

THEOREM ON SEPARATION OF COUPLED DIFFERENTIAL EQUATIONS,
RESONANCE EFFECTS AND THRESHOLD BEHAVIOURSMAIL BOUGOUFFA¹, CAO XUAN CHUAN and PAUL FAUCHER*URA 1362du CNRS, Observatoire de la cote d'Azur, B. P. 229, F-06304, Nice Cedex,
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The aim of this work is to show the importance of the theorem on the separation of coupled differential equations in elastic scattering when the electron energy is below the threshold necessary to produce excitation of the state 1 from the ground state 0. We apply a schematical model to study the resonance effects in electron-hydrogen scattering. We are concerned with the behaviour of various cross-sections in the neighbourhood of the threshold of a new mode of scattering in which the electron possesses any quantized angular momentum, and examine the effects of the change in the centrifugal potentials in the case 1s-2s-2p close-coupling approximation. We conclude by discussing the threshold behaviour and its relation to resonance effects.

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1. Introduction

Previously, we studied the energy variations of cross-section of electron collisions with atoms [1]. The features such as the Ramsauer-Townsend effect have been considered [2] and a theoretical description provided, but some effects in the elastic cross-sections as a function of electron energy have not been explained. The sharp peaks observed with high resolution equipment cannot be understood theoretically in the same way and we now consider how they arise in some cases. In particular, there exist some models which can reproduce well the resonance effects for restricted cases, but a global understanding of these resonance effects still needs to be explicated.

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In this paper, we are concerned with the behaviour of the cross-sections in the neighbourhood of the threshold of new modes of collision. The principal interest in such an investigation arises from the theoretical difficulty in resolving the system of coupled differential equations (CDE) which is related to the resonance effects. These difficulties can be overcome using the theorem on the separation of CDE in some particular cases [3].

We introduce the basic theory of the resonance phenomena where we consider the effects arising from the interaction between the discrete and continuum states. The simplest cases of resonance of concern are those that arise in doubly-excited states of H^- and in elastic scattering when the electron energy is below the threshold value necessary to produce excitation.

The analysis can be extended without difficulties to the cases in which the electron possesses any quantized angular momentum. We obtain the oscillations of the cross-sections in the neighbourhood of the threshold by solving the coupled equations quite accurately, no matter how large the coupling potential may be, so that we have means of determining the positions and level widths of the resonances to a much better accuracy.

The results obtained in this work show the importance of the theorem on separation of the coupled differential equations which governs the problem of collision in cases when the angular momentum $l \neq 0$. We conclude by discussing the threshold behaviour and its relation to resonance effects.

2. Accurate calculation of resonance parameters related to coupled equations

The theory mentioned in Ref. [4] is essentially a perturbation treatment in which the interaction between the discrete and continuum states is assumed to be small. For many purposes, this is a valid approximation for electron collisions with atoms, and in any case it seems to bring out clearly the physical principles involved. The most accurate calculation of resonance parameters to date have been made by using a somewhat more direct approach based on the usual expansion of atomic eigenfunctions.

Recently [5], it has been shown that the system of CDE which are involved in the theory of collisions can be made tractable by the method of the decoupling operations which transform the original problem into a chain of subsystems of two coupled equations which are to be solved successively. These partial solutions can then be recombined afterwards by inverse transformation to reconstruct the exact solutions.

For example, consider the scattering of electron by a hydrogen atom. In order to obtain a collision wave function that includes the effects of resonance due to H^- states based on the 2s and 2p states of neutral atom, it seems reasonable to suppose that only the 2s and 2p atomic wave functions need to be included in the expansion of the eigenfunction. We shall assume the following simplifications:

- Ignore the energy degeneracy between the 2s and 2p states.
- Seek only the resonance effects due to H^- states based on the 2s state.
- Assume that the electron energy E_1 is so low that only s-scattering is involved.
- Neglect exchange effects.

