# Coupled-channels optical calculation of electron-hydrogen resonances

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(Received 30 March 1992)

An application of the coupled-channels optical method to energy-dependent phenomena, electron-hydrogen resonances for $n = 1$ and 2, is given. The equivalent local approximation is made for the optical potential. The calculation includes nine explicitly coupled channels. The optical potential accounts for the target continuum. The good agreement with experiment shows the role played by the optical potential in the coupled-channels calculation. Some additional resonances have been found.

PACS number(s): 34.80.Bm, 34.80.Dp

## I. INTRODUCTION

The coupled-channels optical (CCO) method given by McCarthy and Stelbovics [1] is applied to describing experiments with rapid energy variation. It has been our practice in introducing developments in the method to start with the equivalent local approximation to the optical potential [2]. This is done here in the case of electron scattering on hydrogen to the $n = 1$ and $n = 2$ states. For $n = 1$ and $n = 2$ the energy ranges are, respectively, 9.4–10.2 and 11.66–12.06 eV.

The energy dependence in elastic electron-hydrogen scattering has been investigated by, for example, Taylor and Burke [3] with the close-coupling method; Seiler, Oberoi, and Callaway [4] with the algebraic close-coupling method; and Pathak, Kingston, and Berrington [5] with the $R$-matrix method. The investigation for $n = 2$ has been made by, for example, Morgan, McDowell, and Callaway [6] with the algebraic variational method; Callaway [7] with the variational pseudostates method; Pathak, Kingston, and Berrington [5]; and Fon, Ratnavelu, and Aggarwal [8] with the $R$-matrix method. A complete list of references is given by Pathak, Kingston, and Berrington [5].

In the present calculation nine states (1, 2, 3, 4$s$; 2, 3, 4$p$; 3, 4$d$) are explicitly coupled ($P$ space) and only the target continuum is included in the optical potential ($Q$ space). Optical potentials are used in the couplings $1s-1s$, $1s-2s$, $1s-2p$. Optical potentials in other couplings have a small effect on the $1s$, $2s$, and $2p$ cross sections.

Section II discusses the computational developments that enable fast computations of energy variation to be done in setting up and solving the coupled Lippmann-Schwinger equations. It also discusses the methods used to extract Breit-Wigner resonance parameters from the partial-wave $T$-matrix elements.

## II. FORMALISM AND CALCULATION DETAILS

The coupled integral equations are represented in momentum space:

$$\langle \mathbf{k}i \mid T_S \mid 0\mathbf{k}_0\rangle = \langle \mathbf{k}i \mid V_S^{(Q)} \mid 0\mathbf{k}_0\rangle + \sum_{j\in P}\int d^3q \frac{\langle \mathbf{k}i \mid V_S^{(Q)} \mid j\mathbf{q}\rangle\langle \mathbf{q}j \mid T_S \mid 0\mathbf{k}_0\rangle}{E^{(+)}-\varepsilon_j - q^2/2}, \quad (1)$$

where $i,j$ represent target states, $P$ projects a finite set of target states including the ground state 0, and $Q$ projects the continuum and the remaining discrete states. The subscript $S$ indicates the total spin. $V_S^{(Q)}$ has two parts, the electron-target potential $V_S$ and the complex, nonlocal polarization potential $W_S^{(Q)}$,

$$V_S^{(Q)} = V_S + W_S^{(Q)}, \quad (2)$$

where the basic approximation for the matrix element of $W_S^{(Q)}$ is

$$\langle \mathbf{k}'i \mid W_S^{(Q)} \mid j\mathbf{k}\rangle = \sum_{l\in Q}\int d^3q \langle \mathbf{k}'i \mid V_S \mid l\mathbf{q}\rangle \frac{1}{E^{(+)}-\varepsilon_l - q^2/2}\langle \mathbf{q}l \mid V_S \mid j\mathbf{k}\rangle + \int d^3q' \int d^3q \frac{\langle \mathbf{k}'i \mid V_S \mid \psi^{(-)}(\mathbf{q}_<)\mathbf{q}_>\rangle\langle \mathbf{q}_>\psi^{(-)}(\mathbf{q}_<) \mid V_S \mid j\mathbf{k}\rangle}{E^{(+)}-q^2/2-q'^2/2}. \quad (3)$$

