

Truncated dipole series in the electron-hydrogen and positron-hydrogen systems

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Dipole series in H^- and in the positron-hydrogen system are studied in a coupled-channel calculation, in which the short-range part of the interaction between the electron or positron and the excited hydrogen core is modeled by a local potential, adjusted to reproduce low-lying states of the respective series. Consideration of the fine-structure splitting and radiative corrections enables us to describe the termination of the series towards the nondegenerate threshold. For the $^1S^e$ series below the $N=2$ threshold we give quantitative predictions for the number of resonances and their energies. [S1050-2947(98)06101-0]

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Due to the l degeneracy of energy levels in the hydrogen atom, an electron or positron moving in the potential of an excited hydrogen core asymptotically experiences a dipole potential $V(r) = P/r^2$ for $r \rightarrow \infty$. If the asymptotic potential is sufficiently attractive $P < -1/4$, it binds an infinite series of Feshbach resonances converging to the N th hydrogenic threshold [1–4]. The energies E_n and widths of levels within an ideal dipole series scale exponentially with the series quantum number n , so the level ratio, $R_n := (E_n - E^{\text{thresh}})/(E_{n+1} - E^{\text{thresh}})$ is constant. Due to short-range deviations from a pure $1/r^2$ potential the R_n are not constant, but converge rapidly to the limiting value $R = \exp(2\pi/\sqrt{-P-1/4})$ as $n \rightarrow \infty$.

Experimental advances [5,6] have made highly accurate observation of some of these resonances possible, and further precise data may be expected soon. This has led to increased theoretical activity in the field [7–9]. One question of interest is how a dipole series terminates on approaching the threshold energy E^{thresh} . When the binding energies $|E_n - E^{\text{thresh}}|$ become comparable to the fine-structure and radiative corrections, the thresholds obviously can no longer be regarded as degenerate; threshold splitting leads to a more rapidly decaying potential that can only support a finite number of (resonant) states. Although this has been known for a long time [10,11], theoretical investigations are still generally based on degenerate thresholds. So far the only quantitative studies of the effect of threshold splitting are the preliminary results reported in [12] and a study by Lindroth *et al.*, who predict just one further state to follow two observed resonances in the $^1P^o$ series below the $N=2$ threshold in H^- [13].

In this paper we describe a simple semiempirical approach to reliably predict the properties of higher members of a dipole series in the regime where threshold splitting leads to truncation of the series. The method is to solve the coupled-channel equations for electron or positron scattering, with potentials consisting of the leading long-range terms supplemented by an empirical model in the internal region, with parameters adjusted to reproduce the lowest states of the series, assumed known. Such a procedure is justified because the short-range part of the electron-hydrogen or positron-hydrogen wave function will be essentially energy

independent in the small range of energies where threshold splitting is important [2,11]. We illustrate the method by applying it to the $^1S^e$ series below the $N=2$ threshold.

When the radial coordinate r_1 of the projectile electron or positron is much larger than the coordinate r_2 of the bound target electron we can neglect possible exchange effects and expand the total wave function in terms of radial wave functions $F_\mu(r_1)$ and $R_\mu(r_2)$ and angular functions for the remaining degrees of freedom. When fine-structure and radiative corrections are neglected these are the coupled spherical harmonics $Y_{l_1, l_2}^{LM}(\Omega_1, \Omega_2)$ and the coupled-channel equations for the modified radial wave functions $f_\mu(r_1) = r_1 F_\mu(r_1)$ are

$$\left(-\frac{d^2}{dr_1^2} + V_{\mu\mu}(r_1) \right) f_\mu(r_1) + \sum_{\nu \neq \mu} V_{\mu\nu}(r_1) f_\nu(r_1) = (E - E_\mu^{\text{threshold}}) f_\mu(r_1). \quad (1)$$

