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ELECTRON-HYDROGEN PHASE SHIFTS JUST BELOW THE INELASTIC THRESHOLD

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SUMMARY

The singlet S-wave phase shifts for the scattering of electrons by atomic hydrogen just below the inelastic threshold (10.2 ev) are calculated by using a recently developed nonadiabatic theory. Previous calculations of Burke and Schey based on the much more restricted close-coupling approximation yielded a resonance characterized by the phase shift going through π radians. In view of a theorem of Wigner and a calculation of Holøien this result is indicative of a bound state of the compound system near the energy 9.4 ev. It is argued on the basis of a previous calculation that this resonance must be distinct from another resonance near 10.1 ev. And on this basis it is concluded that this partial cross-section must exhibit two resonances below threshold.

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INTRODUCTION

Burke and Schey (Reference 1) have recently calculated a resonance in the elastic scattering of electrons by atomic hydrogen just below the threshold for inelastic scattering (10.203 ev). The basis of their calculation was the close-coupling approximation with 1s-2s-2p states. The nomenclature refers to hydrogenic states, each of which is multiplied by an initially undetermined function. For S-wave† scattering, their wave function can be written:

$$r_1 r_2 \Psi_{cc} = \left[u(r_1) R_{1s}(r_2) + v(r_1) R_{2s}(r_2) + (1 \rightleftarrows 2)\right] P_0(\cos\theta_{12})$$

$$+ \sqrt{3}\left[w(r_1) R_{2p}(r_2) + (1 \rightleftarrows 2)\right] P_1(\cos\theta_{12}) , \tag{1}$$

where $R_{nl}(r)$ is r times the nl radial wave function of hydrogen. It is clear from Equation 1 that this function is approximate in two ways. First, it contains only 2 of an infinite number of *relative* angular momenta $P_l(\cos\theta_{12})$. Second, the "coefficients" of the included P_l have a comparatively restricted form (which, however, is manifestly symmetric with respect to the interchange of 1 and 2 corresponding to the necessary symmetry of singlet scattering, with which we shall here be concerned).

Clearly the most general function containing P_0 and P_1 can be written:

$$r_1 r_2 \Psi = \Phi_0(r_1 r_2) P_0(\cos\theta_{12}) + \sqrt{3}\, \Phi_1(r_1 r_2) P_1(\cos\theta_{12}) , \tag{2}$$

where the two-dimensional functions Φ_0 and Φ_1 are required to have the correct symmetry. Substitution of Equation 2 into the variational principle, $\delta \int \Psi^* (H - E) \Psi \, d\tau = 0$, yields the following coupled set

†Letters referring to angular momentum states are capitalized when the total angular momentum state (partial wave) is being considered. Lower case l refers to the relative angular momentum within a given total angular momentum state.

of partial differential equations* in the region $r_1 \geq r_2$ with appropriate boundary conditions (References 2 and 3):

$$\left(\Delta_{12} + \frac{2}{r_2} + E\right) \Phi_0 = \frac{2r_2}{\sqrt{3}\, r_1^2} \Phi_1 , \tag{3a}$$

$$\left[\Delta_{12} - 2\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) + \frac{2}{r_2} - \frac{4r_2^2}{5r_1^2} + E\right] \Phi_1 = \frac{2r_2}{\sqrt{3}\, r_1^2} \Phi_0 . \tag{3b}$$

It is the object of the present nonadiabatic theory (References 2 and 3) to identify and directly attack these partial differential equations, and thus avoid the second category of approximation implicit in the close-coupling method. The purpose of this note is to report on results of calculations on the lowest order approximation of the equations and to give some speculations concerning the next higher correction.

The lowest order approximation is the so-called zeroth order problem and is given by the equation:

$$\left(\Delta_{12} + \frac{2}{r_2} + E\right) \Phi_0^{(0)} = 0 . \tag{4}$$

For future reference note that this basic relation can be derived:

$$\sin\left(\delta_{(1)} - \delta_0\right) = \frac{-2}{k\sqrt{3}} \int_0^\infty dr_1 \int_0^{r_1} dr_2\, \Phi_0^{(0)} \frac{r_2}{r_1^2} \Phi_1 , \tag{5}$$

where δ_0 is the phase shift of Equation 4, and $\delta_{(1)}$ is the phase shift of Equations 3.

