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POSITRONIUM FORMATION BY POSITRON IMPACT ON HYDROGEN ATOMS

by

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Abstract

The sensitivity of s and p wave positron-hydrogen atom elastic-phase shifts, to the presence or absence of various multipole components of the adiabatic polarisation potential is discussed. It is concluded that higher multipoles than the quadrupole component are unimportant and support is given to the view of Drachman (1965) that in s-wave scattering the monopole component of the adiabatic potential should be suppressed.

Then the cross-section for positronium formation by positron impact on hydrogen is calculated in the two-state approximation, taking account of the polarisation of the hydrogen and positronium atoms in each channel. It is found that the polarisation forces dominate the cross-section near the threshold for positronium formation and evidence is presented for the existence of a positronium-proton bound state that gives rise to a resonance in elastic e^+ -H scattering just below the formation threshold.

CONTENTS

CHAPTER ONE

Introduction

Theoretical evaluation of cross-sections for slow positrons by hydrogen atoms has received considerable attention recently. The development of high-speed computers and variational methods have made the problem easier.

Unfortunately, experiment has not provided us with data about positron-hydrogen scattering. Nevertheless, there is a growing interest for studying various effects of positron-hydrogen scattering, especially for comparison with electron-hydrogen scattering. For example, the mean static interaction is attractive in the electron case and repulsive in the positron case. The long-range forces are attractive in both cases. The two effects therefore oppose each other in the positron case and combine in the electron case. It is interesting to see which of the effects is the stronger one. We can also compare between exchange in the electron case and positronium formation in the positron case, and between polarization and positronium formation.

It is known that the static field produces negative phase shifts for positron-hydrogen scattering. It is interesting to see the relative importance of the various effects in drawing the phase shift towards the positive region, and to see whether an effect on a combination of effects can alter the sign of it.

Relativistic effects are neglected in this work and the interaction between the particles is purely coulombic. The particles in the interaction are the incident positron, the proton which is assumed to be infinitely heavy compared with the electron, and the electron which occupies the ground state orbit around the proton.

This is a three-body problem. Many-body problems have no exact solution and are associated with mathematical difficulties. After more than thirty years, there is no general method that can be applied to the calculation of cross-sections for particle-atom scattering.

There are various approximation methods for calculating the cross sections of atomic scattering. Not all of these methods are practicable. Some of them are not accurate enough. Some of them are only applicable in restricted conditions. Two very common methods are the "Born Approximation" and the "Hartree-Fock" method. Among other methods which are coming into use now are the "Optical potential" method and the "Perturbed Hartree-Fock expansion".

A considerable amount of work has been concentrated on elastic scattering of electrons, especially electron-hydrogen and electron-helium scattering. Excitation of the target and rearrangement have not received much attention. They have been receiving more attention relatively lately.

In this work the problem is attacked in two stages. The first stage consists of the elastic scattering of positrons by hydrogen atoms treated in a single-channel calculation. Then, as a generalisation, a second stage consists of a two-channel treatment for the rearrangement scattering. In the latter stage positronium is formed, and its formation is coupled with the elastic channel.

The basic feature of multichannel scattering is that, in general, the identities of the scattering systems alter (permanently or intermediately) throughout the collision. Each set of identities (simultaneously) determines a channel.

Channels are coupled if the whole system is able to switch from one of them to another.

Open channels are those channels which are energetically possible. The other channels are the closed ones.

We shall assume that there are two coupled channels (one of them open in the first stage). The coupling between these channels is neglected at first, thus giving the one-channel scattering. i.e. the elastic scattering ignoring positronium formation. An improvement in the results is expected in the second stage where the positronium channel is introduced and coupled with the elastic channel. Nevertheless the one-channel calculation can be compared with the two-channel calculation to learn something about the effect of each of the two channels.

While single-channel scattering is determined by the specification of the phase shift, the multi-channel scattering is determined by the specification of the eigen-phase shifts and of the mixing parameter.