The collision wave function is approximated by

$$\Psi = \psi_0(r_2)F_0(r_1) + \psi_1(r_2)F_1(r_1), \quad (1)$$

where ψ_0 and ψ_1 are the respective wave functions of the 1s- and 2s-states of atomic hydrogen. If k is the incident-electron wave number, which is below the threshold value necessary to produce excitation of the 2s state, then the angular momentum is zero in both initial and final states. By writing

$$F_0 = (kr)^{-1}G_0, \quad (2)$$

$$F_1 = (kr)^{-1}G_1,$$

the coupled equations take the form

$$\left(\frac{d^2}{dr^2} + k^2 - U_{00} \right) G_0 = U_{01}G_1, \quad (3)$$

$$\left(\frac{d^2}{dr^2} - \kappa^2 - U_{11} \right) G_1 = U_{01}G_0. \quad (4)$$

We require solutions for G_0 and G_1 which vanish at $r = 0$ and have the asymptotic

$$G_0 \sim \sin kr + \alpha e^{ikr}, \quad (5)$$

$$G_1 \sim \beta e^{-\kappa r}, \quad (6)$$

where $k^2 - k_0^2 = -\kappa^2$, k_0^2 is written for $2m|E_0 - E_2|/\hbar^2$, and E_0 and E_1 are energies of the 1s- and 2s-states, respectively. The functions U_{00} , U_{01} and U_{11} are given by

$$U_{ij} = \frac{2m\epsilon^2}{\hbar^2} \int \left(-\frac{1}{r_1} + \frac{1}{r_{12}} \right) \psi_i(\vec{r}_2) \psi_j^*(\vec{r}_2) d\vec{r}_2. \quad (7)$$

As both ψ_0 and ψ_1 are real, $U_{ij} = U_{ji}$.

If U_{11} is attractive and sufficiently large in absolute magnitude, there will exist, for certain values of κ , solutions of the homogeneous equations

$$\left(\frac{d^2}{dr^2} - \kappa^2 - U_{11} \right) \phi = 0, \quad (8)$$

which represent bound states.

We denote these bound-state wave functions by $\phi_1, \phi_2, \dots, \phi_n$. Corresponding to each of these states, there will be bound states of energy

$$-\hbar^2 \kappa_1^2 / (2m), \quad -\hbar^2 \kappa_2^2 / (2m), \quad \dots - \hbar^2 \kappa_n^2 / (2m).$$

If the coupling $U_{01} = U_{10}$ were vanishingly small, we would have (with $k^2 - k_0^2 = -\kappa_1^2, -\kappa_2^2, \dots, -\kappa_n^2$) two degenerate solutions of the wave equation describing the collision. One, $\psi_0(r_1)F_0(r_2)$, belongs to a continuum while the other, $\psi_1(r_1)\phi_j(r_2)$ is a discrete function corresponding to a doubly-excited state of H^- .

In fact, resonance effects should be apparent for values of k^2 such that κ^2 is near one of the values $\kappa_1^2, \kappa_2^2, \dots, \kappa_n^2$. Then, the analysis based on approximate solution of Eqs. (3) and (4) leads to the Breit-Wigner formulae [4], which give the partial elastic and inelastic cross-sections as functions of k^2 (the energy of the incident particle) which have a typical resonance shape, and which have been often applied in nuclear physics [6].

On the other hand, it is possible to solve the coupled equations using the theorem on separation of CDE, such as (3) and (4), quite accurately no matter how large the coupling U_{01} may be, so that widths of the resonance can be obtained to a better precision.

3. The model of resonance phenomena

In order to support our conclusions, our model calculations will be improved using two requirements:

(a) The conditions required by the theorem on separation of CDE should be satisfied so that these equations can be solved directly.

(b) The model should, at least schematically, reproduce some new features which are not predicted in the previous approach.

As an illustration, we propose a simple schematic model, in which the potentials U_{00}, U_{01} and U_{11} are constant for $r < a$ and zero for $r > a$. Then the solutions of Eqs. (3) and (4) in the second region ($r > a$) can be obtained in the following forms:

$$G_0 = \sin kr + \alpha e^{ikr}, \quad (9)$$

$$G_1 = \beta e^{-\kappa r}. \quad (10)$$

In the first region ($r < a$), where the direct potentials are constants and $U_{01} = C$, the system (3) and (4) can be solved using the theorem on separation of CDE. The solutions are given by

$$G_0 = A_1 \sin \omega_1 r + A_2 \sin \omega_2 r, \quad (11)$$

$$G_1 = (k'^2 - \omega_1^2)C^{-1}A_1 \sin \omega_1 r + (k'^2 - \omega_2^2)C^{-1}A_2 \sin \omega_2 r, \quad (12)$$

