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Full optical potential for the electron-hydrogen entrance channel

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Differential and total elastic and total reaction cross sections are calculated for electron-hydrogen scattering at 30, 100, and 400 eV using an *ab initio* optical potential that treats bound and continuum nonelastic channels in the distorted-wave Born approximation. Multichannel and partial-wave expansions are carried out to numerical convergence. Convergence criteria and quadratures for the continuum-energy integration are chosen for 1% overall accuracy. Results are compared with experiment and less-detailed calculations.

The electron-hydrogen problem is the simplest nontrivial problem in scattering theory. Nevertheless, it is very difficult to calculate and there are significant discrepancies between experiment and theory, even in the entrance channel.[1]

Most calculations of electron-atom scattering, for which the electron-hydrogen problem is the prototype, are based on the multichannel expansion. For each state of total spin a reaction channel is characterized by a state of the target. A multichannel expansion can be written for a finite discrete set P of channels, but the complementary set Q, including the continuum, has a large effect. For example, for hydrogen at energies well above the ionization threshold the continuum is responsible for about half of the absorption of electrons from the entrance channel into nonelastic channels.

Calculations based on the perturbation series include the unitarized eikonal Born series of Byron, Joachain, and Potvliege.[2] This method does not treat the Q-space channels explicitly. These channels are treated explicitly by Madison, Hughes, and McGinness,[3] where Q space is calculated exactly to second order.

One method of accounting for Q space in a coupled-channels calculation is to represent it by a discrete set of pseudostates chosen to give an accurate description of part of the problem, with the hope that it gives an adequate description of the whole problem. For example, the calculation of van Wyngaarden and Walters[4] uses 20 pseudostates chosen to reproduce the second Born approximation for chosen channels at a chosen energy.

In the present work we represent Q space by an optical potential that makes only two approximations. The first is the use of the distorted-wave Born approximation for the explicitly treated Q-space channels. The second, which will be removed in later work, is the omission of exchange terms in Q-space excitation amplitudes.

The optical potential for the coupling of channels i and j consists of the first-order coupling potential plus a complex polarization potential, whose real and imaginary parts describe respectively virtual and real (on-shell) excitations of the Q-space channels. For the entrance-channel problem considered here, Q space consists of all nonelastic channels. The momentum representation of the complex polarization potential is:

$$\langle \mathbf{q}'0 \,|\, V_S \,|\, 0\mathbf{q}\rangle = \sum_{I \in Q} \int d^3k \langle \mathbf{q}'0 \,|\, v_S \,|\, \Psi_I^{(-)}(\mathbf{k})\rangle \frac{1}{E^{(+)} - H} \times \langle \Psi_I^{(-)}(\mathbf{k}) \,|\, v_S \,|\, 0\mathbf{q}\rangle . \quad (1)$$

Here H is the total Hamiltonian for the scattering problem, E is the total energy, S is the total spin, and $\Psi_I^{(-)}(\mathbf{k})$ is the exact state vector for a three-body state with a continuum electron of momentum $\mathbf{k}$ and the target in a state I whose energy eigenvalue is ε_I. For ionized target states I is a discrete notation for the continuum. We present the continuum integration for each partial-wave state by a quadrature rule. The two-electron interaction v_S is given in the light of the Pauli exclusion principle by

$$v_S = v[1 + (-1)^S P_r] , \quad (2)$$

where v is the Coulomb potential and P_r is the space-exchange operator.

Formally the entrance-channel problem is solved by using (1) as the potential operator in the Lippmann-Schwinger equation for the entrance channel. However, this is really only a rearrangement of the problem, not a

solution, because a solution involves finding $\Psi_I^{(-)}(\mathbf{k})$.