 

Here $q_<$ and $q_>$ represent the lesser and greater of $q$ and $q'$, respectively, and $\psi^{(-)}(\mathbf{q})$ is a Coulomb wave orthogonalized to the $P$ space target orbital involved in the same matrix element. For computational feasibility it is necessary to use the equivalent local exchange amplitude in (3) and to make the angular momentum projection approximation

$$\langle \mathbf{k}'i \mid W_S^{(Q)} \mid j\mathbf{k}\rangle = \sum_{l'',m''} i^{l''} C_{l''l'l}^{m''m'm} U_{l''l'l}(K) Y_{l''m''}(\hat{\mathbf{K}}), \tag{4}$$

where $lm$ and $l'm'$ are the orbital angular momentum quantum numbers of the states $i$ and $j$, respectively, and

$$\mathbf{K} = \mathbf{k} - \mathbf{k}'. \tag{5}$$

The half-on-shell approximation

$$\frac{1}{2}k^2 = E - \varepsilon_j \tag{6}$$

is made for the amplitudes (3), reducing the computation of the optical potential to the function $U_{l''l'l}(K)$ obtained by inverting (4). Details of the calculation are given in Ref. [9] and references therein.

The present calculation was carried out by using the same quadrature points for solving the integral equation (1) over a range of energies, thus making the off-shell potential matrices energy independent. We calculated the slowly varying optical potentials at a few energy points instead of the whole energy range. For computation we make a partial-wave expansion of the $T_S$ and $V_S^{(Q)}$ matrix elements, defining the partial matrix elements

$$\langle k'n'l'L' \parallel T_{JS} \parallel Llnk\rangle \tag{7}$$

for total orbital angular momentum quantum number $J$ by

$$\langle \mathbf{k}'i \mid T_S \mid j\mathbf{k}\rangle = \sum_{L,M,L',M',J,K} \langle \hat{\mathbf{k}}' \mid L'M'\rangle C_{L'l'J}^{M'm'K} \langle k'n'l'L' \parallel T_{JS} \parallel Llnk\rangle C_{LlJ}^{MmK} \langle LM \mid \hat{\mathbf{k}}\rangle, \tag{8}$$

where

$$\langle \hat{\mathbf{k}} \mid LM\rangle \equiv Y_{LM}(\hat{\mathbf{k}}) \tag{9}$$

and $C_{LlJ}^{Mmk}$ is a Clebsch-Gordan coefficient. The definition of

$$\langle k'n'l'L' \parallel V_{JS}^{(Q)} \parallel Llnk\rangle \tag{10}$$

is analogous to (7) with $V_S^{(Q)}$ substituted for $T_S$.

The energies and widths of resonances for particular values of $J$ and $S$ have been found by fitting the Breit-Wigner form with a linear background

$$\sigma_R = aE + b + \frac{c + id}{E - E_R + 0.5i\Gamma_R} \tag{11}$$

TABLE I. Resonance energies and widths in elastic electron-hydrogen scattering.

| State | Experiments | | | Calculations | | | |
|---|---|---|---|---|---|---|---|
| | Williams [10] | Warner *et al.* [11] | Risley, Edward, and Geballe [13] | Taylor and Burke [3] | Seiler, Oberoi, and Callaway [4] | Pathak, Kingston, and Berrington [5] | Present work |
| | | | | Energies (eV) | | | |
| $^1S$ | 9.557(10) | 9.549(13) | 9.59(3) | 9.560 | 9.574 | 9.557 | 9.553 |
| | | | | | | | 9.875 |
| | | | | 10.178 | 10.178 | 10.177 | 10.172 |
| $^3S$ | | | | 10.150 | 10.151 | 10.147 | |
| $^1P$ | | | | | | | 9.531 |
| | | | | 10.177 | 10.185 | 10.176 | 10.177 |
| $^3P$ | 9.735(10) | 9.736(13) | 9.76(3) | 9.74 | 9.768 | 9.741 | 9.743 |
| $^1D$ | | 10.115(13) | | 10.125 | 10.160 | 10.126 | 10.144 |
| | | | | Widths (meV) | | | |
| $^1S$ | 45.0(5) | 63.0(8) | | 47.0 | 54.0 | 52.0 | 48.0 |
| | | | | | | | 8.9 |
| | | | | 2.2 | 2.3 | 2.6 | 2.4 |
| $^3S$ | | | | 0.02 | 0.02 | | |
| $^1P$ | | | | | | | 9.1 |
| | | | | 0.04 | 0.02 | | 0.04 |
| $^3P$ | 6.0(5) | 5.0(2) | | 5.9 | 8.0 | 7.1 | 4.5 |
| $^1D$ | | 6.0(2) | | 8.8 | 7.7 | 8.8 | 6.9 |