where A_1 and A_1 are constants,

$$k'^2 = k^2 - U_{00}, \quad \kappa'^2 = -\kappa^2 - U_{11},$$

$$2\omega_1^2 = (k'^2 + \kappa'^2) + \sqrt{(\kappa'^2 - k'^2)^2 + 4C^2},$$

$$2\omega_2^2 = (k'^2 + \kappa'^2) - \sqrt{(\kappa'^2 - k'^2)^2 + 4C^2}.$$

By matching these solutions at $r = a$ to the asymptotic forms (9) and (10), the values of α and β were obtained. The elastic cross-section is given by

$$Q_0^{\text{el}} = (4\pi/k^2) |\alpha|^2. \quad (13)$$

For numerical calculation, the values $a = 1$, $U_{11} = -6.25$ and $U_{00} = -1$, were assumed, and the solution evaluated for a number of values of the coupling constant $U_{01} = C$ (see Fig. 1). The elastic cross-sections are shown as functions of energy for the case in which the resonance level appears for $k^2 = 0.77$. The excitation energy was chosen so that $k^2 = 2.25 - \kappa^2$, giving the undisplaced level at $k^2 = 1.48$. The resonance effect is clearly seen as well as the increased shift and

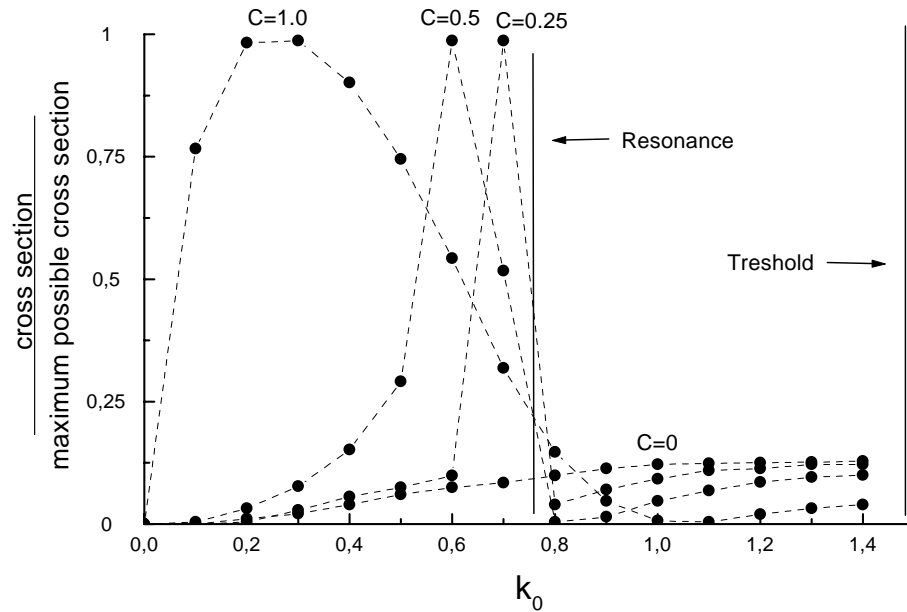


Fig. 1. Resonance effects in elastic scattering below the inelastic threshold for different strengths of the coupling interaction U_{01} . Note the increase in the width of the resonance peak and of the displacement of the maximum from the uncoupled location as U_{01} increases, for the case $l = 0$.

width as U_{01} increases. The maximum cross-section remains $4\pi/k^2$ until the shift is so large that the maximum is displaced to negative values of k^2 . In reality, the form of the cross-section in passing through the resonance region will depend on the interference between the resonance and mean potential scattering terms in Eq. (13).

4. *Extension to scattering of electrons with non-zero angular momentum*

Although we have restricted the analysis in the previous paragraph to scattering of s-electrons, it is not difficult to extend it to the cases in which the electron possesses any quantized angular momentum.