The procedure we adopt is to use the distorted-wave Born approximation to $\Psi_I^{(-)}(\mathbf{k})$. This approximation gives very reasonable descriptions of discrete excitations,[5] of total ionization cross sections,[6] and of larger values of double and triple differential cross sections for ionization.[7] We are actually using the distorted-wave representation to expand the exact channel Green's function $(E^{(+)}-H)^{-1}$. This has been used very successfully to represent on-shell dipole excitations by Madison, Hughes, and McGinness.[3]

For formal purposes we made the exact spectral representation in Eq. (1). However, for computation of the polarization potential we use the representation

$$\langle \mathbf{r},I|(E^{(+)}-H)^{-1}|I,\mathbf{r}'\rangle = -\langle \mathbf{r},I|(E^{(+)}-\varepsilon_I-K-V_1-v)^{-1}|I,\mathbf{r}'\rangle , \quad (3)$$

where K is the projectile kinetic energy operator, v is the two-electron potential, and V_1 is the potential between the continuum electron and the nucleus. We approximate the noncentral potential V_1+v by a central distorting potential $V_D(r)$ for which the Green's function can be calculated. In the present calculation $V_D(r)$ is the static potential of the hydrogen ground state.

A simplified version of the optical potential has been used in the coupled-channels problem by McCarthy and Stelbovics.[8] We call this the half-shell optical potential. Here the integrations in (1) are done by a multidimensional method for which considerations of computational feasibility require an analytic expression for each excitation matrix element. For the continuum case this requires the approximation of a plane wave for the faster electron and a Coulomb wave orthogonalized to the target ground state for the slower electron. In addition, it is necessary to restrict the set of values of $\mathbf{q}'$ and $\mathbf{q}$ for which V_S is calculated to $\frac{1}{2}q^2=E-\varepsilon_0$ and to project out the relevant angular momentum components by integrating over $\hat{\mathbf{q}}'\cdot\hat{\mathbf{q}}$. None of these restrictions apply to the present calculation.

TABLE I. Entrance channel data at 30 eV. Cross sections are in atomic units, angles in degrees. Numbers in square brackets indicate powers of 10. Total errors in the last significant digits are shown in parentheses. Column headings are (A) data of Williams (Ref. 13); (B) present calculation.

Angle (deg)	(A)	(B)
0		1.26[1]
10	5.32(57)	7.52
15	3.51(37)	5.47
20	2.74(28)	3.92
25	2.25(21)	2.79
30	1.60(18)	2.00
40	1.15(12)	1.06
50	6.41(65)[−1]	5.97[−1]
60	4.61(52)[−1]	3.66[−1]
70	3.16(28)[−1]	2.46[−1]
80	2.21(21)[−1]	1.79[−1]
90	1.62(17)[−1]	1.41[−1]
100	1.31(11)[−1]	1.17[−1]
110	1.28(14)[−1]	1.02[−1]
120	1.05(10)[−1]	9.23[−2]
130	9.8(10)[−2]	8.56[−2]
140	9.1(9)[−2]	8.09[−2]
160		7.57[−2]
180		7.39[−2]
σ_{elastic}	6.50	6.93
σ_{reaction}	6.22	8.89

Coupled-channels calculations that use the second-order direct optical potential for a Q space represented by pseudostates have been done by Bransden, Scott, Shingal, and Roychoudhury[9] and by Callaway, Unnikrishnan, and Oza.[10] Bartschat, McEachran, and Stauffer[11] have calculated electron and positron scattering from argon using an explicit direct optical potential for bound states of the target.

In the general coupled-channels case we solve the partial-wave Lippmann-Schwinger equation for P space:

$$T_{lL'L}^{(JS)}(q',q)=V_{lL'L}^{(JS)}(q',q)+\sum_{l',L'}\int dk\,k^2 V_{ll'L'}^{(JS)}(q',k)\frac{1}{E^{(+)}-\varepsilon_{l'}-\frac{1}{2}k^2}T_{l'lL}^{(JS)}(k,q) . \quad (4)$$

For economy of notation we have represented each target state (nonuniquely) by its orbital angular momentum l. The corresponding continuum partial-wave angular momentum is L. The total angular momentum is J. The numerical method of performing the integration over k is described in Ref. 8.