In practice, Equation 4 has been solved by expanding in exact separable solutions (Reference 3), the program for which has been extended to double precision arithmetic (16 significant figures). For this discussion the resultant values for $\Phi_0^{(0)}$ and δ_0 can be considered correct to the significance given in Table 1. A close-coupling approximation of Equation 4 gives results in good accord with δ_0 (Reference 4).

CONJECTURES ON THE SOLUTION OF EQUATIONS 3†

An obvious first step in an iterative attempt to solve Equations 3 would be to use the $\Phi_0^{(0)}$ in the right-hand side of Equation 3b to get an approximate Φ_1 which we can call $\Phi_1^{(0)}$:

$$\left[\Delta_{12} - 2\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) + \frac{2}{r_2} - \frac{4r_2^2}{5r_1^3} + E\right] \Phi_1^{(0)} = \frac{2r_2}{\sqrt{3}\, r_1^2} \Phi_0^{(0)} . \tag{6}$$

*Energy is in rydbergs (1 ryd = 13.605 ev) and length is in Bohr radii.

†The quantitative speculations of this section are quite different from what was calculated in Reference 5. The author is particularly indebted to Dr. T. F. O'Malley for pointing out the usual increase of π of phase shifts at resonances and the analytical derivation of this behavior for some simple nonlocal potentials. This discussion led, directly, to a re-examination of δ_0 (Reference 5) and the discovery that it does indeed go through π. Dr. O'Malley also brought Reference 6 to the author's attention.

This neglects the coupling of Φ_0 to Φ_1 (but not the reverse). Figure 1 gives the close-coupling results, labeled δ_{cc}, as well as the results for δ_0. A possible explanation for the shift in energy at which the resonance in δ_{cc} occurs as compared with δ_0 is that it is due to the coupling of Φ_0 to Φ_1, which is included in some approximate way in the close-coupling approximation. However, the previous calculation (Reference 5) was based on the assumption that all resonances arise directly from the resonance in $\Phi_0^{(0)}$. The calculated results give absolutely no indication of such a shift. The reason for taking the close coupling seriously is explained below. If it is assumed that there must be a resonance at or below the energy corresponding to the close-coupling resonance, a more plausible explanation of the lower resonance would seem to be that it is due to a resonance (change in sign) of Φ_1 in Equation 3b which is fairly independent of the right-hand side.* If this is so then a resonance very close to $k = 0.84$ should also come from Equation 6. Hopefully, solutions of this equation will be obtained by using a noniterative numerical technique for solving partial differential equations (Reference 7). As another test of this hypothesis a close-coupling expansion with only 1s-2p states would also be expected to show a resonance near the lower energy.†

Table 1

Zeroth Order Phases Shifts Below Threshold.

$k\,(\mathrm{ryd}^{1/2})$	k^2 (impacting energy in ev)	δ_0 (radians)
0.85	9.830	0.721
0.855	9.944	0.729
0.860	10.061	0.7545
0.861	10.085	0.768
0.862	10.108	0.793
0.863	10.132	0.853
0.864	10.155	1.25
0.8645	10.169	3.14
0.865	10.180	3.628
0.8656	10.194	3.738
0.866	10.203	3.781