If we are considering the scattering of electrons in the state 1, with insufficient energy to produce excitation, by an atom in the ground state 0, there exists a doublet resonance state of orbital angular momentum $\hbar\sqrt{L(L+1)}$. The discussion of the previous paragraph may readily be generalized to equations of the form

$$\left(\frac{d^2}{dr^2} + k^2 - U_{00} - \frac{l(l+1)}{r^2} \right) G_{0l} = U_{01} G_{1l}, \quad (14)$$

$$\left(\frac{d^2}{dr^2} - \kappa^2 - U_{11} - \frac{l(l+1)}{r^2} \right) G_{1l} = U_{01} G_{0l}, \quad (15)$$

where we ignore the difference in centrifugal potentials in these equations and use the one corresponding to $l_0 = l_1 = l$ in all channels. The states which couple to the initial state must then have also $L = 1$. The solutions of these equations must satisfy the following conditions

$$G_{0l}(0) = G_{1l}(0) = 0, \quad (16)$$

and have either of the asymptotic forms

$$G_{0l} \sim i^l \sin(kr - l\pi/2) + \alpha_l e^{i(kr - l\pi/2)}, \quad (17)$$

$$G_{1l} \sim \beta_l e^{-\kappa r - il\pi/2}. \quad (18)$$

Under these conditions, we may decouple Eqs. (14) and (15) using the theorem on the separation of a system of CDE [3], provided the quantity $\gamma = U_{01}/(U_{00} - U_{11})$ is independent of r .

To illustrate the effects of the partial waves ($l \neq 0$) in the resonance problems, we propose the same schematic model, in which the potentials U_{00} , U_{11} and U_{01} are assumed to be constant for $r < a$ and to be zero for $r > a$.

Then the solutions of these equations, in the second region $r > a$, can be obtained in the following forms, which satisfy the asymptotic conditions (17) and (18)

$$G_{0l} = \sqrt{\pi kr/2} \{i^l J_\nu(kr) + \alpha_l [iJ_{-\nu}(kr) + (-1)^l J_{-\nu}(kr)]\}, \quad (19)$$

$$G_{1l} = i^l \sqrt{\pi kr/2} \beta_l (2/\pi) \sin \nu \pi K_\nu(\kappa r), \quad (20)$$

where $J_{\pm\nu}$ are the Bessel functions of the first kind, and K_ν are the hyperbolic Bessel functions [7].

In the first region ($r < a$) where the direct potential are constants and $U_{01} = C$, the system (14) and (15) can be solved using the theorem on separation of CDE. Then the solutions are given by

$$G_{0l} = A_1 J_\nu(\omega_1 r) + A_2 J_\nu(\omega_2 r), \quad (21)$$

$$G_{1l} = A_2 J_\nu(\omega_1 r) - A_1 J_\nu(\omega_2 r), \quad (22)$$

where $A_2 = -A_1 C / (k^2 - U_{00} - \omega_2^2)$.

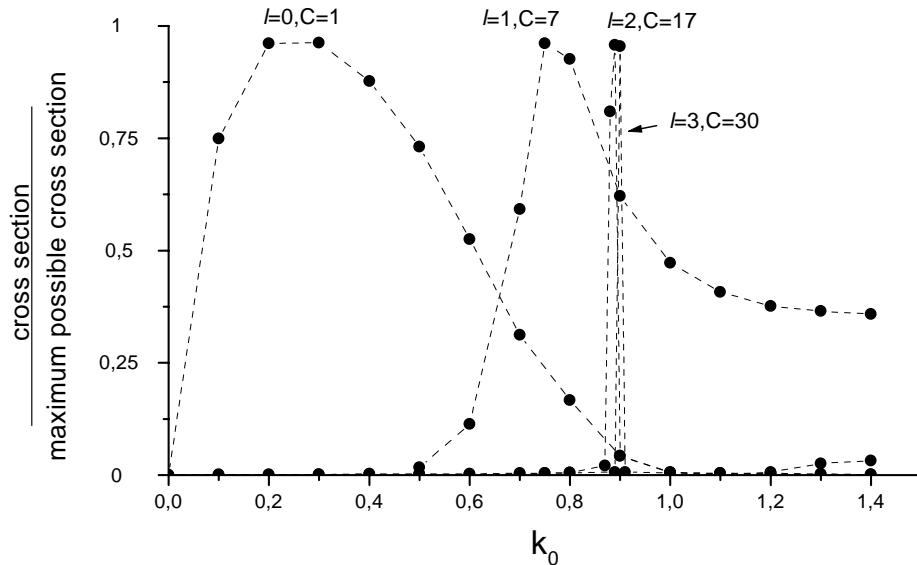


Fig. 2. Resonance effects in the elastic scattering below the resonance threshold for some values of the orbital angular momentum quantum number $l \leq 3$, and for different strengths of the coupling interaction U_{01} as indicated.