The channel label μ stands for $(n_2 l_2, l_1)$, and for a given total orbital angular momentum L and parity $(-1)^L$ there are three channels coupling below the $N=2$ threshold, viz., $(2s, L)$, $(2p, L+1)$, and $(2p, L-1)$. For the $^1S^e$ states ($L=0$) there are only the $l_1=L$ and $l_1=L+1$ channels, and the leading asymptotic terms in the potential are

$$V(r_1) = \frac{1}{r_1^2} \mathbf{V}^D(r_1) + \frac{1}{r_1^3} \mathbf{V}^Q(r_1), \quad (2)$$

with

$$\mathbf{V}^D = \begin{pmatrix} 0 & 6 \\ 6 & 2 \end{pmatrix}, \quad \mathbf{V}^Q = \begin{pmatrix} 0 & 0 \\ 0 & 24 \end{pmatrix}. \quad (3)$$

The case of nondegenerate thresholds is more appropriately described in jj coupling. The angular part of the wave function now consists of jj -coupled generalized spherical harmonics $\mathcal{Y}_{j_1, j_2, l_1, l_2}^{J, M, J}$ and the channel label μ stands for $(n_2, j_2, l_2, j_1, l_1)$. The coupled-channel equations can still be written in the form (1), but the threshold energies E_μ^{thresh} depend not only on $n_2 \equiv N$, but also on l_2 and j_2 . For $r_1 \gg r_2$ the matrix elements of the electron-electron ($-$ positron) interaction are now [14]

$$\begin{aligned}
& \left\langle j_1, l_1, j_2, l_2, J, M \left| \frac{1}{r_{12}} \right| j_3, l_3, j_4, l_4, J, M \right\rangle \\
& \sim \sum_k (-1)^{J+j_2-j_4+1+l_1+l_2} [\hat{j}_1 \hat{j}_2 \hat{j}_3 \hat{j}_4]^{1/2} \\
& \times \begin{Bmatrix} J & j_2 & j_1 \\ k & j_3 & j_4 \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & j_1 & l_1 \\ k & l_3 & j_3 \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & j_2 & l_2 \\ k & l_4 & j_4 \end{Bmatrix} \\
& \times \sqrt{\hat{l}_1} \langle l_1, 0, k, 0 | l_3, 0 \rangle \\
& \times \sqrt{\hat{l}_2} \langle l_2, 0, k, 0 | l_4, 0 \rangle M_{\mu\mu', k}(r_1),
\end{aligned}$$

where \hat{j} stands for $2j+1$ and the radial matrix elements are $M_{\mu\mu', k}(r_1) := \int_0^{r_1} R_{\mu}^*(r_2) R_{\mu'}(r_2) r_2^{k+2} dr_2$. The ${}^1S^e$ states below the $N=2$ threshold(s) are now found in the subspace corresponding to total angular momentum $J=0$ and parity $\pi=+1$. There are three (closed) coupled channels $S_{1/2}$, $P_{1/2}$, $P_{3/2}$, and the leading asymptotic terms in the potential are

$$V(r_1) = \frac{1}{r_1^2} \mathbf{W}^D + \frac{1}{r_1^3} \mathbf{W}^Q, \quad (4)$$

with

$$\mathbf{W}^D = \begin{pmatrix} 0 & 2\sqrt{3} & 2\sqrt{6} \\ 2\sqrt{3} & 2 & 0 \\ 2\sqrt{6} & 0 & 2 \end{pmatrix}$$

and

$$\mathbf{W}^Q = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 12\sqrt{2} \\ 0 & 12\sqrt{2} & 12 \end{pmatrix}. \quad (5)$$

In the approximation of degenerate thresholds, asymptotically diagonal channels can be obtained by diagonalizing the dipole matrix \mathbf{W}^D . Its eigenvalues $2, 1 \pm \sqrt{37}$ are just the eigenvalues $1 \pm \sqrt{37}$ of the dipole matrix (3) in LS coupling together with the eigenvalue $2 = l_2(l_2+1)$ for a further P channel. The asymptotic dipole potential does not depend on the coupling scheme chosen.

