Complete Numerical Solution of Electron-Hydrogen Model Collision Problem above the Ionization Threshold

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(Received 9 June 1999)

Benchmark results are presented for electrons colliding with hydrogen atoms in the S-wave (Temkin-Poet) model collision problem, which neglects angular momentum. Complete results (elastic, inelastic, and ionization), accurate to 1%, are obtained by numerically integrating Schrödinger's equation subject to correct asymptotic boundary conditions. This marks the first time direct matching to asymptotic boundary conditions has been shown to yield convergent ionization amplitudes for a Coulomb three-body problem. Results are presented for impact energies of 54.4 and 40.8 eV, where comparison with other theories is available.

PACS numbers: 34.80.Dp, 31.15.Fx, 34.10.+x, 34.80.Bm

The Temkin-Poet [1,2] model of electron-hydrogen scattering is now widely regarded as an ideal testing ground for the development of general methods intended for the full three-body Coulomb problem. Although only s states are included for both the projectile and the atomic electrons, this model problem still contains most of the features that make the real scattering problem hard to solve. Indeed, even in this simplified model, converged energy distributions for ionization cannot generally be obtained via the close-coupling formalism [3]. Any general method that cannot obtain complete, converged results for this model problem will face similar difficulties when applied to the full electron-hydrogen system. For this reason, we believe it is essential to develop a general numerical method capable of solving the Temkin-Poet model completely *before* angular momentum is included. Here we report such a method. Complete, precision results for $e^- + \mathrm{H}(1s)$, accurate to 1%, are presented for total energies of 3 and 2 Ry, where comparison with other theories is available. Cross sections for the very highest Rydberg transitions, which would require integrating to infinitely large distances, may be accurately obtained from our lower-level Rydberg cross sections using the $1/n^3$ scaling law.

Our numerical method may be summarized as follows. The model Schrödinger equation is integrated outwards from the atomic center on a grid of fixed spacing h. The number of difference equations is reduced each step outwards using an algorithm due to Poet [4], 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. This direct matching of boundary conditions to yield ionization amplitudes is successfully implemented here for the first time.

Let us start by writing Schrödinger's equation for the full electron-hydrogen scattering problem (in atomic units with the total energy E in Rydbergs),

$$\left(\nabla_{\mathbf{x}}^2 + \nabla_{\mathbf{y}}^2 + \frac{2}{x} + \frac{2}{y} - \frac{2}{|\mathbf{x} - \mathbf{y}|} + E\right)\Psi(\mathbf{x}, \mathbf{y}) = 0\,. \tag{1}$$

Expanding Ψ as a complete set of functions in $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$,

$$\Psi(\mathbf{x}, \mathbf{y}) = \frac{1}{xy}\sum_{\ell} \Psi_\ell(x, y) Y_\ell(\hat{\mathbf{x}}, \hat{\mathbf{y}})\,, \tag{2}$$

Schrödinger's equation (1) takes the form

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\Psi_\ell(x, y) + \sum_{\ell'} T_{\ell\ell'}(x, y)\Psi_{\ell'}(x, y) = 0\,, \tag{3}$$

where T contains all the nonderivative terms and the index $\ell = 0, 1, 2, \ldots$ denotes a set of quantum numbers; in particular, $\ell = 0$ corresponds to zero angular momentum for both electrons. Since $\Psi(\mathbf{x}, \mathbf{y})$ must remain finite everywhere, boundary conditions along $x = 0$ and $y = 0$ can immediately be written down for the Ψ_ℓ:

$$\Psi_\ell(x, 0) = \Psi_\ell(0, y) = 0\,. \tag{4}$$

The Pauli exclusion principle demands that Ψ also obey the symmetry condition

$$\Psi(\mathbf{y}, \mathbf{x}) = \pm\Psi(\mathbf{x}, \mathbf{y})\,, \tag{5}$$

depending on whether the two electrons form a singlet $(+)$ or triplet $(-)$ spin state. Because the wave function is symmetric or antisymmetric, we can solve Schrödinger's equation (3) in just the region $x \geq y$; the symmetry condition (5) then plays the role of a spin-dependent boundary condition along $x = y$. Finally, the asymptotic forms of the $\Psi_\ell(x, y)$ for $x \geq y$ are needed to complete the specification of boundary conditions.