1.1 Approximation Methods

To the present, a many-body problem has no exact solution. With the help of some approximation methods, the matter of getting reasonable results for the problem becomes possible. According to the conditions of the scattering problem (as those concerning the energy or the identities of the interacting systems) suitable approximation methods can be used.

For example, if the wave function of the incident particle is expected to remain the same throughout the scattering (as is the case when the kinetic energy of the incident particle is large compared with the interaction potentials), then "Born approximation" provides a very practical tool. Of course, it is expected that the Born approximation breaks down for low energy of scattering.

As well as the Born approximation there is the optical potential method. It is derived from the Lippmann-Schwinger equation. The optical potential method approximates the distortion of the atomic electron and the incident particle by an effective interaction. The method introduces a summation which is impossible to obtain. Usually few terms of this summation are retained, thus making the approximation.

One of the earliest approximations is the eigen function expansion method. The idea of this method is to represent the total wave function by a complete set of eigen functions. It takes the form of the expansion

$$\psi(x,r) = \left[\Sigma + \int\right]\phi_n(x)\ F_n(r) \tag{1.1}$$

Where ϕ_n are the discrete and continuous set of eigen functions used. $F_n(r)$ are the coefficients of the expansion. They are independent of x but dependent on r, the co-ordinates of the scattered particle.

Usually $\phi_n(x)$ are taken to be the eigen functions of the target atom. In positron-hydrogen scattering they satisfy

$$(H_0 - \varepsilon_n)\phi_n = 0 \tag{1.2}$$

where H_0 is the Hamiltonian of the hydrogen atom, and ε_n the energy of the atom in the nth state.

In expansion (1.1) the summation acts on the discrete region, and the integration acts on the continuous region of the atomic energy. When a complete set of eigen functions is used the expression is exact.

It is possible to describe the elastic scattering of a particle by an atom without arbitrarily discarding the continuum. The complete set of eigen functions do not have to be of a physical system. Rotenberg (1962) used what he called Sturmian functions. They are generated by a differential equation closely related to the Schrodinger equation, but in spite of this, they had not been exploited in atomic and nuclear physics. They have an advantage over Schrodinger functions in that they form a complete set without a continuum, regardless of the potentials existing between the particles. Rotenberg used these functions for the scattering of electrons by hydrogen atoms.

Expansion (1.1) leads to an infinite set of coupled integro-differential equations. To make the solution possible, the summation has to be truncated. This reduces the equations to a finite set. The terms neglected in this way are lost, which reduces the accuracy of the solutions. In practice, the number of terms retained is small enough to make the solution possible, but large enough to include atomic levels directly involved in the collision. This succeeded in some calculations of resonances and excitation.

For obtaining the set of integro-differential equations according to theeigen function expansion method, expansion (1.1) is substituted in the Schrodinger equation

$$(H - E)\ \Psi\ (x,r) = 0 \tag{1.3}$$

where E is the total energy of the whole system and H is its Hamiltonian which satisfies

$$H = H_0 - K + V \tag{1.4}$$

where K is the kinetic energy operator and V the interaction between the atom and the scattered particle.

Equation (1.3) is multiplied then by $\emptyset^*$ on the left and integrated over x leading to an infinite set of coupled integro-differential equations as follows:

$$(\nabla_r^2 - \tfrac{1}{2}k^2)F_n(r) = \left[\Sigma + \int\right] U_{nm}\, F_m(r) \tag{1.5}$$

where k is the wave number of the scattered particle and where

$$U_{nm} = \int \emptyset_n^*(x)\ V(x,r)\emptyset_m(x)\,dx \tag{1.6}$$

If no distortion occurs in the atomic orbitals, the first term of (1.1) which describes the state before scattering, continues to do so throughout the collision. Therefore, all the other terms of (1.1) are there to describe distortion, and any truncation is a neglect of part or all of this distortion. This way of describing distortion is very indirect.

