# Resonances in Proton-Hydrogen and Positron-Hydrogen Scattering*

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The problems of resonances in proton-hydrogen and positron-hydrogen scattering are studied. For proton-hydrogen scattering, resonances are predicted at energies just below each of the excitation thresholds. Infinite sequences of resonances are found just as in the electron-scattering case, but the widths are much narrower and these resonances are not presently observable. The positron-hydrogen scattering problem exhibits infinite sequences of resonances just below excitation thresholds, similar to the electron scattering problem. Infinite sequences are also exhibited just below the thresholds for forming excited positronium.

## I. INTRODUCTION

IN previous papers O'Malley and Geltman[1] and Temkin and Walker[2] used the projection-operator formalism of Feshbach[3] to obtain the lowest few resonances in electron-hydrogen scattering. Burke and later Mittleman[4] extended the method to multichannel resonances just below the higher thresholds. In this note we apply the same method to the problems of proton-hydrogen and positron-hydrogen scattering. The spacing formula relating the "resonance" positions below the $N$th state, $\epsilon_{j+1}(N)/\epsilon_j(N)$, are determined. Infinite sequences of resonances are found in both cases. For the proton problem, the resonances lie much closer together. For the positron problem, the spacing formulas are found as for the electron problem but in addition other sequences are found below the excited positronium thresholds. In the next section the proton-hydrogen problem is treated. The positron-hydrogen problem is dealt with in Sec. III.

## II. PROTON-HYDROGEN SCATTERING RESONANCES

The method of Feshbach[3] requires the construction of a projection operator which projects out of the total wave function all the open continuum states below the resonance in question. We first deal with the problem where only elastic scattering is possible.

The total Hamiltonian is

$$\mathcal{H} = -\frac{1}{M}\nabla_R^2 - \frac{1}{2\mu}\nabla_x^2 - \frac{e^2}{|x-R/2|} - \frac{e^2}{|x+R/2|} + \frac{e^2}{R}, \quad (1)$$

$$\mu = 2Mm/(2M+m),$$

where $R$ is the inter-proton coordinate and $x$ is the coordinate of the electron relative to the center of mass of the two protons. The Hamiltonian is symmetric

under interchange of the protons, $R \to -R$, so that the total wave function may be decomposed into parts even and odd under this interchange.

$$\psi^\pm(x,R) = \pm\psi^\pm(x, -R). \quad (2)$$

The asymptotic form of the incident wave for scattering off the ground state is

$$\psi_{in}^\pm = \phi_{1s}(x-R/2)e^{ip_0\cdot(R+\alpha x)}$$
$$\pm \phi_{1s}(x+R/2)e^{-ip_0\cdot(R-\alpha x)}, \quad (3)$$

where $\alpha = 2m/(2M+m) \ll 1$. We shall be interested in center-of-mass energies up to the ionization threshold so that $p_0\alpha x$ is always small compared to unity. Thus, the $x$ dependence in the exponents of (3) can always be dropped. We therefore seek a projection operator $P$ such that $P\psi^\pm$ has the form

$$P\psi^\pm = \phi_{1s}(x-R/2)F_\pm(R) \pm \phi_{1s}(x+R/2)F_\pm(-R). \quad (4)$$

It may easily be shown that

$$P = \frac{\delta(R-R')}{1-S_{1s,1s}^2(R)}\{\phi_{1s}(x-R/2)\phi_{1s}(x'-R/2)$$
$$+ \phi_{1s}(x+R/2)\phi_{1s}(x'+R/2)$$
$$- S_{1s,1s}(R)\phi_{1s}(x-R/2)\phi_{1s}(x'+R/2)$$
$$- S_{1s,1s}(R)\phi_{1s}(x+R/2)\phi_{1s}(x'-R/2)\} \quad (5)$$