TABLE 1. Disappearance of the resonance effects in the elastic cross-sections below the inelastic threshold for $l = 4$ and 5 and for different values of the coupling interaction U_{01} .

$l = 4$	C			
k_0	20	40	60	80
0.2	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$
0.4	$0.50 \cdot 10^{-16}$	$0.90 \cdot 10^{-16}$	$0.24 \cdot 10^{-16}$	$0.39 \cdot 10^{-16}$
0.6	$0.86 \cdot 10^{-15}$	$0.20 \cdot 10^{-13}$	$0.36 \cdot 10^{-14}$	$0.98 \cdot 10^{-16}$
0.8	$0.21 \cdot 10^{-13}$	$0.25 \cdot 10^{-11}$	$0.98 \cdot 10^{-12}$	$0.12 \cdot 10^{-12}$
1.0	$0.90 \cdot 10^{-12}$	$0.15 \cdot 10^{-9}$	$0.49 \cdot 10^{-10}$	$0.67 \cdot 10^{-11}$
1.2	$0.25 \cdot 10^{-10}$	$0.48 \cdot 10^{-8}$	$0.11 \cdot 10^{-8}$	$0.15 \cdot 10^{-9}$
1.4	$0.39 \cdot 10^{-9}$	$0.90 \cdot 10^{-7}$	$0.15 \cdot 10^{-7}$	$0.21 \cdot 10^{-8}$

$l = 4$	C			
k_0	100	120	140	160
0.2	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$
0.4	$0.89 \cdot 10^{-16}$	$0.17 \cdot 10^{-16}$	$0.28 \cdot 10^{-16}$	$0.37 \cdot 10^{-16}$
0.6	$0.13 \cdot 10^{-13}$	$0.76 \cdot 10^{-14}$	$0.18 \cdot 10^{-14}$	$0.27 \cdot 10^{-15}$
0.8	$0.18 \cdot 10^{-11}$	$0.18 \cdot 10^{-11}$	$0.62 \cdot 10^{-12}$	$0.19 \cdot 10^{-12}$
1.0	$0.11 \cdot 10^{-9}$	$0.90 \cdot 10^{-10}$	$0.32 \cdot 10^{-10}$	$0.10 \cdot 10^{-10}$
1.2	$0.38 \cdot 10^{-8}$	$0.20 \cdot 10^{-8}$	$0.77 \cdot 10^{-9}$	$0.24 \cdot 10^{-9}$
1.4	$0.82 \cdot 10^{-7}$	$0.27 \cdot 10^{-7}$	$0.10 \cdot 10^{-7}$	$0.33 \cdot 10^{-8}$

$l = 5$	C			
k_0	20	40	60	80
0.2	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$
0.4	$0.49 \cdot 10^{-16}$	$0.49 \cdot 10^{-16}$	$0.49 \cdot 10^{-16}$	$0.49 \cdot 10^{-16}$
0.6	$0.36 \cdot 10^{-15}$	$0.36 \cdot 10^{-16}$	$0.39 \cdot 10^{-15}$	$0.35 \cdot 10^{-15}$
0.8	$0.14 \cdot 10^{-15}$	$0.19 \cdot 10^{-15}$	$0.10 \cdot 10^{-14}$	$0.26 \cdot 10^{-16}$
1.0	$0.54 \cdot 10^{-16}$	$0.67 \cdot 10^{-15}$	$0.73 \cdot 10^{-13}$	$0.49 \cdot 10^{-14}$
1.2	$0.17 \cdot 10^{-14}$	$0.32 \cdot 10^{-13}$	$0.52 \cdot 10^{-11}$	$0.25 \cdot 10^{-12}$
1.4	$0.27 \cdot 10^{-13}$	$0.83 \cdot 10^{-12}$	$0.23 \cdot 10^{-9}$	$0.66 \cdot 10^{-11}$

