

Hyperspherical close-coupling calculation of electron-hydrogen scattering cross sections

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Elastic phase shifts and scattering cross sections for electron-hydrogen scattering below the $n=2$ threshold are carefully evaluated using the hyperspherical close-coupling (HSCC) method. The results are compared to other benchmark calculations to illustrate the convergence properties of the HSCC method. Elastic and inelastic scattering cross sections between the $n=2$ and $n=3$ thresholds are also calculated and compared to other benchmark calculations. [S1050-2947(97)00709-9]

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In recent years the hyperspherical close-coupling (HSCC) method has been used extensively to study photoionization of helium atoms (see [1], and references therein) and photo-detachment of H^- (see [2], and references therein) over a broad energy region. The HSCC method has been shown to be able to obtain accurate results for the scattering cross sections as well as resonance parameters for two-electron systems. It has also been used recently to study rearrangement collisions such as positron scattering with atomic hydrogen (see [3], and references therein). While results obtained from the HSCC method in the higher-energy region where many channels are open have been shown to be in general in good agreement with experimental data, the method has not been critically examined at the high-precision level. In this Brief Report, we present results from careful HSCC calculations in the low-energy region for electron-hydrogen collisions where a number of other benchmark theoretical calculations are available. We demonstrate that the HSCC method is capable of achieving comparable precise results as well in the energy region where a few channels are open.

The HSCC method has been described elsewhere [4,5] and in a review article [6]. For the present system, the two-electron wave function is expressed in hyperspherical coordinates as $\psi(\vec{r}_1, \vec{r}_2) = \Psi(R, \alpha, \Omega) / (R^{5/2} \sin \alpha \cos \alpha)$ and the Schrödinger equation satisfies

$$\left(-\frac{1}{2} \frac{\partial^2}{\partial R^2} + \frac{H_{\text{ad}}}{R^2} - E \right) \Psi(R, \alpha, \Omega) = 0, \quad (1)$$

where $R = (r_1^2 + r_2^2)^{1/2}$ is the hyperradius, $\alpha = \tan^{-1}(r_1/r_2)$ is the hyperangle, Ω denotes the four angles (\hat{r}_1, \hat{r}_2) , and H_{ad} is the adiabatic Hamiltonian at fixed values of R .

In the HSCC method, the configuration space is divided into two regions, the inner region ($R < R_M$), and the outer or asymptotic region ($R > R_M$). The inner region is further divided into small sectors. Within each sector $[R_{i-1}, R_i]$, the wave function is expanded as

$$\Psi(R, \alpha, \Omega) = \sum_{\mu=1}^{N_{\text{ch}}} F_{\mu}(R) \phi(R_i^m; \alpha, \Omega), \quad (2)$$

with

$$R_{i-1} < R < R_i, \quad (3)$$

where the basis functions $\phi(R_i^m; \alpha, \Omega)$ within the sector are fixed to be the adiabatic eigenstates at R_i^m , often chosen at the midpoint of the sector. Since the basis functions are fixed within each sector, the expansion is called the diabatic-by-sector method. From Eq. (2) a set of coupled second-order differential equations for $F_{\mu}(R)$ are obtained within each sector which are integrated from one end of the sector to the other where it is matched to the wave function expanded in terms of basis functions from the next sector. By matching the wave functions and the derivatives with respect to R at the boundary of the two sectors, this procedure allows us to integrate the coupled equations until it reaches the boundary of the outer region at $R = R_M$, where it is further matched to the asymptotic wave functions expressed in independent particle coordinates to extract the K matrix. The K matrix contains all the information on the scattering process. For more details of the method, the readers are referred to [6].

We first present the elastic phase shifts for electron hydrogen scattering using the HSCC method. Accurate phase shifts for this system have served as a critical test for any theoretical method. In Table I we compare the results of the HSCC calculation with other benchmark calculations. For $1S^e$ and $3S^e$ partial waves, the HSCC results are in good agreement with those obtained from the direct numerical integration of the Schrödinger equation by Wang and Callaway [7], with the results from the R -matrix calculation [8] and the variational calculations [9]. The discrepancies are in the third decimal point in the phase shift at most. To achieve high-precision phase shifts reported here in the HSCC calculation, we have used a matching radius R_M between 115 and 250 a.u. The number of channels N_{ch} included in the inner region is 60–75 and the number of sectors N_{sect} is 1000. Convergence is checked by varying the matching radius and the number of channels.