is such an operator, where the real function $S$ is given by

$$S_{1s,1s}(R) = \int d^3x\, \phi_{1s}(x-R/2)\phi_{1s}(x+R/2). \quad (6)$$

The zero-order positions of the resonances[1] are given by the eigenvalues of the operator $QHQ$, where $Q = 1-P$, which lie below the $n=2$ threshold. An upper bound to the eigenvalues can be obtained by using $QHQ$ in the Kohn variational principle. The trial function which we chose is

$$(Q\Phi)_l = \sum_{l_1 m_1 l_2 m_2} \{\phi_{2l_1 m_1}(x-R/2)Y_{l_2 m_2}(\hat{R})$$
$$\pm \phi_{2l_1 m_1}(x+R/2)Y_{l_2 m_2}(-\hat{R})\}$$
$$\times u_{l_2}^{(\pm)}(R)\langle l_1 m_1 l_2 m_2 | LM_{l_1} l_2\rangle, \quad (7)$$

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[1] T. F. O'Malley and S. Geltman, Phys. Rev. **137**, A1344 (1965).
[2] A. Temkin and J. F. Walker, Phys. Rev. **140**, A1520 (1965).
[3] H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).
[4] P. G. Burke, Advan. Phys. **14**, 521 (1965); M. H. Mittleman, Phys. Rev. **147**, 73 (1966).

where the last factor is the usual vector addition coefficient making this an explicit eigenfunction of the total angular momentum and its $Z$ component. As in Ref. 4, we vary with respect to the functions $u_l^\pm$. The resulting equations are rather complicated, but for large $R$ the overlap terms between the functions $\phi(\mathbf{x}-\mathbf{R}/2)$ and $\phi(\mathbf{x}+\mathbf{R}/2)$ may be dropped since they behave exponentially with $R$. The resulting equations are similar to those of Ref. 4. In rydberg units the equations are

$$\left[-\frac{1}{M}\left(\frac{d^2}{dR^2}-\frac{l(l+1)}{R^2}\right)+\epsilon\right]u_l$$

$$=\sum_{l'}\left[\frac{1}{2M}\mathbf{d}_{ll'}\cdot\nabla_R+\frac{2}{R^2}A_{ll'}{}^{LM}\right]u_{l'}(R),\quad(8)$$

where the distinction between $(\pm)$ may now be dropped. The vector $\mathbf{d}_{ll'}$ contains the vector addition coefficients and is proportional to the matrix element $\langle\phi_{2lm}(x)\nabla_x\phi_{2l'm'}(x)\rangle$ which may easily be shown to vanish by use of the relation

$$\nabla=i\mathbf{p}=-m[H,\mathbf{r}].$$

The eigenvalue $\epsilon$ is now the energy in rydbergs of the resonance below the $n=2$ threshold and $M$ is the proton mass in units of the electron mass, $M\gg1$. Equation (8) may be written

$$\left[\frac{d^2}{dR^2}-\epsilon M\right]u_l=\frac{1}{R^2}\sum_{l'}B_{ll'}{}^{LM}(2)u_{l'},\quad(9)$$

where

$$B_{ll'}{}^{LM}(2)=l(l+1)\delta_{ll'}+2MA_{ll'}{}^{LM}(2),\quad(10)$$

where $A_{ll'}{}^{LM}$ is identical with the analogous matrix occurring in the electron-hydrogen scattering problem.[4] For $S$-wave scattering, the only surviving elements are

$$A_{l,l+1}{}^{0,0}(n)=A_{l+1,l}{}^{00}(n)=\frac{3n}{2}(l+1)\left[\frac{n^2-(l+1)^2}{4(l+1)^2-1}\right]^{1/2}.\quad(11)$$

The matrix $B$ may be diagonalized and the equations (9) decoupled. For positive eigenvalues of $B$ the diagonalized potential in (9) is repulsive and no negative energy (positive $\epsilon$) eigenvalues exist. For negative eigenvalues $b_j(n)$ there are an infinity of negative-energy eigenvalues[5] $\epsilon_s{}^j(n)$ which obey the spacing formula[2]

$$\epsilon_{s+1}{}^j(n)/\epsilon_s{}^j(n)=e^{2\pi/\alpha_j(n)},\quad\alpha_j(n)=[\,|b_j(n)|-\tfrac{1}{4}]^{1/2}.\quad(12)$$