$l = 5$	C			
k_0	100	120	140	160
0.2	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$	$0.67 \cdot 10^{-16}$
0.4	$0.49 \cdot 10^{-16}$	$0.49 \cdot 10^{-16}$	$0.49 \cdot 10^{-16}$	$0.49 \cdot 10^{-16}$
0.6	$0.36 \cdot 10^{-15}$	$0.36 \cdot 10^{-15}$	$0.33 \cdot 10^{-15}$	$0.35 \cdot 10^{-15}$
0.8	$0.83 \cdot 10^{-16}$	$0.19 \cdot 10^{-15}$	$0.45 \cdot 10^{-16}$	$0.27 \cdot 10^{-16}$
1.0	$0.69 \cdot 10^{-15}$	$0.80 \cdot 10^{-15}$	$0.37 \cdot 10^{-13}$	$0.49 \cdot 10^{-14}$
1.2	$0.38 \cdot 10^{-13}$	$0.44 \cdot 10^{-13}$	$0.17 \cdot 10^{-11}$	$0.25 \cdot 10^{-12}$
1.4	$0.11 \cdot 10^{-11}$	$0.13 \cdot 10^{-11}$	$0.40 \cdot 10^{-10}$	$0.70 \cdot 10^{-11}$

To obtain the parameters α_1 and β_1 , we use the connection of these solutions at $r = a$, which leads directly to the elastic partial cross-sections

$$Q_l^{\text{el}} = \frac{4\pi}{k^2} (2l + 1) |\alpha_l|^2. \quad (23)$$

We plot in Fig. 2 the partial cross-sections as a function of energy in terms of the coupling potential $U_{01} = C$. One can see that the resonance effects are more pronounced for low values of l . Thus the curve for $l = 0$ passes through a resonance around $k = 0.3$, for $C = 1$, while for $l = 1$, the partial elastic cross-section does not reach the highest value until $k = 0.8$ for $C = 7$, and the partial cross-sections for higher l require even stronger coupling for complete resonance effects. We have assumed the same values as in the last paragraph for $a = 1$, $U_{11} = -6.25$, $U_{00} = -1$. The excitation energy was chosen so that $k^2 = 2.25 - \kappa^2$, giving the undisplaced level at $k^2 = 1.48$. These effects are also responsible for values of the elastic cross-sections below the conservation limit, and are clearly seen as well as the increased shift and width as C increases. The maximum cross-section remains $4\pi(2l + 1)/k^2$ until the shift is so large that the maximum is displaced to negative values of k^2 .

In Table 1, we give the prediction for the partial cross-sections for $l = 4$ and 5, where we see that the resonance effects disappear for all values of the coupling potential. That shows that the investigation of the partial waves can be neglected in the elastic collisions at energies below the inelastic threshold resonance effects, where the resonance will be missed or at best, broadened. The contribution of these partial waves are important in the inelastic collisions [5].

5. Resonance effects in slow electron collisions

We also consider whether the resonance effects discussed in the previous paragraphs are likely to occur in atomic collisions. Certainly, in the two- and three-state close-coupling approximations, such as the 1s - 2s and 1s - 2s - 2p below the excitation threshold, sharp resonances arise. They correspond to the formation of negative ions which are unstable towards auto-detachment. Thus, an electron may attach to a hydrogen atom in the 2s state to form a negative ion but it is unstable.

It is well known that an interaction that falls off faster than r^{-2} will, in general, support only a finite number of bound states. Therefore, at first sight, it would seem that there could at most be a finite number of doubly-excited states of H^- based on singly-excited orbital of H of the total quantum number n . In fact, as was first proved by Gaillitis and Damburg [8], the situation is affected by the energy degeneracy of the H atom states of different angular momentum associated with a given n . The coupling between these states modifies the effective interaction acting on an additional electron so that it falls as slowly as r^{-1} at large distance r . If the degeneracy were exact, this would lead to an infinite series of doubly-excited states associated with a given n , but only for certain values of the total orbital angular momentum quantum number L . Thus, if $E_{nl}^{(1)}$ is the energy of the lowest level of a series associated with particular values of n and L , the energy of the higher levels

are given by $E_{nl}^{(1)}(\alpha, \alpha^2, \alpha^3, \dots)$, where $\alpha < 1$. In fact, the degeneracy between the s,p,d... levels of H for a given n is not exact because of the Lamb shift. It may be shown that if ϵ is the actual energy difference between the nearly degenerate states, the above considerations remain applicable provided the energy $E_n^{(s)}$ of a particular state below the corresponding ionization threshold satisfies