In the case of electron-atom scattering expansion (1.1) is replaced by the following expansion:

$$\psi(x,r) = \sum_n A\left[\emptyset_n(x)F_n(r)\right] \tag{1.7}$$

where A antisymmetrizes the function with respect to electron co-ordinate exchange. In this case any truncation of (1.7) neglects exchange as well as distortion. Usually a few terms of either of the expansions are retained, giving the so called

"Close coupling" approximation.

In the optical potential method all steps of the previous approximation are done. Further, to surmount the error arising from truncation, an effective interaction potential is added to the original potential. The Schrodinger equation then becomes

$$(H_0 - K + \gamma - E)\ \psi'(x,r) = 0 \qquad (1.8)$$

where the interaction V is replaced by the optical potential γ.

1.2 Variational Methods

The application of variational principles for scattering problems was developed in the 1940's by employing procedures analogous to those of the bound state problems.

One starts with a trial function which includes adjustable parameters. Then one adjusts these parameters in the best way possible. From the obtained function it is possible to extract some scattering parameter and consequently the cross section is determined.

A certain class of variational methods go as far as defining upper or lower bounds on the scattering parameters. Principles of this class are extremum principles. Most of them are minimum principles.

Stationary variational principles are attributed to Hulthen and Kohn. Extremum variational principles include two methods. The first method was derived by Schwinger, for the values of $k \cot \eta_\ell$, where η_ℓ is the partial wave phase shift; and gives an upper (lower) bound for an attractive (repulsive) potential that is not strong enough to form a bound state. The second method is a development from the Kato identity developed by Spruch et. al. (1960) to obtain a minimum principle for $\tan \eta$

Variational principles suffer from the weakness that they can only be applied over a narrow range of conditions.

The reason for this is that unless the number of adjustable parameters in the trial wave function is unreasonably large, the function fails to describe the complete effects of distortion. The Hartree-Fock method is excluded from this as it leaves these effects to be determined in the solutions of the differential equations.

Hulthen's method starts by defining the quantity I_ℓ as follows

$$I_\ell = \int u_\ell \ (L - k^2) \ u_\ell(r)\,dr \tag{1.9}$$

for the ℓth partial wave of the scattered particle. Then the method assumes independent variations of the parameters of the trial wave function. This leads to the equations

$$\delta(I_\ell + k\eta_\ell) = 0 \qquad \text{or} \tag{1.10}$$

$$k\eta_\ell = k\eta_{\ell_t} + I_{\ell_t} \tag{1.11}$$

which is a variational principle correct to the second order. The parameters are determined from the fact that this η_ℓ of (1.11) is stationary. This is expressed in the following equations

$$\frac{\partial \eta_\ell}{\partial \eta_{\ell_t}} = 0 \tag{1.12}$$

$$\frac{\partial \eta_\ell}{\partial C_i} = 0 \qquad (i=1,\ldots\ldots n) \qquad (1.13)$$

where C_i are the variational parameters. Equation (1.12) has been suggested by Hulthen as an improvement to his original method in which he used the equation

$$I_t = 0 \qquad (1.14)$$

instead of the first equation of (1.12).

Hulthen's equations are quadratic. Kohn's equations which are linear are

$$\delta\lambda = \delta(I_\ell - k \tan \eta_\ell) = 0 \qquad (1.15)$$

$$k \tan \varepsilon_1 = k \tan \eta_\ell - \int_0^\infty \phi_\ell (L-k^2)\phi_\ell dr \qquad (1.16)$$

The Hulthen and Kohn variational principles have been used by Massey and Moiseiwitsch (1951) who obtained for electron-hydrogen scattering, satisfactory agreement with the results of the exact solution of the static approximation(see section 1.4).

The value of variational principles in scattering problems is increased when the principles are extremum. The earliest principles of this class suffered from very strict restrictions concerning potentials angular momentum and energies of the incident particle. Further development widened the range of application.

1.3 Hartree-Fock Method

The importance of Hartree-Fock equations lies in their connection with variational methods and with the eigen function expansion method. The latter method is the generalisation of the Hartree-Fock method. Instead of using the target's set of eigen functions one can use any complete set of eigen functions. In the following, the Hartree-Fock equations will be derived from a variational principle.

