r\to\infty}{\sim} \delta_{jk}[S_j'^{-1/2}\exp(\mathrm{i}S_j)] \tag{31}$$

to the accuracy of the JWKB approximation. This suggests the choice of functions

$$\tilde{\boldsymbol{\varphi}}=[\tilde{\varphi}_1\tilde{\varphi}_2\ldots\tilde{\varphi}_M] \tag{32}$$

where, for open channels,

$$\tilde{\varphi}_j=[\cos(S_j)\tilde{t}\ \sin(S_j)\tilde{t}]. \tag{33}$$

In (32) M is the number of non-degenerate channels and the S_j are the action integrals that have distinct k_j values. In (33) t is a vector, of dimension N_t, that contains suitable amplitude functions. For $R_3\leqslant r\leqslant R_2$ we have chosen these to be Chebyshev polynomials in r^{-1}, and for $R_1\leqslant r\leqslant R_3$ to be the same polynomials in the variable r. For the closed channels we have chosen

$$\tilde{\varphi}_j=[r^{\gamma}\exp(-k_j r)\tilde{t}] \tag{34}$$

where $\gamma=k_j^{-1}$. In choosing the collocation points there are two 'natural' choices. One choice is the Chebyshev zeros which, in the range $-1\leqslant x\leqslant 1$, are given by

$$x_j=\cos[(2j-1)\pi/2N] \qquad 1\leqslant j\leqslant N. \tag{35}$$

The other choice that we have used is the Chebyshev–Lobatto set given by

$$x_j=\cos[(j-1)\pi/(N-1)] \qquad 1\leqslant j\leqslant N. \tag{36}$$

5. Illustrative calculations

We consider two typical test cases. The first is a six-channel case with $Z=0$ that occurs in the calculation of electron–hydrogen atom scattering with three open and three closed channels. The second is a five-channel case with $Z=1$ that arises in electron–Ca^+ scattering with three open and two closed channels (cf Norcross 1969). We refer to these as case 1 and case 2, respectively. We define the discrepancy matrix Δ by

$$\mathbf{F}''+[V_0+V]\mathbf{F}=\Delta \tag{37}$$

and take two measures of the size of Δ. We define

$$\delta_1=\operatorname*{Max}_{ij}(|\Delta_{ij}|) \tag{38}$$

and

$$\delta_2^2=N^{-2}\sum_{ij}(\Delta_{ij})^2. \tag{39}$$

In figure 1 we show, for case 1, δ_1 and δ_2 as a function of basis size in the outer region ($R_3\leqslant r\leqslant R_2$). In figure 1, the upper curves display δ_1 and δ_2 for $N_t=4$ and the lower for $N_t=8$. In figure 2 we illustrate the effect of using the two choices of collocation points (35) and (36) in the inner region ($R_1\leqslant r\leqslant R_3$) for case 1. In both these cases, the number of Chebyshev polynomials is kept constant at six. In figures 3 and 4 the same comparisons are made for case 2 in which $Z=1$.

6. Concluding remarks

It can be seen clearly from figures 1 and 3 that high accuracy can be obtained using a relatively small number of basis functions. The use of four polynomials gives an error of about 10^{-7} for the $Z=1$ case and of about 10^{-8} for the $Z=0$ case. This decreases to about 10^{-11} and 10^{-14}, respectively, when the number of basis functions is doubled.

