

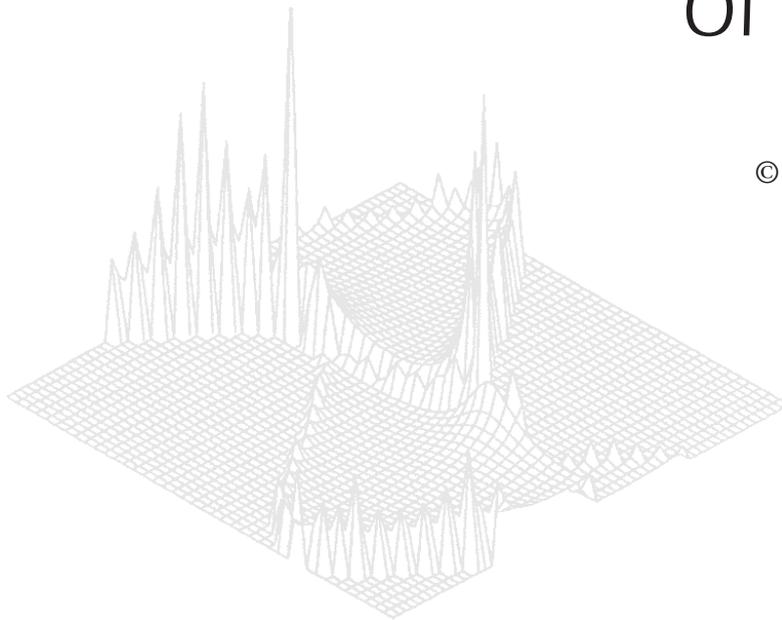
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## Towards a Direct Numerical Solution of Schrödinger's Equation for $(e, 2e)$ Reactions\*

*S. Jones and A. T. Stelbovics*

Centre for Atomic, Molecular and Surface Physics, Division of Science and Engineering,  
Murdoch University, Perth, WA 6150, Australia.

### *Abstract*

The finite-difference method for electron–hydrogen scattering is presented in a simple, easily understood form for a model collision problem in which all angular momentum is neglected. The model Schrödinger equation is integrated outwards from the atomic centre on a grid of fixed spacing  $h$ . The number of difference equations is reduced each step outwards using an algorithm due to Poet, resulting in a propagating solution of the partial-differential equation. By imposing correct asymptotic boundary conditions on this general, propagating solution, the particular solution that physically corresponds to scattering is obtained along with the scattering amplitudes. Previous works using finite differences (and finite elements) have extracted scattering amplitudes only for low-level transitions (elastic scattering and  $n = 2$  excitation). If we are to eventually extract ionisation amplitudes, however, the numerical method must remain stable for higher-level transitions. Here we report converged cross sections for transitions up to  $n = 8$ , as a first step towards obtaining ionisation  $(e, 2e)$  results.

### 1. Introduction

In this paper, we report progress towards a direct numerical solution of the Schrödinger equation for electron–atom ionisation [the  $(e, 2e)$  problem]. This problem has remained unsolved even for the simplest case of atomic hydrogen as target. The primary obstacle to obtaining accurate  $(e, 2e)$  cross sections is that correct three-particle boundary conditions need to be imposed in the asymptotic region. A direct approach (as opposed to e.g. close-coupling methods) can make this part of the problem much easier. We have chosen to use the finite-difference method, which was introduced by Poet (1980) for a simplified ‘ $S$ -wave model’ in which all angular momentum is neglected. Wang and Callaway (1993, 1994) extended Poet’s (1980) method to real electron–hydrogen scattering, but only for energies below the  $n = 3$  threshold. The similar finite-element method has been employed by Botero and Shertzer (1992) and Shertzer and Botero (1994) to describe real scattering below the  $n = 3$  threshold. Neither method has yet been extended to ionisation.

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When developing a general method for solving the six-dimensional three-body Schrödinger equation, it makes sense to consider first, simplified models of lower dimensionality. An ideal, two-dimensional, three-body model is the  $S$ -wave, or Temkin–Poet model (Temkin 1962; Poet 1978) mentioned above. Although only  $s$ -states are included for both projectile and atomic electrons, this model problem contains most of the features that make the real scattering problem hard to solve. Indeed, even in this simplified model, converged  $(e, 2e)$  energy distributions have never been obtained (see e.g. Bray 1997). We want to be sure our numerical method can obtain ionisation amplitudes for this simplified model before we include angular momentum.