The exact wave function of the whole system satisfies the equation

$$I \equiv \int \Psi^{*} (H - E) \Psi d\nu = 0 \tag{1.17}$$

where Ψ is the total wave function and the integration acts on the co-ordinates of the target electrons and the scattered particles. If Ψ is expanded in terms of the target atom wave functions

$$\Psi = \sum_{n} \psi_{n}(x, \hat{r}) \; F_{n} (r) \tag{1.18}$$

where Ψ_n describes the target and the angular relative motion and $F_n(r)$ describes the radial relative motion it has the asymptotic form

$$F_{n}(r) \sim C_{n} \left[S_{n}(kr) + R_{n} \; C_{n}(kr) \right] \tag{1.19}$$

Then for a variation $\delta\Psi = \Psi_t - \Psi$ we have

$$\delta I = C^2 \frac{\delta R}{2k} + \int \delta\psi (H - E) \delta\psi \, d\nu \qquad (1.20)$$

Neglecting the term in $\delta\psi^2$ equation (1.20) becomes

$$\delta (I - C^2 \frac{R}{2k}) = 0 \qquad (1.21)$$

which means that the quantity $(I - C^2 \frac{R}{2k})$ is stationary with respect to the variations $\delta\Psi$. Equation (1.21) can be written in the alternative form

$$R = R_t - 2I_t \, k/C^2 \qquad (1.22)$$

which is the Kohn variational principle. It is apparent that neglecting the term in $\delta\Psi$ is responsible for the second order error in Kohn's variational principle.

Hartree-Fock equations are obtained when we apply the variation $\delta\psi$ on equation (1.17). For electron-hydrogen scattering these equations are:

$$\left[\frac{d^2}{dr^2} - \frac{\ell 2(\ell 2 + 1)}{r^2} + k_n^2 \right] F_\nu^{Ls}(r)$$

$$= \sum_{\nu'} \left[V^L_{\nu\nu'} - W^{Ls}_{\nu\nu'} \right] F^{Ls}_{\nu'}(r)$$

where all quantities are defined by Percival and Seaton (1957). In the positron-hydrogen atom the equations are:

$$\left[\frac{d^2}{dr^3} - \frac{\ell 2(\ell 2 + 1)}{r^2} + k_n^2\right] F_\nu^{Ls}(r) = \sum_{\nu'} V_w^L(r)\ F_{\nu'}(r) +$$

$$\sum_{\mu'} \int_0^\infty K^L_{\nu\mu'}(r,R)\, G_{\mu'}(R)\, dR$$

$$\left[\frac{d^2}{dR^2} - \frac{P2(P2 + 1)}{R^2} + K_m^2\right] G_\mu^{Ls}(R) = \sum_{\mu'} V^L_{\mu\mu'}(R)\, G_{\mu'}(R) +$$

$$\sum_{\nu'} \int_0^\infty K_{\mu\nu'}(R,r)\ F_{\nu'}(r)\, dt$$

where all the quantities are defined by Smith (1961).

1.4 Static Field Approximation

This approximation is a special case of the eigenfunction expansion method where only one term of the expansion (1.1) is taken. The eigenfunction expansion method yields the set of equations

$$\left[\nabla_1^2 + k_n^2\right]F_n(r_1) = \frac{2m}{\hbar^2}\sum_m F_m(r_1)V_{nm}(r_1) \qquad (1.25)$$

with $k_n^2 = \frac{2m}{\hbar^2}(E - \varepsilon_n)$ (1.26)

and

$$V_{nm}(r_1) = \int \psi_n^*(r_2)\left(\frac{1}{r_{12}} - \frac{1}{r_1}\right)\psi_m(r_1)\,dr_2 \qquad (1.27)$$