In the Temkin-Poet model, the infinite set of coupled equations (3) is reduced to a single equation,

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{2}{x} + \frac{2}{y} - \frac{2}{\max(x, y)} + E\right)\Psi_0(x, y) = 0\,, \tag{6}$$

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by keeping only the first term in the expansion (2). For this model problem, the asymptotic boundary condition is easily written down and is given in terms of unknown S-matrix elements by

$$\Psi_0(x,y) \underset{x\to\infty}{\sim} \psi_{\epsilon_m}(y)\phi^*_{k_{\epsilon_m}}(x) - \sum_{n=1}^{\infty} S_{\epsilon_n\epsilon_m}\psi_{\epsilon_n}(y)\phi_{k_{\epsilon_n}}(x) - \int_0^E d\epsilon_b\, S_{\epsilon_b\epsilon_m}\psi_{\epsilon_b}(y)\phi_{k_{\epsilon_b}}(x), \quad (7)$$

where $\phi_k(x) = (1/\sqrt{k})\exp(ikx)$ and the ψ_ϵ are bound and continuum states of the hydrogen atom with zero angular momentum,

$$\psi_\epsilon(y) = N_\epsilon[\, y e^{-qy}\, {}_1F_1(1 - 1/q, 2; 2qy)]. \quad (8)$$

Here $q^2 = -\epsilon$, where ϵ is the energy of the atomic electron, ${}_1F_1$ is the confluent hypergeometric function, and N_ϵ normalizes bound states to unity and continuum states to a delta function in energy. The momenta in (7) are fixed by energy conservation according to

$$\epsilon_m + k^2_{\epsilon_m} = \epsilon_n + k^2_{\epsilon_n} = \epsilon_b + k^2_{\epsilon_b} = E. \quad (9)$$

To convert the partial-differential equation (6) into difference equations, we impose a grid of fixed spacing h and approximate derivatives by finite differences. Applying the Numerov finite-difference scheme [4] in both the x and y directions, our difference equations take the form

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

Here we have collected the various $\Psi^{(i)}_j, j = 1, 2, \ldots, i$, where $\Psi^{(i)}_j \equiv \Psi_0(x_i = ih, y_j = jh)$, into a vector $\mathbf{\Psi}^{(i)}$. The matrices $\mathbf{A}^{(i)}$, $\mathbf{B}^{(i)}$, and $\mathbf{C}^{(i)}$ are completely determined by the formulas given by Poet [4].

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

$$\mathbf{\Psi}^{(i)} = \mathbf{D}^{(i)} \cdot \mathbf{\Psi}^{(i+1)}. \quad (11)$$

We can obtain a recursion relation for $\mathbf{D}^{(i)}$ by using (11) to eliminate $\mathbf{\Psi}^{(i-1)}$ from Eq. (10):

$$[\mathbf{B}^{(i)} + \mathbf{A}^{(i)} \cdot \mathbf{D}^{(i-1)}] \cdot \mathbf{\Psi}^{(i)} = -\mathbf{C}^{(i)} \cdot \mathbf{\Psi}^{(i+1)}. \quad (12)$$

Comparing (12) with (11), we see that

$$\mathbf{D}^{(i)} = -[\mathbf{B}^{(i)} + \mathbf{A}^{(i)} \cdot \mathbf{D}^{(i-1)}]^{-1} \cdot \mathbf{C}^{(i)}. \quad (13)$$

Thus each $\mathbf{D}^{(i)}$ is determined from the previous one; to start the recursion, one calculates $\mathbf{D}^{(1)} = -\mathbf{B}^{(1)-1} \cdot \mathbf{C}^{(1)}$.