This is a work in progress and we have just finished testing our code for energies below the ionisation threshold. Our cross sections for  $1s$ – $1s$  elastic scattering,  $1s$ – $2s$  and  $1s$ – $3s$  excitation are in excellent agreement with the convergent close-coupling (CCC) results of Bray and Stelbovics (1994) for electron–hydrogen scattering. We also present detailed results *at* the ionisation threshold, where we obtained converged cross sections for transitions up to  $n = 8$ .

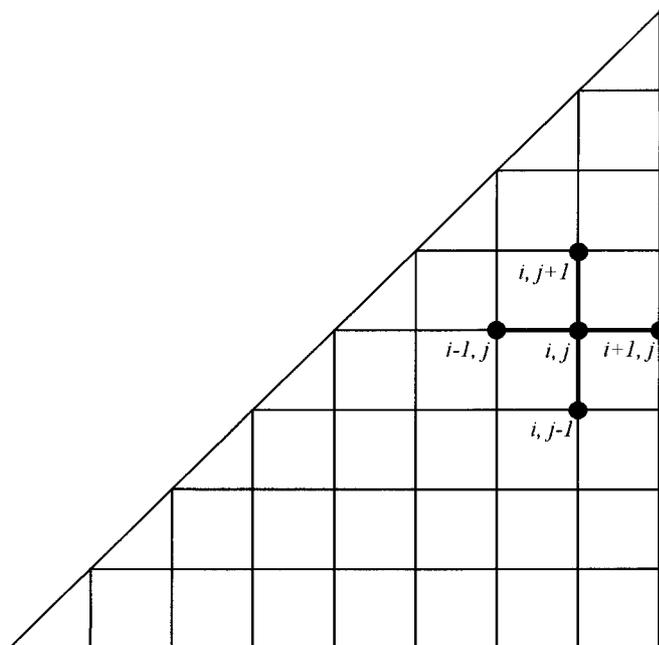


Fig. 1. Schematic diagram of the grid.

## 2. Finite-difference Method

The simplest finite-difference scheme involves solving Schrödinger's equation on a grid of fixed spacing  $h$ , with only nearest-neighbour points contributing with the central grid point to each difference equation (see Fig. 1). Since the wave function is symmetric (singlet spin state) or antisymmetric (triplet) about  $x = y$ , the region of integration reduces to a triangle. Although the triplet case

is easier, we consider the singlet case here since it provides a better test of the numerical method. The electron–hydrogen ‘*S*-wave model’ Schrödinger equation reads (Temkin 1962), in atomic units (a.u.)

$$\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{2}{y} + 2E \right) \Psi(x, y) = 0, \quad x \geq y. \quad (1)$$

Here the wave function, which must remain finite, has been multiplied by  $xy$ , so that

$$\Psi(x, 0) = 0, \quad (2)$$

$$\Psi(0, y) = 0. \quad (3)$$

Because we are integrating over a triangular region, the symmetry condition

$$\Psi(y, x) = \Psi(x, y) \quad (4)$$

must be imposed as well (this will come into play only when nearest-neighbour points lie above the triangular region, i.e. when the central grid point is on the line  $x = y$ ). If the atom is initially in a state  $m$ , then for impact energies at or below the ionisation threshold, the asymptotic behaviour of the wave function is given in terms of unknown *S*-matrix elements  $S_{nm}$  by

$$\Psi(x \rightarrow \infty, y) \sim \phi_{k_m}^*(x) \psi_m(y) - \sum_n S_{nm} \phi_{k_n}(x) \psi_n(y). \quad (5)$$

Here  $\psi_n(y)$  is the (*s*-state) wave function for the hydrogen atom with principal quantum number  $n$  and  $k_n$  is the corresponding wave number of the free electron described by  $\phi_{k_n}(x) = N_n \exp(ik_n x)$ , where  $N_n$  is a normalisation factor. Singlet cross sections are given by

$$\sigma_{nm} = \frac{1}{4k_m^2} |S_{nm} - \delta_{nm}|^2. \quad (6)$$

Note that this is just the usual expression for the real electron–hydrogen cross section with all angular momentum set equal to zero.