For $n=2$ there is one negative eigenvalue $b$ which is

$$b(2)=-6M[1+O(1/M)]\quad(13)$$

then $\alpha\simeq(6M)^{1/2}\simeq105$, which results in

$$\epsilon_{s+1}{}^j(2)/\epsilon_s{}^j(2)=1+\frac{2\pi}{(6M)^{1/2}}+\cdots.\quad(14)$$

Thus, the proton-hydrogen and electron-hydrogen problems have similar resonance structures but in the former the resonances are much more closely spaced. The result (14) is for the unshifted resonance. The shift may actually raise these values above the $n=2$ energy level, in which case these would no longer be resonances.[1]

We may also expect that the widths of the resonances are much narrower for the proton problem. The width is given by

$$\Gamma=2\pi\,|\langle\Psi'PHQ\Phi\rangle|^2,\quad(15)$$

where $Q\Phi$ is the eigenfunction of $QHQ$ and the precise definition of $\Psi'$ is given in Ref. 1. (Our normalization of $\Psi'$ is the usual one, a unit amplitude plane wave at infinity, which accounts for the difference of (15) and the definition given in Ref. 1.) $\Psi'$ is roughly the scattering function averaged over the resonance. The fact that the proton mass is so large will make $\Psi'$ oscillate more rapidly in the proton case than the electron case. This will result in a reduction of at least $M^{-1/2}$ for the matrix element in (15) so that the resonance will be at least of the order $M^{-1}$ narrower for protons. This is well beyond the limits of present observation.

For resonances below the higher thresholds the projection operator (5) becomes much more complicated; additional overlap terms $S_{n,n'}$ are introduced. However, this will not enter in the large $R$ limit and just as in the electron case we arrive at Eq. (9) where the definition (11) applies. As in the electron case,[4] multiple sequences of resonances arise. To lowest order in $M^{-1}$ the negative eigenvalues of $B$ are given by $b(3)=-9M$, $b_1(4)=-6M$, $b_2(4)=-18M$. Thus, just as in the electron case, multiple sequences of resonances appear for $n\ge4$.

## III. POSITRON-HYDROGEN SCATTERING RESONANCES

The projection operator for this problem is more complicated because of the positronium channels. However, forms have been given by Mittleman,[6] and Chen and Mittleman[7] which will project out the open channels. The former seems simplest here. It is given by

$$P=\phi_{1s}(r_2)\left[\delta(\mathbf{r}_1-\mathbf{r}_1')+\sum_\lambda\frac{u_\lambda(r_1)u_\lambda}{\lambda^2-1}{}^*(r_1')\right]\phi_{1s}(r_2')$$

$$+\chi_{1s}(r)\left[\delta(\mathbf{R}-\mathbf{R})+\sum_\lambda\frac{v_\lambda(R)v_\lambda}{\lambda^2-1}{}^*(R')\right]\chi_{1s}(r')$$

$$+\sum_\lambda\frac{\lambda}{\lambda^2-1}[\phi_{1s}(r_2)u_\lambda(r_1)v_\lambda{}^*(R')\chi_{1s}(r')$$

$$+\chi_{1s}(r)v_\lambda(R)u_\lambda{}^*(r_1')\phi_{1s}(r_2')],\quad(16)$$

[5] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Press, London, 1958), p. 118 *et seq.*

[6] M. H. Mittleman, Ann. Phys. (N.Y.) **28**, 43 (1964).
[7] J. C. Y. Chen and M. H. Mittleman, Ann. Phys. (N.Y.) **37**, 269 (1966).

where $\chi_{1s}$ is the ground state of positronium. Here $r_2$ is the electron and $r_1$ the positron coordinate, both taken relative to the infinitely heavy proton. They are given in terms of the alternative coordinates by

$$r_1 = R + r/2,$$
$$r_2 = R - r/2. \qquad (17)$$

The functions $u_\lambda$ and $v_\lambda$ satisfy a homogeneous integral equation[6] with eigenvalue $\lambda$. Their only property which is relevant here is that they vanish exponentially as their argument becomes large. The projection operator given by (16) projects out the ground state of hydrogen and the ground state of positronium. It may be used to investigate the resonance structure just below the $n=2$ level of hydrogen.