The polarization part of the optical potential consists of a direct term and three exchange terms. We give the computational form of the direct term. The other terms are related to it by appropriate space exchanges:

$$\bar{V}_{lL'L}^{(J)}(q',q)=(q',q)^{-1}\int dr\int dr' U_{\bar{L}}(q',r)W_{lL'L}^{(J)}(r,r')U_L(q,r') , \quad (5)$$

where $U_L(q,r)$ is the partial wave of a plane wave (Riccati-Bessel function) and the nonlocal coordinate-space component of the polarization potential is

$$W_{lL'L}^{(J)}(r,r')=\left(\frac{2}{\pi}\right)^2(-1)^{J+l_i L-\bar{L}}\sum_{j,L',\lambda,\bar{\lambda}}\hat{j}\hat{L}'\hat{L}\hat{l}\begin{pmatrix}L&\lambda&j\\0&0&0\end{pmatrix}\begin{pmatrix}L'&\lambda&l\\0&0&0\end{pmatrix}\begin{Bmatrix}j&J&L'\\l&\lambda&L\end{Bmatrix}\hat{j}\hat{L}'\hat{\bar{L}}\hat{\bar{l}}\begin{pmatrix}\bar{L}&\bar{\lambda}&j\\0&0&0\end{pmatrix}\begin{pmatrix}L'&\bar{\lambda}&\bar{l}\\0&0&0\end{pmatrix}\begin{Bmatrix}j&J&L'\\\bar{l}&\bar{\lambda}&L\end{Bmatrix}$$
$$\times\mathcal{P}\int dk\left(\int dr''\,u_l(r'')v_{\bar{\lambda}}(r,r'')u_{L'}(k,r'')\right)$$
$$\times rr' g_j(E-\tfrac{1}{2}k^2;r,r')\left(\int dr'''\,u_{L'}(k,r''')v_\lambda(r''',r')u_l(r''')\right) . \quad (6)$$

TABLE II. Entrance channel data at 100 eV. Column headings are (A) data of van Wingerden *et al.* (Ref. 14); (B) data of Williams (Ref. 13); (C) present calculation; (D) half-shell optical calculation of McCarthy, Saha, and Stelbovics (Ref. 16); (E) pseudostate calculation of van Wyngaarden and Walters (Ref. 4); and (F) unitarized eikonal Born series calculation of Byron *et al.* (Ref. 2).

Angle (deg)	(A)	(B)	(C)	(D)	(E)	(F)
0	· · ·	· · ·	7.40	· · ·	7.55	8.2
10	· · ·	· · ·	2.17	· · ·	2.20	2.4
15	1.59(11)	· · ·	1.30	1.29	· · ·	· · ·
20	1.17(8)	1.10(10)	8.28[−1]	8.9[−1]	8.79[−1]	8.5[−1]
25	· · ·	6.92(71)[−1]	5.48[−1]	· · ·	5.91[−1]	· · ·
30	5.25(35)[−1]	5.09(49)[−1]	3.70[−1]	4.4[−1]	4.06[−1]	3.6[−1]
40	2.57(21)[−1]	2.88(27)[−1]	1.80[−1]	2.1[−1]	2.01[−1]	1.7[−1]
50	1.31(10)[−1]	1.32(12)[−1]	9.47[−2]	1.04[−1]	1.06[−1]	· · ·
60	7.4(8)[−2]	7.22(71)[−2]	5.44[−2]	6.1[−1]	6.07[−2]	5.3[−2]
70	4.8(5)[−2]	4.91(46)[−2]	3.38[−2]	3.9[−2]	· · ·	· · ·
80	3.19(34)[−2]	2.95(30)[−2]	2.26[−2]	2.6[−2]	· · ·	2.3[−2]
90	2.27(20)[−2]	2.09(20)[−2]	1.60[−2]	1.81[−2]	1.77[−2]	· · ·
100	1.62(20)[−2]	1.55(15)[−2]	1.20[−2]	1.32[−2]	· · ·	1.2[−2]
110	1.30(15)[−2]	1.15(12)[−2]	9.43[−2]	1.02[−2]	1.01[−2]	· · ·
120	1.07(12)[−2]	9.2(9)[−3]	7.71[−3]	8.3[−3]	8.26[−3]	8.0[−3]
130	8.4(9)[−3]	7.8(7)[−3]	6.51[−3]	6.8[−3]	· · ·	· · ·
140	· · ·	6.5(7)[−3]	5.69[−3]	· · ·	6.15[−3]	5.9[−3]
160	· · ·	· · ·	4.80[−3]	· · ·	5.32[−3]	5.0[−3]
180	· · ·	· · ·	4.51[−3]	· · ·	5.07[−3]	4.7[−3]
$\sigma_{elastic}$	1.83	1.85	1.42	1.50	1.51	1.46
$\sigma_{reaction}$	· · ·	5.53	5.77	5.28	5.18	5.58