The limiting values R of the level ratios corresponding to all eigenvalues of the dipole matrix less than $-1/4$ are summarized in [3] for orbital angular momenta up to $L=6$ and principal quantum numbers up to $n_2 \equiv N=4$. For the ${}^1S^e$ dipole series below the $N=2$ threshold we have $R = 17.4289 \dots$

The short-range potential is modeled in the representation in which the dipole potential is diagonal. In the channels with an eigenvalue of the dipole matrix less than $-1/4$ we add a box potential of the depth V^{box} and width r^{box} (see Fig. 1) [11]. The potentials in the other channels and the coupling potentials are set at the constant value $V(r^{\text{box}})$ for $r < r^{\text{box}}$. The model thus has two free parameters, namely, the

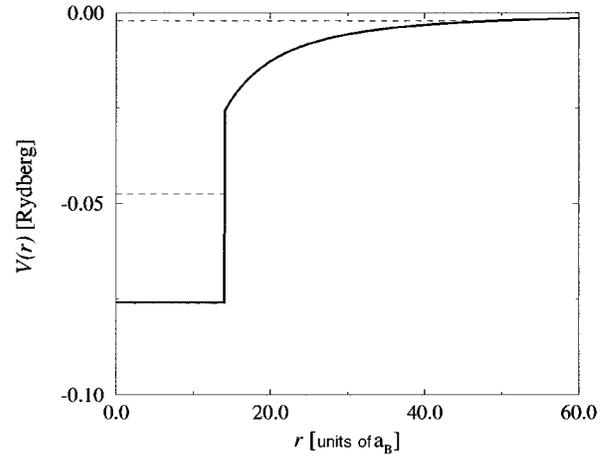


FIG. 1. Dipole asymptotics with additional short-range potential $V(r) = -V^{\text{box}}$ for $r \leq r^{\text{box}}$. The dashed levels denote the lowest two ${}^1S^e$ resonances of H^- below $N=2$.

depth V^{box} and the width r^{box} , which can be adjusted to reproduce the energies of the two lowest-lying states, assumed known.

For the H^- system recent calculations [7,15,16] essentially agree on the lowest two energies. We choose as reference the numbers in [15], where the most significant digits are given. For a given width r^{box} of the box potential we initially determine its depth V^{box} so that only the lowest resonance position E_1 matches the value in [15]. The higher-lying levels are then obtained by solving the coupled-channel equations (1) for the three closed channels. This yields the energies E_n and hence the ratios R_n as functions of r^{box} . The results obtained with the assumption of degenerate thresholds are shown as dashed lines in Fig. 2. The ratio R_1 derived from [15] is 23.41, which is somewhat larger than the limiting value 17.43, showing that the short-range part of the electron-hydrogen interaction has a substantial influence on the level ratio for the lowest two states of the series. We reproduce the lowest two energies by choosing $r^{\text{box}} = 13.36a_B$ and $V^{\text{box}} = 0.053874$ Ry, or $r^{\text{box}} = 14.25a_B$ and $V^{\text{box}} = 0.053813$ Ry. The inclusion of the quadrupole term in Eq. (2) is essential for reproducing the comparatively

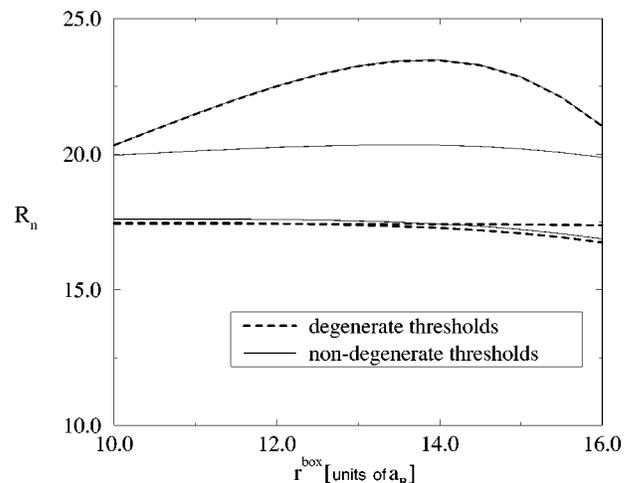


FIG. 2. Level ratios R_n in H^- as functions of r^{box} . Dashed and solid lines from top to bottom denote R_1, R_3, R_2 with degenerate and nondegenerate thresholds, respectively.