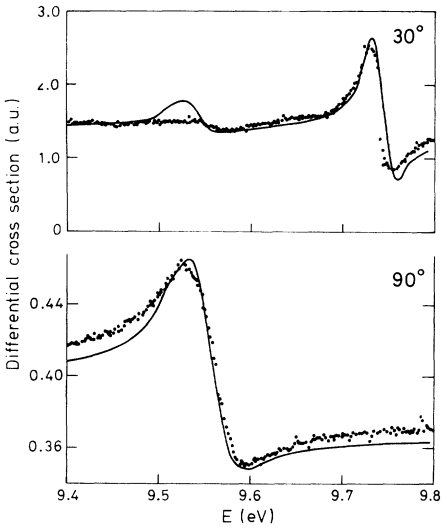


FIG. 1. Comparison between the experiment of Williams [10] for the elastic integrated cross sections and the present calculation at 30° and 90°. The solid lines are the CCO calculations.

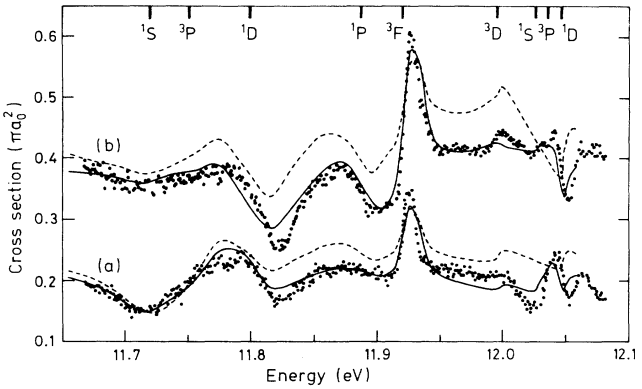


FIG. 2. Comparison between the experiment of Williams [12] for the 2s (a) and 2p (b) integrated cross sections and the present calculation with and without the optical potential. Solid lines are the calculation with the optical potential and dashed lines without the optical potential. The energies of resonances are shown at the top of the diagram.

to the partial cross section $\sigma_R$ for each resonance over the resonant energy range, where $E$ is the incident energy, and $E_R$, $\Gamma_R$, $a$, $b$, $c$, and $d$ are the fitting parameters. $E_R$ is the resonant energy and $\Gamma_R$ the width.

## III. RESULTS AND DISCUSSION

A table of calculated and observed resonances below the first inelastic threshold has been given in Ref. [10]. However, there is little theoretical work on the angular behavior of the cross sections in the resonance region. The present work has calculated electron-hydrogen resonances in elastic scattering over the energy range 9.4–10.2 eV at angles of 30° and 90°. Figure 1 shows the comparison of the experiment [10] for the energy dependence of the differential cross section at 30° and 90° and the present calculation folded with the experimental resolution, 0.012 and 0.02 eV. The resonances found in the present calculation are compared with experiment and with earlier calculations in Table I. Two possible resonances, which have not been reported before, have been found at 9.531 and 9.875 eV, belonging to the symmetry manifolds $^1P$ and $^1S$ with widths 0.0091 and 0.0089 eV, respectively. The first one is very close to the $^1S$ resonance at 9.553 eV with width 0.0048 eV. The latest two experiments [10,11] observed resonances at 9.557 and 9.549 eV, with energy resolutions 0.02 and 0.025 eV. Therefore it is possible that the experimental cross section here is due to two resonances, $^1P$ at 9.531 eV and $^1S$ at 9.553 eV. For the other new resonance at 9.875 eV there is a very weak sign of resonance in the vicinity of this energy in the experiment [11]. It still needs the confirmation of further experiments. Some other calculations mentioned in Table I found a $^3S$ resonance near 10.150 eV. However, we cannot find it. We have done the calculation from 10.149 91 to 10.150 10 eV at intervals of 0.01 meV. From 10.147 00 eV to 10.151 00 eV, intervals were 0.03 meV. The width quoted by other authors is 0.02 meV [5]. Note that the $^1P$ resonance at 10.177 eV, which has a comparable width, was found by the present calculation.