In the asymptotic region,

$$\mathbf{\Psi}^{(i)} \underset{x\to\infty}{\sim} \mathbf{I}^{(i)} - \mathbf{R}^{(i)} \cdot \mathbf{S}. \quad (14)$$

Here the matrix $\mathbf{I}^{(i)} = \mathbf{R}^{(i)*}$ contains incident waves while $\mathbf{R}^{(i)}$ contains reflected waves:

$$R^{(i)}_{j,n} = \begin{cases} \psi_{\epsilon_n}(y_j)\phi_{k_{\epsilon_n}}(x_i), & n \le N_d, \quad (15) \\ \int_0^E d\epsilon_b\, \epsilon_b^p \psi_{\epsilon_b}(y_j)\phi_{k_{\epsilon_b}}(x_i), & n > N_d, \quad (16) \end{cases}$$

where $p = n - N_d - 1$. Note that the infinite summation over discrete channels is truncated to some finite integer N_d and that the quadrature over the two-electron continuum is performed prior to matching by first writing the $S_{\epsilon_b\epsilon_m}$ as a power series in ϵ_b,

$$S_{\epsilon_b\epsilon_m} \approx \sum_{p=0}^{N_c-1} s_{pm}\epsilon_b^p. \quad (17)$$

The matching procedure [insertion of Eq. (14) into both sides of Eq. (11) and solving for $\mathbf{S}$] then determines the (in practice, much smaller set of) coefficients s_{pm}, rather than $S_{\epsilon_b\epsilon_m}$ directly, which eliminates ill conditioning [4].

To extract an $N \times N$ coefficient matrix $\mathbf{S}$, where $N = N_d + N_c$, we need only N of the i equations (11). Alternatively, one may use all i equations as in Poet [4]. In this case, the system of equations is overdetermined. Nevertheless, a solution can be found by the standard method of minimizing the sum of the squares of the residuals [the differences between the left- and right-hand sides of equations (11)]. Previously we found [5] that the least-squares method is generally stabler than keeping any subset of just N equations (11).

Our numerical method is stable and rapidly convergent. For a given grid spacing h, we established convergence in propagation distance by performing the matching every 40 a.u. until convergence was obtained. At each matching radius, both the number of discrete channels N_d and the number of expansion functions for the continuum (N_c) were varied to obtain convergence. Finally, the entire calculation was repeated for a finer grid (using one-half the original grid spacing h).

The biggest advantage of having a general, propagating solution is that once the grid spacing is chosen, a single D-matrix calculation is all that is needed to establish convergence for the remaining numerical parameters. This is because the D matrix, the calculation of which consumes nearly all the computational effort, is independent of asymptotic boundary conditions. Thus, in a typical calculation, the same D matrix is used for $N_c = 0, 1, \ldots, 9$, while N_d runs from 1 to 30. This would have required 300 completely separate calculations (each taking about the same time as our one D-matrix calculation) had we solved our finite-difference equations (10) globally (for all values of i at once).

We have performed complete calculations for electrons colliding with hydrogen atoms at impact energies of 54.4 and 40.8 eV (total energies of 3 and 2 Ry, respectively). In Table I, we present our calculated cross sections for $e^- + \mathrm{H}(1s) \to e^- + \mathrm{H}(ns), n \le 8$. The grid spacing is

TABLE I. $e^- + \mathrm{H}(1s) \rightarrow e^- + \mathrm{H}(ns)$ cross sections (πa_0^2) for impact energies of 54.4 and 40.8 eV (superscripts indicate powers of 10).