TABLE I. Energies of electron-hydrogen $J^\pi=0^+$ resonances from a closed channel calculation including fine-structure splitting and the Lamb shift. The left and right halves of the table correspond to the two sets of model parameters (see the text for values) reproducing the lowest two energies in [15]. (The energies are given relative to the unperturbed $N=2$ state in the hydrogen atom. The level ratios are, of course, calculated using the correct $2P_{1/2}$ threshold at -4.16×10^{-6} Ry.)

n	$-E_n$ (Ry)	R_n	$-E_n$ (Ry)	R_n
1	4.7579×10^{-2}	23.41	4.7579×10^{-2}	23.41
2	2.0361×10^{-3}	17.51	2.0361×10^{-3}	17.39
3	1.202×10^{-4}	20.36	1.210×10^{-4}	20.32
4	9.86×10^{-6}		9.91×10^{-6}	

large value of R_1 ; if only the dipole part of the long-range potential is included, the maximum value obtainable for R_1 in this model is about 20.

If we include the fine-structure splitting that lifts the $2P_{3/2}$ threshold 3.33×10^{-6} Ry above the $2P_{1/2}$ threshold, but assume for the time being that the $2S_{1/2}$ and $2P_{1/2}$ thresholds are still degenerate, then the asymptotic dipole potential is determined by the eigenvalues of the 2×2 submatrix of \mathbf{W}^D [Eq. (5)],

$$\mathbf{W}_{S_{1/2}P_{1/2}} = \begin{pmatrix} 0 & 2\sqrt{3} \\ 2\sqrt{3} & 2 \end{pmatrix}. \quad (6)$$

Its eigenvalues are $1 \pm \sqrt{13}$ and the eigenvalue $1 - \sqrt{13}$ fulfills the condition ($< -1/4$) for supporting a dipole series, but the corresponding limiting value of the level ratio is now $\tilde{R} = 59.971$. We thus expect level ratios close to $R \approx 17.43$ for low-lying states, for which the $N=2$ thresholds are effectively degenerate, whereas the ratio should be enhanced and approach $\tilde{R} \approx 59.97$ for high-lying states for which only the residual degeneracy of the $S_{1/2}$ and the $P_{1/2}$ thresholds contributes to an attractive dipole potential.

Finally, the series is truncated because of $S_{1/2}P_{1/2}$ splitting, essentially due to the Lamb shift by which the $S_{1/2}$ threshold is moved upward in energy by 0.32×10^{-6} Ry. Solving the coupled-channel equations now yields exactly four states; their energies are given in Table I for the two model potentials reproducing the energies of the two reference states. All higher states are shifted above the $P_{1/2}$ threshold and therefore disappear out of the series. The behavior of the level ratios R_n allows us to identify three different regimes of the dipole series. The ratio $R_1 = 23.41$ of the lowest two levels is strongly affected by the short-range potential, whereas the ratio $R_2 = 17.39$ (or 17.51) is already quite close to the asymptotic value 17.43 of an ideal dipole series. The enhanced ratio $R_3 = 20.3$ is due to beginning influence of the fine-structure splitting.