Figure 2 shows the comparison between the experi-

TABLE II. Resonance energies and widths below the n=3 threshold for electron-hydrogen scattering.

| State | Experiment [12] | | | | Present work | | | | Callaway [7] | | Pathak, Kingston, and Berrington [5] | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 2p | | 2s | | 2p | | 2s | | | | | |
| | $E_R$ (eV) | $\Gamma_R$ (meV) | $E_R$ (eV) | $\Gamma_R$ (meV) | $E_R$ (eV) | $\Gamma_R$ (meV) | $E_R$ (eV) | $\Gamma_R$ (meV) | $E_R$ (eV) | $\Gamma_R$ (meV) | $E_R$ (eV) | $\Gamma_R$ (meV) |
| $^1S$ | 11.722(9) | 45(9) | 11.724(12) | 37(8) | 11.726 | 39.01 | 11.726 | 37.03 | 11.7218 | 38.89 | 11.7218 | 40.93 |
| $^3P$ | | | | | 11.751 | 46.10 | 11.753 | 45.8 | 11.7513 | 44.74 | 11.7515 | 46.64 |
| $^1D$ | 11.807(9) | 45(8) | 11.803(9) | 37(8) | 11.805 | 49.41 | 11.803 | 47.80 | 11.8048 | 44.46 | 11.8049 | 43.52 |
| $^1P$ | 11.902(6) | 33(10) | | | 11.892 | 29.70 | 11.891 | 30.92 | 11.8929 | 32.50 | 11.8930 | 34.13 |
| $^3F$ | 11.925(2) | 4(2) | 11.926(2) | 4(2) | 11.927 | 3.74 | 11.927 | 3.51 | 11.9255 | 2.96 | 11.9258 | 3.10 |
| $^3S$ | | | | | 11.993 | 0.24 | 11.994 | 0.24 | 11.9943 | 0.24 | 11.9944 | 0.23 |
| $^3D$ | 11.997(5) | 10(3) | 12.00(5) | 15(10) | 11.996 | 10.00 | 11.996 | 12.01 | 11.9949 | 10.20 | 11.9952 | 10.50 |
| $^1S$ | 12.029(5) | 9(3) | 12.024(5) | 9(3) | 12.028 | 9.50 | 12.030 | 9.80 | 12.0272 | 8.31 | 12.0273 | 7.89 |
| $^3D$ | | | | | 12.024 | 0.23 | 12.024 | 0.23 | 12.0283 | 0.23 | 12.0286 | 0.22 |
| $^3P$ | 12.040(6) | 10(4) | 12.036(4) | 10(4) | 12.037 | 12.65 | 12.028 | 13.00 | 12.0369 | 8.31 | 12.0370 | 8.25 |
| $^1D$ | 12.049(4) | 7(3) | 12.048(4) | 7(3) | 12.047 | 7.9 | 12.046 | 7.9 | 12.0532 | 6.57 | 12.0534 | 5.82 |

ment [12] for the $2s$ and $2p$ integrated cross sections in the energy range 11.66–12.06 eV and the present calculation with and without the optical potential, folded with experimental resolution, 9 meV. We can see clearly that the continuum plays a role in the scattering, especially in the higher energy range. Its effect on the background increases with increasing energy. The energies and widths of the calculated resonances below the $n = 3$ threshold are presented in Table II. They are compared with experiment and other calculations. There is a good agreement among them.

## IV. CONCLUSION

An application of the CCO method to energy-dependent phenomena, electron-hydrogen resonances, gives good agreement with experiments and other calculations. It shows that the continuum plays a role in the relevant energy region. Resonances have been found that are yet to be obtained experimentally.

## ACKNOWLEDGMENTS

We are grateful for the support of this work by the Australian Research Council. One of us (B.S.) would like to thank Flinders University and The Australian Federation of University Women–South Australia Inc. Trust Fund for support.

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