	54.4 eV		40.8 eV	
n	Singlet	Triplet	Singlet	Triplet
1	6.47^{-2}	4.07^{-1}	8.58^{-2}	6.34^{-1}
2	4.66^{-3}	4.04^{-3}	8.09^{-3}	5.08^{-3}
3	1.22^{-3}	8.39^{-4}	2.15^{-3}	9.88^{-4}
4	4.92^{-4}	3.13^{-4}	8.74^{-4}	3.59^{-4}
5	2.48^{-4}	1.52^{-4}	4.41^{-4}	1.71^{-4}
6	1.42^{-4}	8.52^{-5}	2.53^{-4}	9.55^{-5}
7	8.89^{-5}	5.27^{-5}	1.58^{-4}	5.88^{-5}
8	5.94^{-5}	3.49^{-5}	1.06^{-4}	3.88^{-5}

$h = 0.2$ a.u. (results using one-half this spacing differed by less than 0.1% for excitation and 0.5% for elastic scattering). Another advantage of our direct approach is that we are able to obtain the amplitudes for higher-level (Rydberg) transitions as easily as those for low-level excitations, provided the matching radius is large enough to enclose the final Rydberg state of interest.

In Figs. 1–4, we present our ionization results (labeled FDM for finite-difference method) for the singly differential cross section (SDCS). For a total energy of 3 Ry, 240 a.u. proved to be a sufficient matching radius to get convergence of the SDCS, and for $E = 2$ Ry, a radius of 360 a.u. was required. The SDCS is more sensitive to the number of expansion functions for the continuum than the other observables, particularly about $\epsilon_b = E/2$. Nevertheless, convergence to better than 1% was readily obtained using eight functions (the largest discrepancy in the SDCS between $N_c = 7$ and $N_c = 8$ was smaller than 0.3%; even using just six expansion functions gave results accurate to 1%).

Some very recent results from Baertschy *et al.* [6] have also been included in the figures. Baertschy *et al.* rearrange the Schrödinger equation to solve for the outgoing scattered wave. They use a two-dimensional grid like ours, but scale the coordinates by a complex phase factor beyond a certain radius where the tail of the Coulomb potential is ignored. As a result, the scattered wave decays like an ordinary bound state beyond this cutoff radius, which makes the asymptotic boundary conditions very simple. By computing the outgoing flux directly from the scattered wave at several large cutoff radii, and extrapolating to infinity, they obtain the single-differential ionization cross section without having to use Coulomb three-body boundary conditions. This method, called exterior complex scaling (ECS), has just been extended to the full electron-hydrogen ionization problem [7]. It is seen from Figs. 1–4 that the ECS results are in good agreement with our FDM results except when the energy fraction ϵ_b/E approaches 0 or 1. Baertschy *et al.* [6] note that their method may be unreliable as ϵ_b approaches 0 or E due to "contamination" of the ionization flux by contributions from discrete excitations.

Also shown in Figs. 1–4 are the results of convergent close-coupling (CCC) calculations [3]. Comparison with the FDM shows that CCC is accurate only for the triplet case (in general, CCC does not yield convergent amplitudes for the triplet case either, except for total angular momentum $L = 0$, since it is only for $L = 0$ that the cross section vanishes at $\epsilon_b = E/2$).

We note also the recent work of Miyashita *et al.* [8], who have presented SDCS for total energies of 4, 2, and 0.1 Ry using two different methods. One produces an asymmetric energy distribution similar to that of CCC while the other gives a symmetric distribution. Both contain oscillations. The mean of their asymmetric curve at $E = 2$ Ry (40.8 eV impact energy) is in reasonable agreement (up to $\epsilon_b = E/2$) with our calculations.

In conclusion, we have presented complete, precision results for the Temkin-Poet electron-hydrogen model collision problem by numerically integrating Schrödinger's

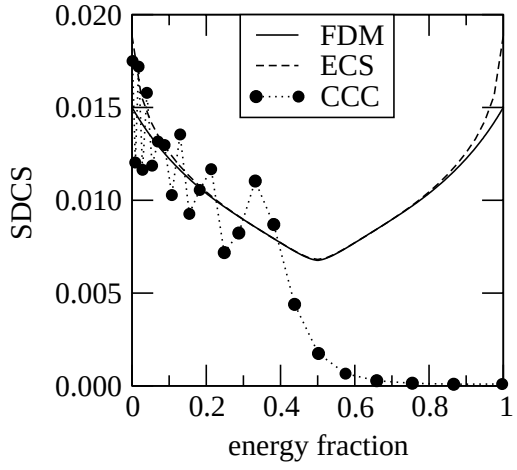

FIG. 1. Singlet SDCS (πa_0^2/Ry) vs the energy fraction ϵ_b/E for an impact energy of 54.4 eV. The total ionization cross section from the FDM is 0.0150 (πa_0^2).