As a trial function for minimizing $QHQ$ we chose

$$(Q\Phi)_t = \sum_{l_1 m_1 l_2 m_2} \phi_{2l_1 m_1}(r_2) u_{l_2}(r_1) \frac{1}{r_1} Y_{l_2 m_2}(\hat{r}_1)$$

$$\times \langle l_1 m_1 l_2 m_2 | L M l_1 l_2 \rangle. \qquad (18)$$

The variation with respect to $u_l$ yields a complicated equation but again for $r_1 \to \infty$ the equation simplifies. The terms with $u_\lambda$ and $v_\lambda$ drop out as do the overlap of hydrogen and positronium wave functions. The resulting equation is identical with that for electron hydrogen scattering except that the sign of $A_{ll'}$ is changed. This does not affect the eigenvalues of the matrix $B_{ll'}$ so the resonance spacing formula is the same as for the electron-hydrogen case. This, of course, does not mean that the resonances fall at the same positions. It is easily shown that the positron resonance spacing formula below the high $n$ thresholds is also identical with that obtained in the electron scattering case.

We may also investigate the regions below the positronium formation thresholds. The projection operator is much more complicated than (16) when higher states of hydrogen and positronium are included but again in the limit of large $R$ (i.e., when the positronium atom is far from the proton) great simplification results. In effect, the projection operator becomes

$$P = \delta(R - R') \sum_n \chi_n(r) \chi_n^*(r'), \qquad (19)$$

where the sum runs over all the open positronium channels. Then a suitable trial function for the energy region below the $n$th level of positronium is

$$(Q\Phi)_t = \sum_{l_1 m_1 l_2 m_2} \chi_{n l_1 m_1}(r) u_{l_2}(R) \frac{1}{R} Y_{l_2 m_2}(\hat{R})$$

$$\times \langle l_1 m_1 l_2 m_2 | L M l_1 l_2 \rangle. \qquad (20)$$

Again minimization of $\langle QHQ \rangle$ with respect $u_l$ yields an equation which for large $R$ becomes

$$\left( \frac{d^2}{dR^2} - 2\epsilon \right) u_l = \frac{1}{R^2} \sum_{l'} B_{ll'}{}^{LM}(n) u_{l'}, \qquad (21)$$

where now

$$B_{ll'}{}^{LM}(n) = l(l+1)\delta_{ll'} + 8 A_{ll'}{}^{LM}(n), \qquad (22)$$

where the matrix $A$ is identical with the electron hydrogen case. For $L=0$ it is given by (11). This relation to the electron matrix element is obtained from the scaling relation

$$\chi_n(r) = (1/\sqrt{8}) \phi_n(r/2). \qquad (23)$$

The factor of 8 in front of $A$ in (22) results from the mass of positronium $(2m)$ and the fact that the dipole matrix element of positronium is twice as large as that for hydrogen. The parameter $b(n)$ which enters in the spacing formula (12) is again obtained from the negative eigenvalues of $B_{ll'}$. For $n=2$ the negative eigenvalue is $b(2) = -[(1 + (24)^2)^{1/2} - 1] \simeq 23$. For $n=3$ the equation determining the eigenvalues is $b^3 - 8b^2 - 5172b + (144)^2 = 0$ which has one negative root $b(3) \simeq -70$.

These results depend on the existence of degenerate eigenfunctions of different angular momenta. So there are no resonances of this sort below the $n=1$ positronium formation threshold. A resonance in this energy region may exist but this must be explored by detailed numerical calculation.[8]

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[8] Such a calculation is presently in progress, A. Temkin and A. K. Bhatia (private communication).