Table I also shows the phase shifts for the $1P^o$ and $3P^o$ symmetries and the results are compared to the calculations of Wang and Callaway [7] and the R -matrix method of Scholz *et al.* [8] and the earlier variational calculations of Das and Rudge [10]. All four calculations are in good agree-

TABLE I. Phase shifts for e -H scattering.

| State | k | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 |
|---------|----------------------|---------|--------|---------|--------|---------|---------|--------|--------|
| $^1S^e$ | Present | 2.555 | 2.066 | 1.695 | 1.413 | 1.197 | 1.036 | 0.925 | 0.881 |
| | Direct numerical [7] | 2.555 | 2.066 | 1.695 | 1.415 | 1.200 | 1.041 | 0.930 | 0.887 |
| | R matrix [8] | 2.550 | 2.062 | 1.691 | 1.410 | 1.196 | 1.035 | 0.925 | |
| | Variational [9] | 2.553 | 2.067 | 1.691 | 1.415 | 1.202 | 1.041 | 0.930 | 0.886 |
| $^3S^e$ | Present | 2.941 | 2.718 | 2.499 | 2.292 | 2.101 | 1.929 | 1.775 | 1.638 |
| | Direct numerical [7] | 2.939 | 2.717 | 2.500 | 2.294 | 2.104 | 1.933 | 1.780 | 1.644 |
| | R matrix [8] | 2.939 | 2.717 | 2.500 | 2.294 | 2.105 | 1.933 | 1.780 | |
| | Variational [9] | 2.939 | 2.717 | 2.500 | 2.294 | 2.105 | 1.933 | 1.780 | 1.643 |
| $^1P^o$ | Present | 0.0059 | 0.0157 | 0.0168 | 0.0098 | -0.0019 | -0.0124 | -0.016 | -0.007 |
| | Direct numerical [7] | 0.006 | 0.016 | 0.017 | 0.010 | -0.002 | -0.012 | -0.015 | -0.007 |
| | R matrix [8] | 0.006 | 0.015 | 0.016 | 0.009 | -0.002 | -0.012 | -0.016 | |
| | Variational [10] | 0.006 | 0.015 | 0.017 | 0.010 | -0.001 | -0.011 | -0.014 | -0.006 |
| $^3P^o$ | Present | 0.010 | 0.046 | 0.107 | 0.188 | 0.272 | 0.342 | 0.392 | 0.426 |
| | Direct numerical [7] | 0.010 | 0.046 | 0.107 | 0.188 | 0.271 | 0.342 | 0.394 | 0.429 |
| | R matrix [8] | 0.010 | 0.045 | 0.107 | 0.187 | 0.270 | 0.341 | 0.392 | |
| | Variational [10] | 0.010 | 0.045 | 0.107 | 0.187 | 0.271 | 0.341 | 0.393 | 0.427 |
| $^1D^e$ | Present | 0.0011 | 0.0056 | 0.011 | 0.018 | 0.027 | 0.038 | 0.052 | 0.074 |
| | Direct numerical [7] | 0.0012 | 0.0056 | 0.011 | 0.018 | 0.027 | 0.038 | 0.052 | 0.075 |
| | R matrix [8] | 0.0013 | 0.0051 | 0.011 | 0.018 | 0.027 | 0.038 | 0.052 | |
| | Finite element [11] | 0.0007 | 0.0048 | 0.011 | 0.018 | 0.027 | 0.038 | 0.052 | 0.074 |
| $^3D^e$ | Present | 0.0012 | 0.0052 | 0.011 | 0.018 | 0.027 | 0.038 | 0.052 | 0.075 |
| | Direct numerical [7] | 0.0012 | 0.0059 | 0.011 | 0.019 | 0.030 | 0.042 | 0.055 | 0.069 |
| | R matrix [8] | 0.0013 | 0.0052 | 0.011 | 0.020 | 0.030 | 0.042 | 0.055 | |
| | Finite element [11] | 0.0007 | 0.0049 | 0.011 | 0.020 | 0.030 | 0.042 | 0.055 | 0.070 |
| $^1F^o$ | Present | 0.0013 | 0.0052 | 0.011 | 0.020 | 0.030 | 0.042 | 0.055 | 0.070 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0066 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0067 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0067 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0067 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0067 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0067 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0067 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |
| $^3F^o$ | Present | | | 0.0038 | 0.0067 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Direct numerical [7] | 0.00016 | 0.0015 | 0.00378 | 0.0063 | 0.0105 | 0.0146 | 0.020 | 0.025 |
| | Direct numerical [7] | 0.0001 | 0.0015 | 0.0038 | 0.0064 | 0.010 | 0.015 | 0.020 | 0.026 |
| | Finite element [11] | 0.0000 | 0.0016 | 0.0037 | 0.0065 | 0.010 | 0.015 | 0.020 | 0.026 |