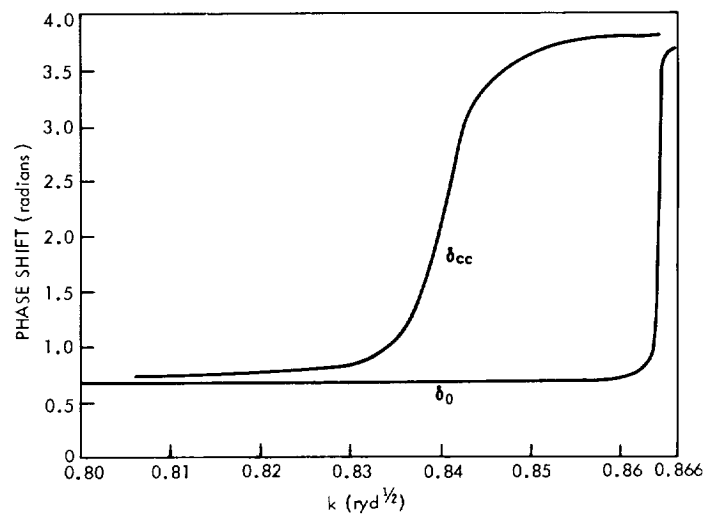

Figure 1—The 1s-2s-2p close-coupling phase shift (δ_{cc}) and δ_0 as a function of k.

Mathematically a resonance in $\Phi_1^{(0)}$ manifests itself in $\delta_1^{(0)}$, the first approximation of $\delta_{(1)}$, whereby in the expression

$$\sin\left(\delta_1^{(0)} - \delta_0\right) = \frac{-2}{k\sqrt{3}}\int_0^\infty dr_1 \int_0^{r_1} dr_2\, \Phi_0^{(0)} \frac{r_2}{r_1^2}\, \Phi_1^{(0)}\,, \tag{7}$$

*Mr. John Cooper pointed out the importance of the energy shift of the lower resonance.

†Schey and Burke are now examining this point.

a change in sign of $\Phi_1^{(0)}$ would mean a change in sign of the integral, since $\Phi_0^{(0)}$ is varying very slowly at the lower energy. This *could* (see below) mean an increase of $\delta_1^{(0)}$ by π which would be the mathematical statement of the resonance.

Along this mathematical line, it might be expected that as the energy increases toward k = 0.8645, $\Phi_0^{(0)}$ would undergo a change of sign and that there the integral would again change sign, corresponding to an increase of δ_0 into the same quadrant as $\delta_1^{(0)}$. This would be in accord with $\delta_1^{(0)}$ exhibiting only one increase of π corresponding precisely to what Burke and Schey calculated. *However,* here Equation 6 must be considered more carefully; it has been presumed to have a resonance due to the structure of the left-hand side at the lower energy. At the higher energy, however, the right-hand side has been shown here to exhibit a resonance and this could cause a second resonance in $\Phi_1^{(0)}$. Mathematically, this would mean that at the same energy at which $\Phi_0^{(0)}$ undergoes a change of sign $\Phi_1^{(0)}$ undergoes a second change in sign. Thus, the integral on the right-hand side of Equation 7 undergoes no change of sign because of the simultaneous changes in sign of $\Phi_0^{(0)}$ and $\Phi_1^{(0)}$. This could correspond to a second increase of $\delta_1^{(0)}$ by π. It is problematical whether or not this second phenomenon will correspond, in fact, to a second increase of the phase shift by π (see below). However, it is quite likely that the phase shift will have a sufficiently uneven behavior to appear in the cross-section as a resonance. (It is only a matter of definition whether a resonance is called a sudden increase of the phase shift by π or a sudden up and down behavior in the cross-section.)