We performed various checks to confirm the reliability of the results in Table I. The sensitivity to model assumptions can be checked by studying the dependence of the level ratios on the potential parameter r^{box} as illustrated in Fig. 2. The ratio R_1 is unaffected by the threshold splitting, so the available results of various *ab initio* calculations based on degenerate thresholds can be assumed to be accurate for the

lowest two levels. Threshold splitting has a noticeable effect on R_2 and a dramatic effect on R_3 . However, the dependence of R_2 and R_3 on r^{box} is very weak, in particular if we restrict r^{box} to values between $13.3a_B$ and $14.3a_B$ yielding realistic values of R_1 . Thus we can conclude that the effect of threshold splitting on the ratios R_2 and R_3 does not depend crucially on the model assumptions. The reliability of the model calculation can also be confirmed by comparing the results obtained in the approximation of degenerate thresholds with recent extensive numerical calculations using the same approximation. Matching to the lowest two levels of a recent complex rotation calculation [9], we obtain for the third level $E_3 = -1.175 \times 10^{-4}$ Ry or $E_3 = -1.187 \times 10^{-4}$ Ry, depending on the choice of r^{box} . This compares favorably with the value $E_3 = -1.158 \times 10^{-4}$ Ry calculated in [9].

In order to study the effect of coupling to the open $1S_{1/2}$ channel, we performed a scattering phase shift calculation including this channel. We also used a two-parameter box potential in the asymptotic dipole representation to describe the short-range part of the coupling of this channel to the closed channels. We chose various box radii r^{open} and adjusted the depth in such a way that not only the energies of the two lowest-lying states but also the width of the lowest resonance agreed with the value in [15]. For values of r^{open} varying between $0.1a_B$ and $15.125a_B$ we obtained resonance positions between -1.185×10^{-4} Ry and -1.21×10^{-4} Ry for E_3 and between -9.75×10^{-6} Ry and -9.91×10^{-6} Ry for E_4 . We therefore estimate that including the open channel will affect our prediction of the energy levels E_3 and E_4 by no more than 2%.

It is worth commenting also on the effect of assuming infinite proton mass. It has recently been argued [17] that finite mass effects will result in a shift of the $1S^e$ resonance levels by about 5 meV relative to the $N=1$ threshold. This shift is readily explained as a reduced mass effect since taking into account the finite proton mass by the substitution $\mathcal{R} = \mathcal{R}_\infty / (1 + m_e/m_p) \approx \mathcal{R}_\infty (1 - m_e/m_p)$ shifts the $N=1$ threshold up by about 7.4 meV and the $N=2$ threshold up by about 1.85 meV relative to the ionization threshold of hydrogen, so that their difference is comparable to the 5-meV effect. Since our calculation yields resonance energies relative to the $2P_{1/2}$ threshold the reduced mass effect is only about 0.05% of these small energies and therefore negligible. Consideration of the above uncertainties leads us to expect that the energies of the third and fourth states listed in Table I are accurate to within a few percent.

The positron-hydrogen system is similar in many ways to the electron-hydrogen system, especially at large distances of the positron, but there are important differences [18]. The short-range part of the positron-hydrogen interaction is free of exchange effects, but it is influenced by the positronium rearrangement channels [19].

We focus again on the dipole series with total angular momentum $J=0$ and parity $\pi=+1$ corresponding to the $1S^e$ series below the $N=2$ threshold. The electron-positron interaction is attractive, so the nondiagonal elements of \mathbf{W}^D and the elements of \mathbf{W}^Q in Eq. (5) now change sign; this does not affect the eigenvalues of \mathbf{W}^D describing the leading asymptotic dipole potential.

Reference energies for the lowest two states are taken from the recent calculation of Gien [8], which is of very high

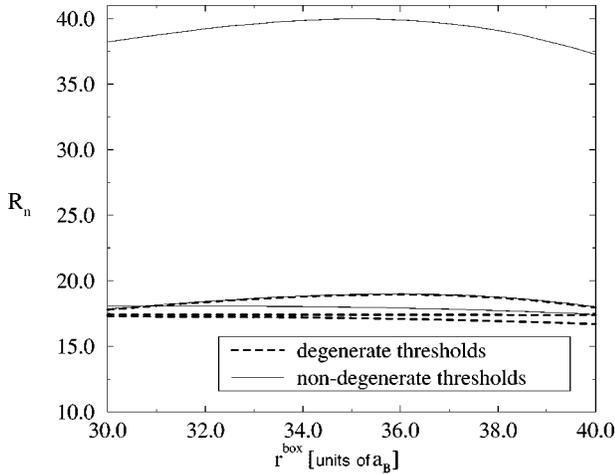


FIG. 3. Level ratios R_n in the positron-hydrogen system as functions of r^{box} . Dashed lines from top to bottom denote R_1, R_3, R_2 with degenerate thresholds; solid lines from top to bottom denote R_3, R_1, R_2 with nondegenerate thresholds.