TABLE II. Cross sections (in units of πa_2^2) at $k^2=0.78$ Ry.

| | | (LS) | | | | | | | |
|---------|----------------------|-------|--------|--------|-------|-------|--------|--------|--------|
| | | (00) | (01) | (10) | (11) | (20) | (21) | (30) | (31) |
| $1s-1s$ | Present | 0.621 | 3.841 | 0.0009 | 2.043 | 0.055 | 0.122 | 0.009 | 0.028 |
| | Direct numerical [7] | 0.622 | 3.841 | 0.001 | 2.073 | 0.058 | 0.131 | 0.010 | 0.033 |
| $1s-2s$ | Present | 0.040 | 0.0009 | 0.0031 | 0.044 | 0.055 | 0.0005 | 0.0003 | 0.0039 |
| | Direct numerical [7] | 0.041 | 0.001 | 0.0032 | 0.044 | 0.056 | 0.0004 | 0.0003 | 0.0035 |
| $1s-2p$ | Present | 0.034 | 0.0003 | 0.048 | 0.041 | 0.092 | 0.0015 | 0.001 | 0.011 |
| | Direct numerical [7] | 0.035 | 0.0004 | 0.048 | 0.042 | 0.092 | 0.0017 | 0.001 | 0.011 |
| $2s-2s$ | Present | 5.515 | 0.275 | 53.88 | 66.94 | 65.36 | 90.00 | 20.04 | 38.38 |
| | Direct numerical [7] | 5.313 | 0.570 | 51.47 | 66.18 | 64.15 | 81.39 | 19.56 | 37.36 |
| $2s-2p$ | Present | 1.893 | 3.66 | 16.78 | 6.933 | 16.85 | 120.77 | 48.23 | 122.2 |
| | Direct numerical [7] | 0.960 | 6.854 | 18.00 | 7.218 | 17.29 | 118.94 | 47.81 | 120.8 |
| $2p-2p$ | Present | 8.712 | 30.16 | 11.38 | 164.2 | 55.28 | 139.4 | 49.02 | 193.0 |
| | Direct numerical [7] | 9.334 | 27.98 | 11.33 | 164.2 | 55.49 | 134.8 | 49.29 | 192.1 |

TABLE III. Cross sections (in units of πa_0^2) at $k^2=0.85$ Ry.

| | | (LS) | | | | | | | |
|-------|----------------------|----------|--------|--------|-------|-------|--------|--------|-------|
| | | (00) | (01) | (10) | (11) | (20) | (21) | (30) | (31) |
| 1s-1s | Present | 0.512 | 3.505 | 0.0027 | 1.864 | 0.062 | 0.127 | 0.010 | 0.030 |
| | Direct numerical [7] | 0.518 | 3.508 | 0.0029 | 1.898 | 0.065 | 0.137 | 0.012 | 0.036 |
| 1s-2s | Present | 0.057 | 0.0013 | 0.0064 | 0.053 | 0.074 | 0.0061 | 0.0022 | 0.013 |
| | Direct numerical [7] | 0.055 | 0.0017 | 0.0060 | 0.055 | 0.074 | 0.0059 | 0.0021 | 0.012 |
| 1s-2p | Present | 0.025 | 0.0006 | 0.066 | 0.045 | 0.152 | 0.011 | 0.0072 | 0.047 |
| | Direct numerical [7] | 0.025 | 0.0010 | 0.067 | 0.046 | 0.152 | 0.011 | 0.0069 | 0.048 |
| 2s-2s | Present | 7.238 | 13.23 | 5.870 | 8.393 | 17.75 | 84.91 | 7.75 | 27.3 |
| | Direct numerical [7] | 7.032 | 13.28 | 6.033 | 7.791 | 18.09 | 83.58 | 8.524 | 27.33 |
| 2s-2p | Present | 0.638 | 3.426 | 2.183 | 18.32 | 0.578 | 20.51 | 14.94 | 14.97 |
| | Direct numerical [7] | 0.686 | 2.785 | 2.049 | 17.69 | 0.490 | 21.45 | 15.31 | 14.84 |
| 2p-2p | Present | 0.586 | 3.342 | 8.822 | 27.15 | 21.58 | 31.06 | 11.47 | 73.30 |
| | Direct numerical [7] | 0.599 | 3.685 | 8.860 | 27.99 | 21.54 | 30.71 | 11.47 | 73.38 |

ment. In the HSCC calculations presented for these two partial waves, we used $R_M=197-534$, $N_{\text{ch}}=114-145$, $N_{\text{sect}}=1600$.