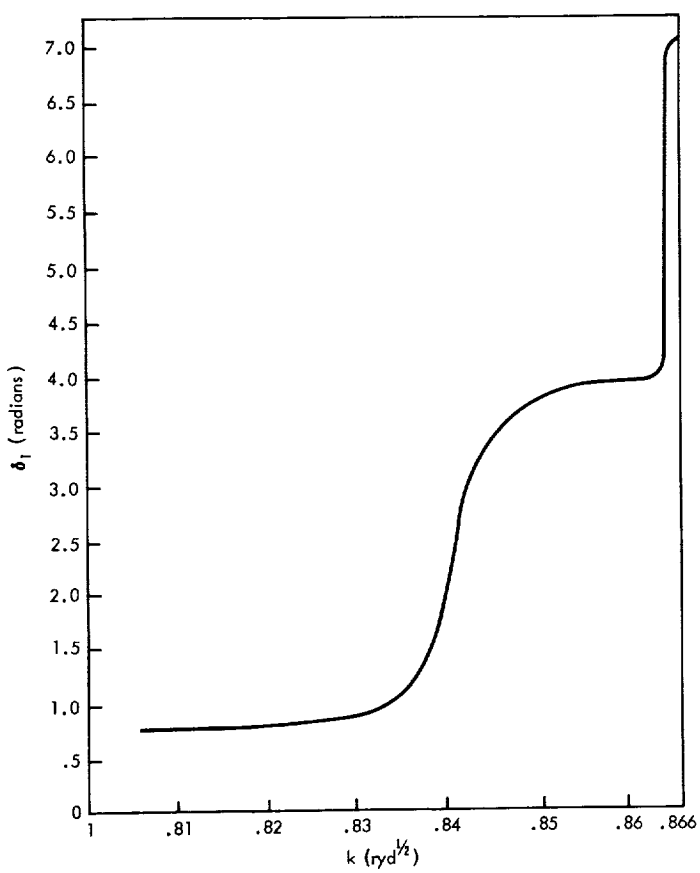

Figure 2—Conjecture of the first order (Equations 3) phase shifts according to the arguments in the text.

In Figure 2 the conjectured behavior of $\delta_1^{(0)}$ showing two increases of π is given. The actual values were gotten by superposing the δ_0 resonance (modulo π) on δ_{cc} at the second resonant energy. In Figure 2 it has been assumed that resonances correspond to increases of the phase shifts by π (in the case of δ_0 this has been calculated to be the case). This is based on a theorem of Wigner and Eisenbud (Reference 6) which says

$$\frac{d\delta}{dk} \geq -R \ .$$

This statement is derived from the fact that $2(d\delta/dk)$ is the delay time of a particle striking a target. Although there is no upper limit on this quantity, its negative value, which is the time advancement of the scattered wave, is optimal if there is a

hard core in the region of interaction. Thus, under any reasonable process of the formation of the compound state corresponding to a sticking of the incoming particle to the atom, the phase shift must exhibit a sharp rise. A calculation by Holøien gives an upper limit of $E = 9.4$ ev on such a state of the compound H^- ion (Reference 8). A more direct argument that there must be a resonance at or below the close-coupling resonance is afforded by theorems on bounds for phase shifts which have recently been proved (Reference 9).* As it applies in the present case it says that $\delta_1 \geq \delta_0$ up to the inelastic threshold.†

Figure 3 shows the plot of the cross-section corresponding to the phase shift curve in Figure 2. This is meant to apply only to the S-wave part of the singlet scattering. In view of the fact that the cross-section contains two resonances, it is felt that the physical reasons for such a behavior which were included in Reference 5 still apply. That argument assumes a correspondence of each state of the target with a state of the compound system (with possible shifts in energy). The main reason for thinking that this correspondence does hold in this case is the large energy difference of the lower resonance from the upper one. The previous calculation (Reference 5) indicates that otherwise this energy shift would be much smaller.