Here the symbols in parentheses and braces are Wigner $3j$ and $6j$ symbols, respectively, $u_l(r)$ is the radial wave function of a bound state in P space. For the discrete Q-space state k, $u_{L'}(k,r)$ is a radial bound-state wave function. For a continuum Q-space state it is the L' partial wave of the solution of the elastic scattering problem at momentum k in the target potential. The symbol $\sum\!\!\!\!\!\!\int$ represents a sum over discrete and integral over continuum Q-space states. The λ multipole of the Coulomb potential is $v_\lambda(r,r')$ and $g_j(E;r,r')$ is the j multipole of the Green's function for elastic scattering at energy E by the distorting potential V_D.

In the present calculation, convergence in the Q-space sum and integral is achieved by including bound states up to $n=6$, $L'=3$, and using continuum energies suitably chosen for 12-point Gaussian quadratures for partial waves up to $L'=10$. The convergence criteria have been chosen with the object of producing final results accurate to 1%.

We report results for a calculation of (4) using the direct polarization potential of (5) and (6) but including exchange in the first-order term. There is some justification for the omission of exchange terms in a preliminary calculation. Exchange has a small effect on the long-range real polarization potential so that forward differential cross sections are weakly affected. There is also some evidence[12] that its overall effect on cross sections is small. While exchange will be fully included in future coupled-channels calculations, the unprecedented detail of the present optical potential makes it interesting to see whether there is a sign of a reduction in the discrepancies between experiment and previous calculations.

Tables I, II, and III give results at 30, 100, and 400 eV. The discrepancy between experiment and previous calculations has been greatest at 100 eV. 30 and 400 eV are included to test the calculation at significantly lower and higher energies. Experimental data are due to Williams[13] and van Wingerden *et al.*[14] Total elastic and reaction

TABLE III. Entrance channel data at 400 eV. Column headings are (A) data of Williams (Ref. 13); (B) present calculation.

Angle (deg)	(A)	(B)
0	· · ·	3.35
10	· · ·	6.28[−1]
20	1.96(21)[−1]	1.70[−1]
30	6.17(62)[−2]	5.10[−2]
40	2.06(15)[−2]	1.89[−2]
50	9.47(132)[−3]	8.52[−3]
60	4.38(62)[−3]	4.43[−3]
70	2.35(24)[−3]	2.57[−3]
80	1.57(27)[−3]	1.64[−3]
90	1.04(24)[−3]	1.11[−3]
100	9.16(192)[−4]	8.09[−4]
110	7.65(158)[−4]	6.21[−4]
120	6.03(122)[−4]	4.93[−4]
130	4.70(107)[−4]	4.10[−4]
140	5.06(115)[−4]	3.56[−4]
160	· · ·	2.96[−4]
180	· · ·	2.83[−4]
$\sigma_{elastic}$	2.45[−1]	2.79[−1]
$\sigma_{reaction}$	2.19	2.15

cross sections are taken from semiempirical estimates by de Heer, McDowell, and Wagenaar[15] whose errors are of the order of 10%.

At 30 eV, differential cross sections do not exhibit detailed agreement with experiment. Perhaps the most serious deficiency of the model is in the total reaction cross section which is overestimated by 40% in comparison with the semiempirical number of de Heer *et al.* The 20% discrepancy between calculated and measured differential cross sections at 100 eV remains. This is well outside experimental error. The total reaction cross section is in excellent agreement with experiment at this energy. All cross sections agree within experimental error at 400 eV.

The major disadvantage of the distorted-wave Born-approximation method, as with other approaches to the electron-hydrogen Q space, is that it does not incorporate the exact boundary conditions[17] for three charged particles. However, it is a major attraction of the method that this may be feasible with minor modifications. The present calculation will be improved in the near future by including full exchange and a larger P space.

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