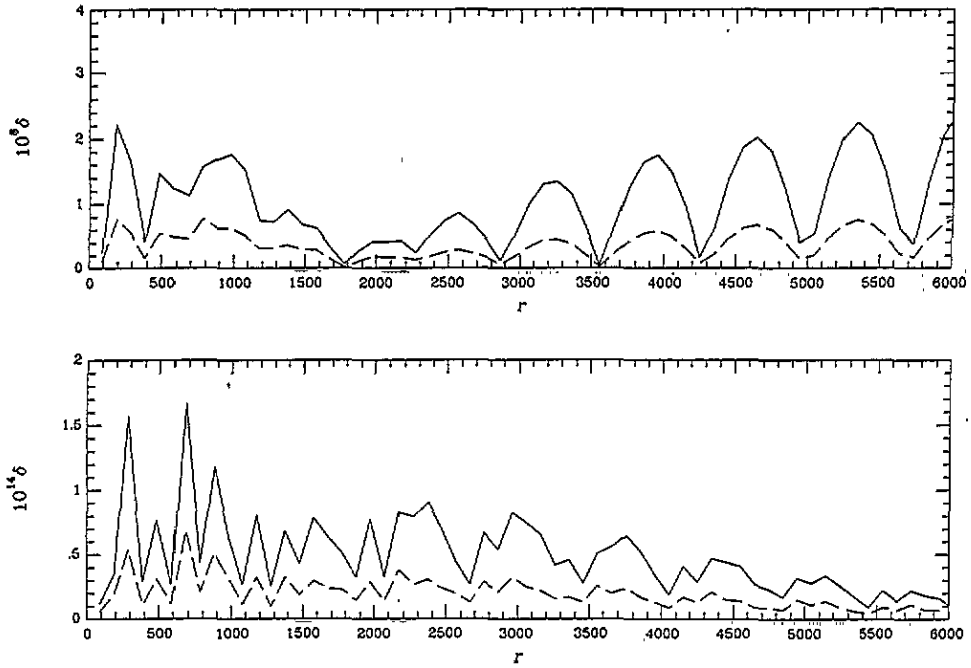

Figure 1. Case 1: plot of δ_1 (full line) and δ_2 (broken line) as a function of r for $R_3 \leqslant r \leqslant R_2$. Upper curves $N_t = 4$, lower curves $N_t = 8$.

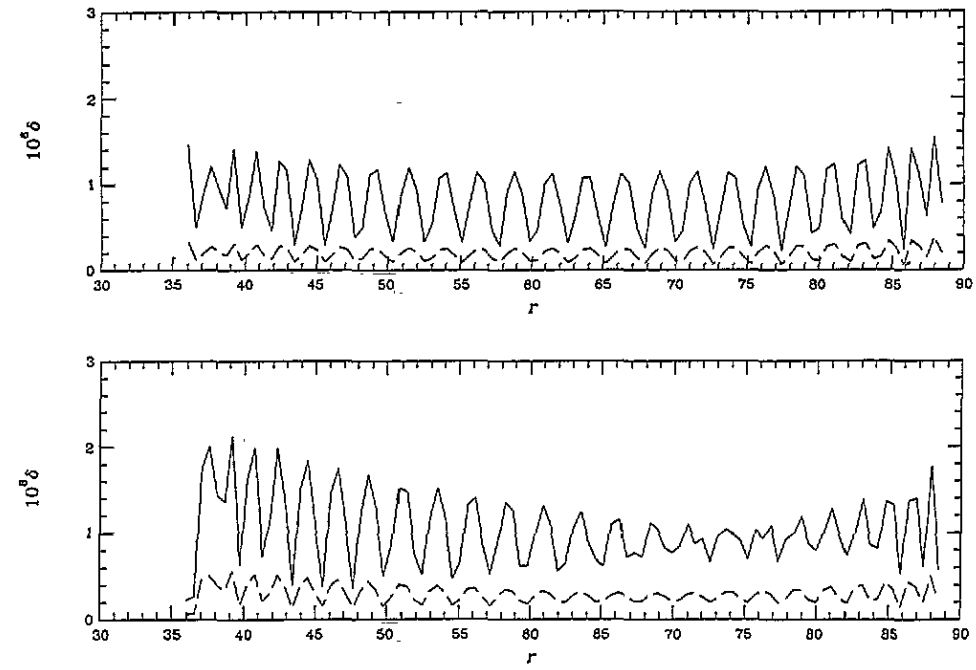

Figure 2. Case 1: plot of δ_1 (full line) and δ_2 (broken line) as a function of r for $R_1 \leqslant r \leqslant R_3$. Upper curves using the set (35), lower curves using the set (36). $N_t = 6$.