For the $^1D^e$ and $^3D^e$ partial waves, the HSCC results are also compared to the calculations of Shertzer and Botero [11] using the finite-element method, in addition to the results of [7,8,12]. The results of Shertzer and Botero at $k=0.1$ and 0.2 appear to be too low. Otherwise there is good overall agreement among the calculations. In the HSCC calculations, we used $R_M=195-644$, $N_{\text{ch}}=85-108$, $N_{\text{sect}}=1900$.

For the $^1F^o$ and $^3F^o$ partial waves, the phase shifts calculated are compared to those from [7,11,13]. The overall agreement among the calculations can be seen clearly in Table I. In the HSCC calculation, we used $R_M=190-602$, $N_{\text{ch}}=100-133$, $N_{\text{sect}}=1400$.

We have not calculated the phase shifts for partial waves beyond $L=3$. The phase shifts for these higher partial waves are quite small because of the centrifugal barrier. Such small phase shifts in general are more easily calculated using perturbative approaches. We note that in this respect the HSCC method is similar to the finite-element method of Shertzer and Botero [11] and the direct numerical solution of Wang and Callaway [7] in that they are suitable for lower partial waves where electron correlation is more significant. For higher partial waves the independent particle picture is rather adequate, then perturbative approaches or methods based on the close-coupling approximation will be able to achieve accurate results with less effort.

We have also calculated all the elastic and inelastic scattering cross sections for a few energy points between the $H(n=2)$ and $H(n=3)$ thresholds using the same set of parameters R_M , N_{ch} , and N_{sect} as in the calculation of the elastic phase shifts. In Table II and Table III the results are compared to those from Wang and Callaway [7] at $k^2=0.78$ Ry and 0.85 Ry, respectively. Results from other calculations can be found in the work of Wang and Callaway and will not be repeated here. From the two tables, we first note that the $1s-1s$, $1s-2s$, and $1s-2p$ cross sections between the two calculations agree quite well for all the partial waves. For the transitions $2s-2s$, $2s-2p$, and $2p-2p$ there are large discrepancies between the two calculations at $k^2=0.78$ Ry, especially for $(LS)=(00),(01)$. The discrepancy is not as serious at $k^2=0.85$ Ry. In general we have observed that the

discrepancy occurs at lower energies when k^2 is close to the excitation threshold (at 0.75 Ry) but the errors become smaller at higher energies.

We remark that the elastic or resonant scattering cross sections (such as $2s-2p$) at low energies are more difficult to obtain accurately using the diabatic-by-sector approach of the HSCC method. Recall that in Eq. (2) the wave functions are expanded in terms of diabatic basis functions within each sector, i.e., the basis functions remained fixed within each sector. This is not a good representation of the physical system for those channels which are barely open. These low-energy channels, as expected, are better represented by suitable adiabatic basis functions. To achieve high-precision calculations for these channels within the diabatic-by-sector scheme, a large increase in the number of diabatic basis functions would be needed to represent the adiabatic channel functions. This is not easy to implement directly since in the same calculation other channels which have higher kinetic energies are more diabatic in nature. The poor elastic and resonant scattering cross sections in the HSCC calculations near the opening of the new thresholds are thus expected. From Tables II and III, however, we notice that the inelastic scattering cross sections converge much faster and even the $1s-1s$ elastic channels are well converged. The inelastic transitions occur at smaller hyperradius and for the $1s-1s$ elastic channel the kinetic energy is not small such that diabatic basis function is a good approximation.

In summary, we illustrated that the HSCC method indeed can be carried out to the comparable precision of the existing benchmark calculations for the basic electron-hydrogen-atom collisions. The main power of the HSCC method, however, is in its application to the higher-energy region where many channels are open, as illustrated in the previous applications [14,2]. In the higher-energy region, there are few benchmark calculations available for comparison, but the results from the HSCC method have been compared most favorably with most detailed experiments from photoionization studies [1].

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