### (2a) Difference Equations

To convert the partial-differential equation (1) into difference equations, we impose a grid of fixed spacing  $h$  (Fig. 1) and approximate derivatives by finite differences:

$$\frac{\partial^2 \Psi(x, y)}{\partial x^2} \approx \frac{\Psi(x+h, y) - 2\Psi(x, y) + \Psi(x-h, y)}{h^2}, \quad (7)$$

$$\frac{\partial^2 \Psi(x, y)}{\partial y^2} \approx \frac{\Psi(x, y+h) - 2\Psi(x, y) + \Psi(x, y-h)}{h^2}. \quad (8)$$

Thus the wave function at grid point  $(i, j)$  is related to nearest neighbours by the difference equation

$$\Psi_j^{(i-1)} + \Psi_{j-1}^{(i)} + (h^2 T_j - 4)\Psi_j^{(i)} + \Psi_{j+1}^{(i)} + \Psi_j^{(i+1)} = 0. \quad (9)$$

Here  $\Psi_j^{(i)} = \Psi(x = ih, y = jh)$  and  $T_j = 2/(jh) + 2E$  is the non-derivative part of the Schrödinger equation. There will be as many equations as there are grid points.

Our difference equations (9) have the form (Poet 1980)

$$\mathbf{A}^{(i)} \cdot \bar{\Psi}^{(i-1)} + \mathbf{B}^{(i)} \cdot \bar{\Psi}^{(i)} + \mathbf{C}^{(i)} \cdot \bar{\Psi}^{(i+1)} = 0, \quad (10)$$

where we have collected the various  $\Psi_j^{(i)}, j = 1, 2, \dots, i$  for a given value of  $i$  into a vector  $\bar{\Psi}^{(i)}$ . By comparing (9) with (10), the matrix elements of  $\mathbf{A}^{(i)}$ ,  $\mathbf{B}^{(i)}$  and  $\mathbf{C}^{(i)}$  are easily determined. At the first grid point  $i = j = 1$ , equation (9) is

$$\Psi_1^{(0)} + \Psi_0^{(1)} + (h^2 T_1 - 4)\Psi_1^{(1)} + \Psi_2^{(1)} + \Psi_1^{(2)} = 0. \quad (11)$$

Using the boundary conditions (2), (3) and the symmetry condition (4), this simplifies to

$$(h^2 T_1 - 4)\Psi_1^{(1)} + 2\Psi_1^{(2)} = 0. \quad (12)$$

Comparing (12) with (10),  $\mathbf{A}^{(1)} = \mathbf{0}$ , and the only non-zero elements of  $\mathbf{B}^{(1)}$  and  $\mathbf{C}^{(1)}$  are given by

$$B_{1,1}^{(1)} = h^2 T_1 - 4, \quad (13)$$

$$C_{1,1}^{(1)} = 2. \quad (14)$$

At a general grid point  $(i, j)$ ,  $j \neq i$ , we have [comparing (9) with (10)]

$$A_{j,j}^{(i)} = 1, \quad (15)$$

$$B_{j,j-1}^{(i)} = 1, \quad (16)$$

$$B_{j,j}^{(i)} = h^2 T_j - 4, \quad (17)$$

$$B_{j,j+1}^{(i)} = 1, \quad (18)$$

$$C_{j,j}^{(i)} = 1. \quad (19)$$

For  $j = i \neq 1$ , the symmetry condition (singlet) is again needed and the non-zero elements are

$$B_{i,i-1}^{(i)} = 2, \quad (20)$$

$$B_{i,i}^{(i)} = h^2 T_i - 4, \quad (21)$$

$$C_{i,i}^{(i)} = 2. \quad (22)$$

### (2b) Propagation Method

At each value of  $i$  we can solve our equations if we apply symbolic boundary conditions at  $i + 1$  [solve for  $\Psi_j^{(i)}$  in terms of  $\Psi_j^{(i+1)}$  ( $j = 1, 2, \dots, i$ )]. This procedure yields a propagation matrix  $\mathbf{D}^{(i)}$ :

$$\bar{\Psi}^{(i)} = \mathbf{D}^{(i)} \cdot \bar{\Psi}^{(i+1)}. \quad (23)$$

We can obtain a recursion relation for  $\mathbf{D}^{(i)}$  by using (23) to eliminate  $\bar{\Psi}^{(i-1)}$  from equation (10):

$$[\mathbf{B}^{(i)} + \mathbf{A}^{(i)} \cdot \mathbf{D}^{(i-1)}] \cdot \bar{\Psi}^{(i)} = -\mathbf{C}^{(i)} \cdot \bar{\Psi}^{(i+1)}. \quad (24)$$