$$E_n^{(s)} \gg (L + 1)\Delta\epsilon/2. \quad (24)$$

In particular, in the three-state case, there exists an infinite number of resonances for $n = 2$ and $L \leq 2$ where L is the total orbital angular momentum quantum number, and the 2s - 2p coupling includes a term which falls off as r^{-2} . For example, for $L = 0$, we have asymptotically in the 2s and 2p channels

$$F_{2s} = G_{2s}/r, \quad (25a)$$

$$F_{2p} = G_{2p}/r, \quad (25b)$$

$$\left(\frac{d^2}{dr^2} - \kappa^2\right)G_{2s} = \frac{6}{r^2}G_{2p}, \quad (26)$$

$$\left(\frac{d^2}{dr^2} - \kappa^2 - \frac{6}{r^2}\right)G_{2p} = \frac{6}{r^2}G_{2s}, \quad (27)$$

where $G_{2s, 2p}$ satisfy the condition

$$G_{2s, 2p} \sim \beta_{2s, 2p} \exp(-\kappa r) \quad (r \rightarrow \infty). \quad (28)$$

It will be seen that the coupling term falls off only as r^{-2} . The equations may be separated using the theorem on the separation [3] when the conditions, which are imposed by this theorem, are satisfied, i.e., the quantity $\gamma = U_{01}/(U_{00} - U_{11}) = -1$ is independent of r . The separated equations are now

$$\left(\frac{d^2}{dr^2} - \kappa^2 + \frac{(\pm\sqrt{37} - 1)}{r^2}\right)\phi^\pm = 0, \quad (29)$$

where $\mathbf{G} = \mathbf{T}^{-1}\phi$ and \mathbf{T} is defined in Ref. [3]. Then, for ϕ^+ , we have a repulsive potential which does not give a bound state, while for ϕ^- , the potential is attractive and may yield a bound state which leads to the resonance effects we have discussed earlier.

If we put

$$\nu(\nu + 1) = -(\pm\sqrt{37} - 1), \quad (30)$$

then this apparently corresponds to four alternative values for ν , but the ambiguity in the form $\nu(\nu + 1)$ does not lead to anything new. We may thus take

$$\nu_1 = -\frac{1}{2} + \sqrt{\frac{5}{4} + \sqrt{37}}, \quad \nu_2 = -\frac{1}{2} + i\sqrt{\sqrt{37} - \frac{5}{4}}. \quad (31)$$

To solve the system (29) for small κ , we may distinguish three ranges of r in which different approximation can be made.

In the discrete region, we may neglect κ for values such that $\kappa r \ll 1$, and the coupling terms are ignored in (26), (27), but in (29) must be taken into account. This means that, for $r = r_0$,

$$\frac{\phi_{1\nu}}{\phi'_{1\nu}} = c, \quad (32)$$

where c is a constant independent of κ , but depending on the internal interactions and $\phi' = d\phi/dr$.

In the second region, we suppose that κ^2 is negligible compared with $\nu(\nu+1)/r^2$, and the general solution is

$$\phi_{II\nu} = ar^{\nu+1} + br^{-\nu}. \quad (33)$$

The constants a and b are determined by fitting the solutions at $r = r_0$, and so their ratio is independent of κ ,

$$\frac{a}{b} = -r^{-2\nu-1} \frac{r_0 + c\nu}{r_0 - c(\nu + 1)}. \quad (34)$$

Finally, there is the outermost region in which $\kappa r \approx 1$, and the required solution of this equation can now be expressed in terms of the Bessel functions,

$$\phi_{III\nu} = \sqrt{i\kappa r} \{AJ_{(\nu+1/2)}(i\kappa r) + BJ_{(-\nu-1/2)}(i\kappa r)\}. \quad (35)$$

As this solution must have the asymptotic form (28), then

$$B = -i \exp(i\nu\pi). \quad (36)$$

When κ is small so that $\kappa r \ll 1$, we may use the series expansions of the Bessel functions [7]

$$J_n(x) \approx \frac{x^n}{2^n \Gamma(n+1)}. \quad (37)$$

Substitution in (35) and comparison with (33) gives

$$\frac{a}{b} = \left(\frac{\kappa}{2}\right)^{2\nu+1} \frac{\pi}{(\nu + \frac{1}{2}) \cos \nu\pi} \frac{1}{[\Gamma(\nu + 1/2)]^2}. \quad (38)$$