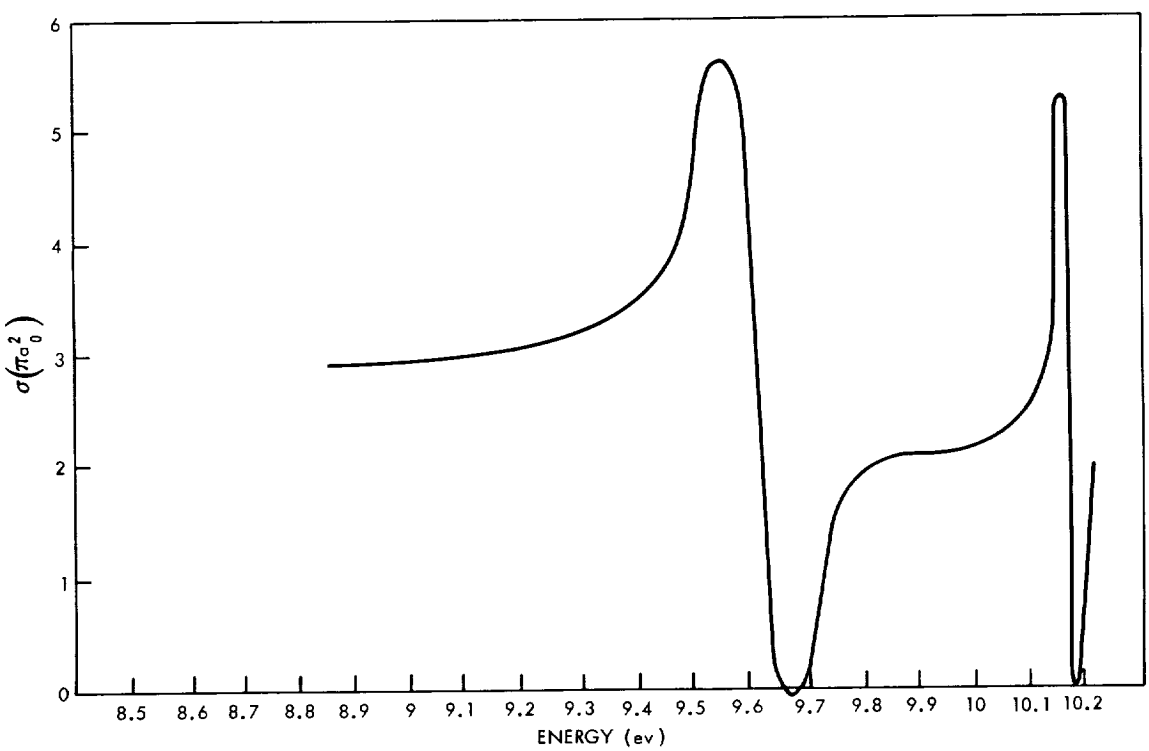

Figure 3—Singlet S-wave cross-section corresponding to the phase shifts in Figure 2. The value a_0 is the Bohr radius.

*Burke and Schey have obtained very narrow resonances (private communication) at low energies (≈ 1 ev), whereas careful calculations by Schwartz (private communication) show no resonances. This is not necessarily a contradiction to the theorem of Hahn, O'Malley, and Spruch (Reference 9), since the numerical method of Burke and Schey may occasionally show some aberrations. However, other logical possibilities, including a contradiction to the theorem in Reference 3, cannot be dismissed at this point.

†Private communication from T. F. O'Malley.

However, the present heuristic considerations give a more explicit indication of what the physical argument means in terms of the nonadiabatic formalism. The $\Phi_0^{(0)}$ equation (4) is the two-dimensional analogue of the one-particle 2s equation. To say that the one-particle 2s equation corresponds to a resonance in the compound system means that the $\Phi_0^{(0)}$ inherently contains zero resonance near the 2s energy. The present calculation for δ_0 explicitly yields this resonance. By the same token the left-hand side of Equation 3b or Equation 6 is a two-particle analogue of the single particle 2p equation; therefore, by the same kind of correspondence, this left-hand side is expected also to contain a spontaneous resonance. It should be emphasized that this latter resonance has not as yet been found in the author's calculations. However, the author believes that Burke and Schey have found it (Reference 1), but that they misinterpreted it to be the shifted $\Phi_0^{(0)}$ resonance. The author further believes that if the 1s-2s-2p close-coupling calculation is extended even closer to the 2s threshold, it will reveal the second resonance. In this context it should be noted that Holøien's calculation gives evidence of two compound states. (Reference 8).

It may be inquired whether or not the higher L equations, of which Equations 3 are the first two, might also reveal spontaneous resonances. They probably do; however, the one-particle target state energies to which they correspond are higher than p states. Therefore, their principal quantum number is $n \geq 3$ and, thus, their energies should be significantly above the $n = 2$ threshold.

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