Comparing (24) with (23), we get

$$\mathbf{D}^{(i)} = -[\mathbf{B}^{(i)} + \mathbf{A}^{(i)} \cdot \mathbf{D}^{(i-1)}]^{-1} \cdot \mathbf{C}^{(i)}. \quad (25)$$

Thus each  $\mathbf{D}^{(i)}$  is determined from the previous one.  $\mathbf{D}^{(1)}$  is just a  $1 \times 1$  matrix and can be determined by inspection of equations (12), (13), (14) and (23):

$$D_{1,1}^{(1)} = -C_{1,1}^{(1)} / B_{1,1}^{(1)} = -2 / (h^2 T_1 - 4). \quad (26)$$

### (2c) Asymptotic Solutions

In the asymptotic region, the form of the wave function is known and is given in terms of the S-matrix  $\mathbf{S}$  by [refer to equation (5)]

$$\bar{\Psi}^{(i)} \sim \mathbf{I}^{(i)} - \mathbf{R}^{(i)} \cdot \mathbf{S}. \quad (27)$$

Here the matrix  $\mathbf{I}^{(i)}$  contains the incident part of the asymptotic solution,

$$I_{j,n}^{(i)} = \phi_{k_n}^*(x_i) \psi_n(y_j), \quad (28)$$

while  $\mathbf{R}^{(i)}$  contains the reflected part,

$$R_{j,n}^{(i)} = \phi_{\kappa_n}(x_i)\psi_n(y_j). \quad (29)$$

Here  $x_i = ih$  and  $y_j = jh$ .

(2d) *Matching Procedure*

To extract an  $N \times N$  S-matrix, we need only  $N$  of the  $i$  equations (23). We can solve for the S-matrix by substituting the asymptotic solutions (27) into  $N$  of equations (23):

$$\mathbf{S} = [\tilde{\mathbf{R}}^{(i)} - \tilde{\mathbf{D}}^{(i)} \cdot \mathbf{R}^{(i+1)}]^{-1} \cdot [\tilde{\mathbf{I}}^{(i)} - \tilde{\mathbf{D}}^{(i)} \cdot \mathbf{I}^{(i+1)}]. \quad (30)$$

Here the tildes on  $\mathbf{I}^{(i)}$ ,  $\mathbf{R}^{(i)}$  and  $\mathbf{D}^{(i)}$  indicate that only  $N$  rows are now being retained in these matrices. In principle, *any*  $N$  rows will do. Perhaps the simplest choice is to just take the first  $N$  rows, but this is a poor choice since the  $\psi_n(y)$  become linearly dependent near  $y = 0$ . We have found that the most stable choice is to keep the rows corresponding to the global maxima of  $|\psi_n(y)|$ ,  $n = 1, 2, \dots, N$ . Let us label the  $y$ -value where this maximum occurs by  $y_m(n)$ . One can consider rather large variations about this stable choice without affecting the final results. If the variation is too large [e.g. if we take the rows corresponding to  $y_m(n)/10$ ] the results are unstable and there is no convergence (using double-precision arithmetic; presumably, higher precision would bring back stability).