This shows that

$$\kappa^{2\nu+1} = \text{constant}.$$

When $\nu = -1/2 + i\mu$, this condition becomes

$$\kappa^{2i\mu} = \text{constant}.$$

This is satisfied by

$$2\mu \ln \kappa = 2s\pi + 2\mu \ln \kappa_0, \quad s = 0, \pm 1, \pm 2, \dots$$

or

$$\kappa^2 = \kappa_0^2 \exp(2s\pi/\mu),$$

showing that if $\kappa^2 h^2/(2m)$ is an allowed energy, then it is also

$$\exp(2s\pi/\mu) \kappa_0^2 h^2/(2m).$$

This will be true provided κ_0^2 is such that κ^2 is neither too small for Eq. (24) to hold, nor too large for κr_1 to be too large. In this case, $\Delta\epsilon = 4 \times 10^{-6}$ eV for $n = 2$ and $L = 0$, and we have considered the progression of energy levels below the ionization threshold, which will be of the form

$$E(1, \alpha, \alpha^2, \alpha^3, \dots)$$

where

$$\alpha = \exp(-2\pi/\mu),$$

Since $\mu = \sqrt{\sqrt{37} - 5/4} = 2.198$, we have $1/\alpha = 17.428$ as is shown in Ref. [4].

6. Conclusions

We have applied the theorem on separation of coupled differential equations to the resonance effects, with neglect of the effect of exchange between the incident and atomic electrons. It has been shown how the coupled-channel equations, which may arise in the elastic scattering when the electron energy is below the threshold excitation, can be decoupled. We expect that our calculation is fairly realistic.

It is clear from the figures and tables that the behaviour of the cross-sections is in qualitative agreement with the considerations expressed in the second section. The elastic cross-section below the threshold shows resonances.

We have described the elastic collisions at energies below the inelastic threshold in terms of the simple model. It is not difficult to extend this analysis to the interaction of a discrete state with any number of continua. In the general case,

in which collision processes occur through the formation of a complex of a finite lifetime as an intermediate stage, we may write for the cross-section for the inelastic process the formulae which were derived by Breit and Wigner [4].

In principle, the analysis can be extended to more complicated sets of coupled equations, including electron exchange. In that case, the corresponding procedure would be to determine the bound states that arise as eigenfunctions for the reduced set of coupled equations that involve the closed channels only, the coupling with the open channels being ignored. Example of such calculations are given in the previous section.

We considered an electron incident on hydrogen ion in the ground state, where $L = 1$ is the angular momentum quantum number of the motion of the electron relative to the ion. The states which couple with this initial state must then also use the rule for combination of angular momenta. When $L = l = 0$, the states which couple may be written $2s, l = 0, 2p, l = 1$, where l refers to the angular momentum relative to the atom in the $2s$ - or $2p$ -state, respectively. In this case, the treatment involves two equations associated with closed channels. The resonance states obtained from these channels correspond to the doubly-excited series $2sns$ and $2pnp$, respectively. Some information about the identification of any resonance state in these terms are given in the last paragraph. When $l = 1$, the states which couple are $2s, l = 1, 2p, l = 0$, and $2p, l = 1$, corresponding to the series $2snp, 2pns$ and $2pnd$, respectively. $2pnp$ does not contribute, because such states are of even parity, whereas the initial state is odd. In this case, there will be four coupled equations. Resonance effects in the first-order phase shift will arise from the interaction with states of the three series of states mentioned above. Investigations on these topics are in progress.

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TEOREM O RAZDVAJANJU VEZANIH DIFERENCIJALNIH JEDNADŽBI,
REZONANTNI UČINCI I SVOJSTVA OKO PRAGA

Cilj je ovog rada pokazati važnost teorema o razdvajanju vezanih diferencijalnih jednadžbi za opis elastičnog raspršenja elektrona kada je energija elektrona ispod praga za uzbuđenje iz osnovnog stanja 0 u stanje 1. Primijenili smo aproksimativni model radi proučavanja rezonantnih učinaka koji se opažaju u raspršenju elektron – vodik. Razmatraju se svojstva raznih udarnih presjeka u blizini praga nove vrste raspršenja u kojemu elektron ima bilo koji impulsni moment i ispituju se učinci promjene centrifugalnog potencijala u slučaju približenja bliskog vezanja 1s-2s-2p. Zaključujemo raspravom o svojstvima oko praga i njihovom odnosu s rezonantnim učincima.