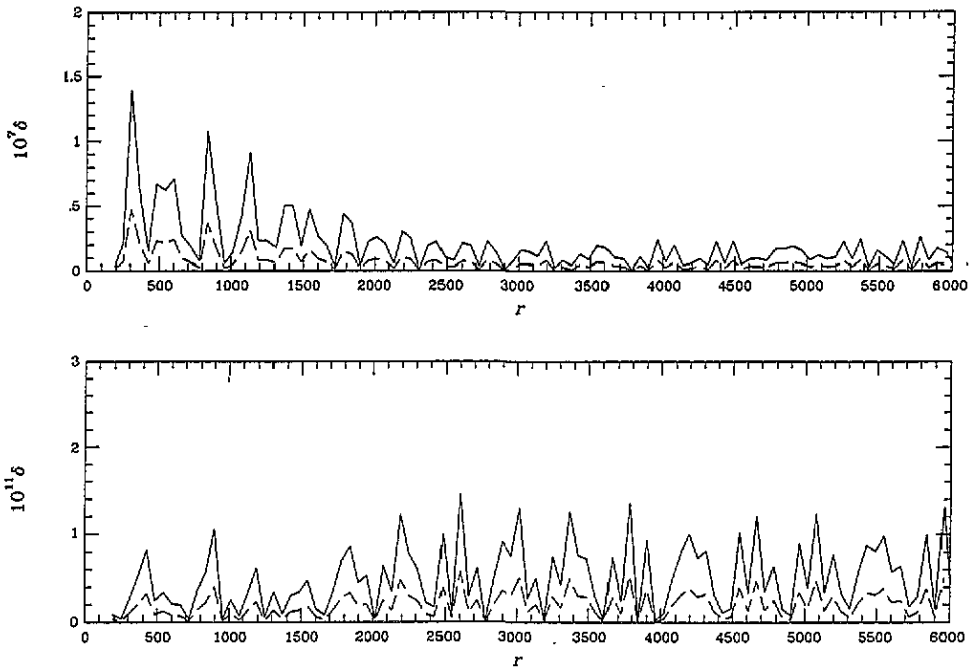

Figure 3. Case 2: plot of δ_1 (full line) and δ_2 (broken line) as a function of r for $R_3 \leqslant r \leqslant R_2$. Upper curves $N_t = 4$, lower curves $N_t = 8$.

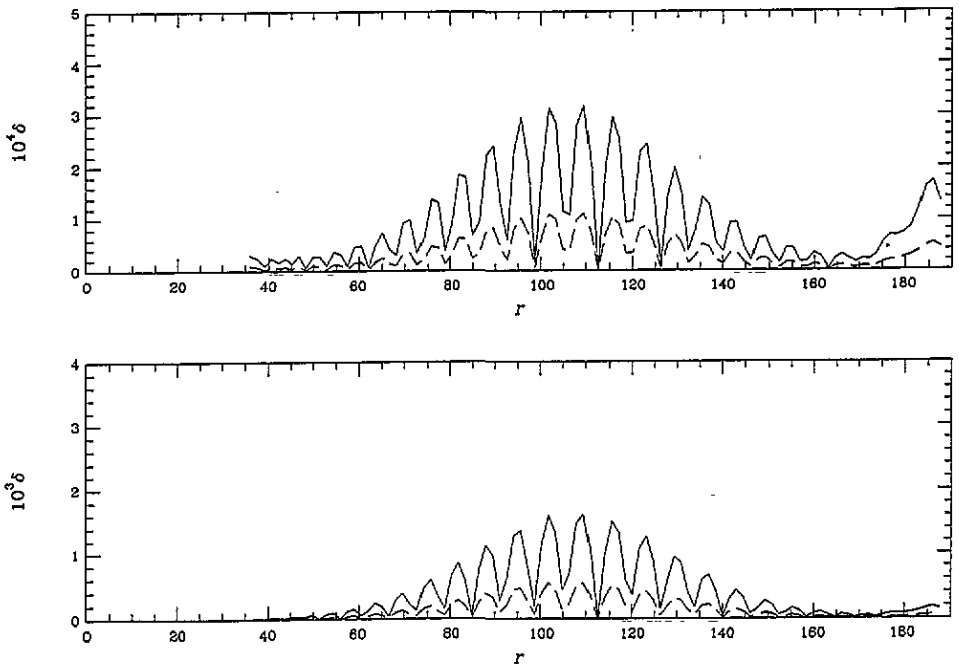

Figure 4. Case 2: plot of δ_1 (full line) and δ_2 (broken line) as a function of r for $R_1 \leqslant r \leqslant R_3$. Upper curves using the set (35), lower curves using the set (36). $N_t = 6$.

In figures 2 and 4 we illustrate the effect of the two choices of collocation points. It can be seen from figure 2 that in the $Z=0$ case the use of the Chebyshev–Lobatto points (36) gives an error that is smaller (by two orders of magnitude) than that obtained using the Chebyshev zeros (35). Figure 4, however, shows the opposite effect for the $Z=1$ case in which higher accuracy is achieved by using the Chebyshev zeros.

We conclude that the method is both stable and accurate for both sets of collocation points. For a given basis size the $Z=0$ results are superior to those obtained for $Z\neq 0$. This is probably due to the difference in the accuracy of (33) in the two cases.

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