**Table 1.** Singlet 1s, 2s, 3s cross sections (in units of  $\pi a_0^2$ ) of the Temkin–Poet electron–hydrogen scattering problem for different impact energies  $E_0$  (eV)

The present results using the finite-difference method (FDM) are compared with the convergent close-coupling (CCC) calculations of Bray and Stelbovics (1994)

| $E_0$  | $\sigma_{1s,\text{FDM}}$ | $\sigma_{1s,\text{CCC}}$ | $\sigma_{2s,\text{FDM}}$ | $\sigma_{2s,\text{CCC}}$ | $\sigma_{3s,\text{FDM}}$ | $\sigma_{3s,\text{CCC}}$ |
|--------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 1      | 13.6                     | 13.6                     |                          |                          |                          |                          |
| 2      | 6.35                     | 6.35                     |                          |                          |                          |                          |
| 3      | 3.68                     | 3.68                     |                          |                          |                          |                          |
| 4      | 2.39                     | 2.39                     |                          |                          |                          |                          |
| 5      | 1.68                     | 1.68                     |                          |                          |                          |                          |
| 6      | 1.24                     | 1.24                     |                          |                          |                          |                          |
| 7      | 0.964                    | 0.965                    |                          |                          |                          |                          |
| 8      | 0.780                    | 0.781                    |                          |                          |                          |                          |
| 9      | 0.659                    | 0.659                    |                          |                          |                          |                          |
| 10.885 | 0.476                    | 0.476                    | 0.0326                   | 0.0326                   |                          |                          |
| 12.245 | 0.390                    | 0.391                    | 0.0417                   | 0.0415                   | 0.00322                  | 0.00320                  |

### 3. Results

For impact energies below 13 eV, where only a few (1, 2, or 3) channels are open, we have calculated cross sections for  $1s$ – $1s$  elastic scattering as well as  $1s$ – $2s$  and  $1s$ – $3s$  excitation. In Table 1, our results are compared with those of the convergent close-coupling (CCC) method (Bray and Stelbovics 1994). The simple low-order scheme used here requires a small step size to obtain accurate

results ( $h = 0.02$  a.u.). It is seen from Table 1 that the present results and the CCC results agree to better than 1%.

Since presenting Table 1 at the AIP Congress (Jones and Stelbovics 1998), we have implemented the higher-order Numerov scheme, which brings in next-nearest-neighbour points to each difference equation. The spacing  $h$  can now be six times larger to obtain approximately the same accuracy. Thus the Numerov scheme reduces storage by a factor of  $6^2 = 36$  and is  $6^4 = 1296$  times faster. Nevertheless, we would still recommend developing one's code using the simpler scheme presented in Section 2 since it is considerably easier to understand and implement. Once this code is working, it is not difficult to upgrade to the Numerov scheme. All the necessary formulas for the Numerov scheme have been given by Poet (1980) and need not be discussed here. We have also implemented Poet's (1980) technique of using *all* rows of the matrices  $\mathbf{I}^{(i)}$ ,  $\mathbf{R}^{(i)}$  and  $\mathbf{D}^{(i)}$ . In this case, the system of equations is overdetermined. Nevertheless, a solution can be found by the standard method of minimising the sum of the squares of the residuals [the differences between the left- and right-hand sides of equations (D)]. This 'least-squares' method works even better than the simpler method described earlier. Although both methods converged to the same final result, the least-squares results converged in a quicker, more stable fashion. In Table 2, we present our results for  $e^- + \text{H}(1s) \rightarrow e^- + \text{H}(ns)$ ,  $n \leq 8$ , using the Numerov scheme at the ionisation threshold (the grid spacing is  $h = 1/14$  a.u.). Here we present the calculated cross sections every 10 a.u., so that convergence in propagation distance may be readily ascertained. In contrast to the cases presented in Table 1,

**Table 2.** Singlet cross sections (in units of  $\pi a_0^2$ ; superscripts indicate powers of 10) of the Temkin-Poet electron-hydrogen scattering problem for an impact energy of 1 Rydberg versus propagation distance  $x$  (atomic units)