precision and identifies more resonances (in the degenerate threshold case) than any other work to date. Using the same model box potential as in the electron-hydrogen case we solve the coupled channel equations (1) for various box radii r^{box} with the box depth adjusted to reproduce the energy of the lowest state. The resulting values of the level ratios R_1, R_2 , and R_3 in the degenerate threshold approximation are shown as dashed lines in Fig. 3. Note that the maximum value of R_1 attainable within this model is now only near 19.0, which is consistent with the ratio derived from the lowest two levels in [8]. The lowest two energies in [8] are reproduced for $r^{\text{box}} = 36.0a_B$ and $V^{\text{box}} = 0.00737$ Ry, corresponding to a much wider and shallower short-range part of the potential than in the electron-hydrogen case. With these parameter values, solution of the coupled equations for the three closed channels below the $N=2$ threshold, including threshold splitting due to the fine structure and the Lamb shift, again yields a total of four $^1S^e$ states; their energies and level ratios are listed in Table II. Again, there are three qualitatively different regimes characterized by different values of the level ratio. R_1 is affected noticeably by the short-range part of the potential, much less however, than in the electron-hydrogen case; R_2 is again quite close to the

TABLE II. Energies of positron-hydrogen $J=0, \pi=+1$ resonances from a closed channel calculation including fine-structure splitting and the Lamb shift. The potential parameters are adjusted to reproduce the lowest two energies in [8]. (The energies are given relative to the unperturbed $N=2$ state in the hydrogen atom. The level ratios are, of course, calculated using the correct $2P_{1/2}$ threshold at -4.16×10^{-6} Ry.)

n	$-E_n$ (Ry)	R_n
1	7.243×10^{-3}	19.0
2	3.85×10^{-4}	17.9
3	2.54×10^{-5}	40.0
4	4.69×10^{-6}	

asymptotic ratio 17.4 for the ideal dipole series. Finally, R_3 is enhanced substantially as a consequence of threshold splitting because the fourth state is already very close to the $2P_{1/2}$ threshold at -4.16×10^{-6} Ry; the fourth state is in fact bound by only 0.53×10^{-6} Ry, corresponding to about $7 \mu\text{eV}$.

In Fig. 3 we see that the level ratio R_1 involving the lowest two states is essentially unaffected by threshold splitting, while the ratio R_2 is affected noticeably and R_3 dramatically. The comparatively weak dependence of the level ratios R_2 and R_3 on the box size, in particular when it is restricted to values giving a realistic value for R_1 , gives us confidence that the predicted energy levels do not depend sensitively on the model assumptions. Note that the ratio R_3 would have to become infinite for the fourth state of the series to be pushed above the $2P_{1/2}$ threshold. The reliability of the model calculations is also supported by comparing the results we obtain in the approximation of degenerate thresholds with the results of [8]. For two different choices of r^{box} (viz., $34.1a_B$ and $37.5a_B$) we obtain the energy of the third state at -2.24×10^{-5} and -2.27×10^{-5} Ry, respectively, which compares very favorably with the value -2.2×10^{-5} Ry given in [8].

We have thus presented a quantitative analysis of how threshold splitting due to fine-structure and radiative corrections modifies and terminates dipole series of resonant states in the electron-hydrogen and the positron-hydrogen systems. For the $^1S^e$ series below the $N=2$ threshold we predict in each case a total of four states with energies given in Tables I and II, respectively.

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