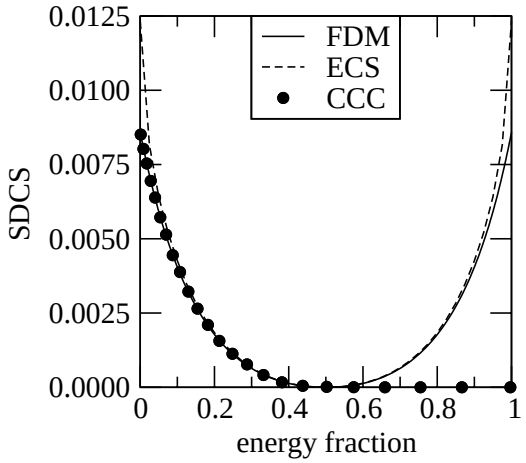

FIG. 2. Same as Fig. 1 for the triplet case. The total ionization cross section from the FDM is 0.003 11 (πa_0^2).

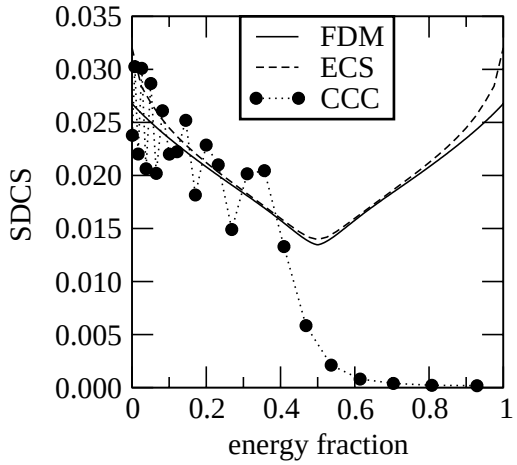

FIG. 3. Singlet SDCS (πa_0^2/Ry) vs the energy fraction ϵ_b/E for an impact energy of 40.8 eV. The total ionization cross section from the FDM is 0.0197 (πa_0^2).

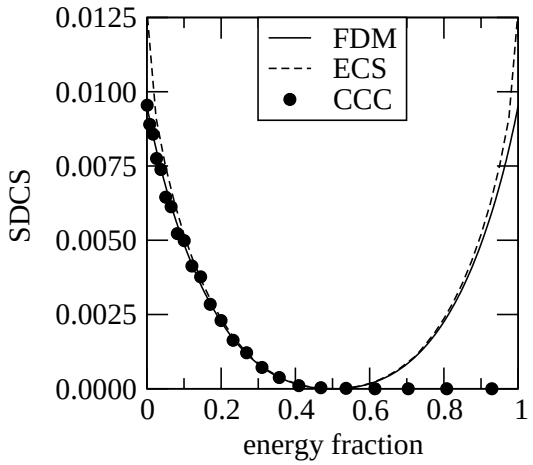

FIG. 4. Same as Fig. 3 for the triplet case. The total ionization cross section from the FDM is 0.002 47 (πa_0^2).

equation subject to correct asymptotic boundary conditions. To our knowledge, this work represents the first time the formal scattering theory has successfully been used to directly extract ionization amplitudes. It may be possible to improve the speed of the present method by using a variable-spaced grid, like that used by Botero and Shertzer [9] in their finite-element analysis (this would greatly reduce storage requirements as well). Once we have optimized our code for this simplified model we will proceed to include angular momentum. When angular momentum is included, the ionization boundary condition will be considerably more complicated, and this is the major challenge for generalizing the present approach to the full electron-hydrogen scattering problem (which has already been accomplished for energies *below* the ionization threshold [10]).

The authors gratefully acknowledge the financial support of the Australian Research Council for this work.

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