| $x$ | $N$ | $\sigma_{1s}$     | $\sigma_{2s}$     | $\sigma_{3s}$     | $\sigma_{4s}$     | $\sigma_{5s}$     | $\sigma_{6s}$     | $\sigma_{7s}$     | $\sigma_{8s}$     |
|-----|-----|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| 10  | 3   | $3 \cdot 30^{-1}$ | $4 \cdot 33^{-2}$ | $5 \cdot 94^{-2}$ |                   |                   |                   |                   |                   |
| 20  | 5   | $3 \cdot 30^{-1}$ | $4 \cdot 00^{-2}$ | $6 \cdot 18^{-3}$ | $8 \cdot 76^{-2}$ | $1 \cdot 09^{-1}$ |                   |                   |                   |
| 30  | 5   | $3 \cdot 30^{-1}$ | $4 \cdot 03^{-2}$ | $7 \cdot 23^{-3}$ | $3 \cdot 81^{-3}$ | $5 \cdot 71^{-3}$ |                   |                   |                   |
| 40  | 6   | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $7 \cdot 04^{-3}$ | $1 \cdot 60^{-3}$ | $4 \cdot 03^{-3}$ | $4 \cdot 92^{-3}$ |                   |                   |
| 40  | 6   | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $7 \cdot 04^{-3}$ | $1 \cdot 60^{-3}$ | $4 \cdot 03^{-3}$ | $4 \cdot 92^{-3}$ |                   |                   |
| 50  | 8   | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 96^{-3}$ | $1 \cdot 77^{-3}$ | $2 \cdot 21^{-5}$ | $3 \cdot 25^{-2}$ | $1 \cdot 86^{-1}$ | $7 \cdot 65^{-2}$ |
| 60  | 9   | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 95^{-3}$ | $1 \cdot 78^{-3}$ | $6 \cdot 27^{-4}$ | $4 \cdot 16^{-3}$ | $1 \cdot 69^{-1}$ | $5 \cdot 20^{-1}$ |
| 70  | 10  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 94^{-3}$ | $1 \cdot 79^{-3}$ | $6 \cdot 46^{-4}$ | $9 \cdot 25^{-4}$ | $6 \cdot 94^{-2}$ | $9 \cdot 32^{-1}$ |
| 80  | 12  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 84^{-4}$ | $6 \cdot 34^{-4}$ | $1 \cdot 10^{-1}$ | $7 \cdot 57^{+0}$ |
| 90  | 12  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 79^{-3}$ | $5 \cdot 97^{-4}$ | $2 \cdot 67^{-4}$ | $5 \cdot 65^{-3}$ | $4 \cdot 34^{-1}$ |
| 100 | 12  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 94^{-4}$ | $2 \cdot 42^{-4}$ | $6 \cdot 11^{-4}$ | $3 \cdot 13^{-2}$ |
| 110 | 13  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 30^{-4}$ | $2 \cdot 01^{-4}$ | $1 \cdot 35^{-2}$ |
| 120 | 13  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 20^{-4}$ | $1 \cdot 43^{-3}$ |
| 130 | 14  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $9 \cdot 46^{-5}$ | $4 \cdot 74^{-4}$ |
| 140 | 14  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 00^{-4}$ | $1 \cdot 15^{-4}$ |
| 150 | 14  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 01^{-4}$ | $6 \cdot 47^{-5}$ |
| 160 | 14  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 01^{-4}$ | $5 \cdot 38^{-5}$ |
| 170 | 14  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 01^{-4}$ | $5 \cdot 02^{-5}$ |
| 180 | 14  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 02^{-4}$ | $4 \cdot 89^{-5}$ |
| 190 | 15  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 02^{-4}$ | $4 \cdot 83^{-5}$ |
| 200 | 15  | $3 \cdot 30^{-1}$ | $4 \cdot 07^{-2}$ | $6 \cdot 93^{-3}$ | $1 \cdot 80^{-3}$ | $5 \cdot 95^{-4}$ | $2 \cdot 32^{-4}$ | $1 \cdot 02^{-4}$ | $4 \cdot 83^{-5}$ |

here we have an infinite number of channels open. An interesting and useful result of this work is that we have found that the rate at which states become important in the matching procedure as the solution is propagated outwards is about three times faster than the rate that their global maxima come onto the grid (in Table 2 we have indicated the total number of states  $N$  included at each stage of the calculation).

#### 4. Conclusion and Outlook

We have presented a simple finite-difference scheme for electron–hydrogen scattering that can be easily upgraded to improve efficiency. Matching boundary conditions to yield a stable system of difference equations when many channels were open proved to be a difficult task. This may explain why other investigators, since Poet, have not yet presented results of their direct methods in this energy regime. We can now proceed to higher energies by applying ionisation boundary conditions. Once we have optimised our code for this simplified model we will include angular momentum.

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