The static approximation yields the equation

$$\left[\nabla^2 + k_n^2 - \frac{2m}{\hbar^2}V_{nn}(r)\right]F_n(r) = 0 \qquad (1.28)$$

which is reduced to the radial equation

$$\left[\frac{d^2}{dr^2} + k_n^2 - \frac{2m}{\hbar^2}V_{nn}(r) - \frac{(\ell + 1)\ell}{r^2}\right]\emptyset_{n',\ell}(r) = 0 \qquad (1.29)$$

by expanding F_n in terms of Legendre polynomials

$$F_n(r) = \frac{1}{r}\sum_\ell i^\ell(2\ell + 1)e^{i\eta_{n,\ell}}\emptyset_{n,\ell}(r)P_\ell(\cos\theta) \qquad (1.30)$$

At sufficiently low incident energy the dominant contribution to the total elastic cross section comes from the zero order partial wave. It was McDougall (1931) who first solved the radial equation (1.29). He obtained values for the elastic scattering of electrons by hydrogen. Breen (1946) has obtained the same results.

1.5 Correlation

Let us consider the expansion

$$\psi(r_1,r_2) = \sum_n \psi_n (r_2)\, F_n (r_1) \tag{1.31}$$

where $\psi_n(r_2)$ represents the wave function of the atom in its nth state. If we write the first term as representing the zero-order wave function, as in the static field approximation, we make no allowance for the mutual interaction of the atomic electron and the incident particle during the collision. Such an interaction would be accounted for if r_{12}, the distance between the electron and the incident particle, is inserted in the wave function. One would naturally think of employing variational methods to determine the dependence.

Massey and Moiseiwitsch (1951), who used Hulthen's and Kohn's variational methods, investigated the effect of correlation simply by inserting a term depending on r_{12} in their trial function as follows;

$$\psi_t(r_1,r_2,r_{12}) = e^{i n_0} r_1^{-1}\, \phi_t(r_1,r_{12})\, \psi_0(r_2) \tag{1.32}$$

where

$$\begin{aligned}\phi_t(r_1,r_2) = {} & k_0^{-1}(1+a^2)^{-\frac{1}{2}} \times \Big[\sin k_0 r_1 + {} \\ & \{a + (b+cr_{12})e^{-r_1/a_0}\} \quad (1-e^{-r_1/d_0}) \cos k_0 r_1 \Big]\end{aligned} \tag{1.33}$$

They have shown that correlation is not important for low energy scattering.

1.6 Resonance Scattering

When the energy of the incident particle is large enough to excite the target atom then there is a possibility of producing a resonance. Another possibility of a resonance arises when the incident particle is captured by the target atom. This state can decay either into the incident channel or other channels. These possibilities can be illustrated in the following equations;

$$a + b \rightarrow a + b^* \rightarrow a + b^+ + e^- \tag{1.34}$$

$$a + b \rightarrow (a + B) \rightarrow a + b \tag{1.35}$$

$$a + b \rightarrow (a + b) \rightarrow a + b^*$$

where a is the incident particle b the target atom and (a + b) is the bound state formed by a and b, the star * represent excitation. Equation (1.34) describes the first possibility and Equation (1.35) describes the second possibility. These are two examples of situations where we have resonance.

Let us consider the scattering of an electron by a potential V(r). The ℓth order partial wave satisfies the following radial equation;

$$\left[\frac{d_2}{d_r{}^2} + k^2 - \ell\left(\frac{\ell+1}{r^2}\right) - V(r)\right]\phi_\ell(k_\nu r) = 0 \tag{1.36}$$

Here V(r) is spherically symmetrical. One example of it is the static field potential. It is assumed to satisfy (Newton 1960): (To ensure that $V \rightarrow 1/r$ at zero and $1/r^2$ at ∞).

$$\int_0^\infty r\,|v\ (r)|\,dr \quad < \quad \infty \tag{1.37}$$

$$\int_0^\infty r^2\ |\ v\ (r)|\,dr \quad < \quad \infty \tag{1.38}$$

Let $S(\ell k)$ be the scattering matrix. Then the following statements are true (Burke 1965)

A - $S(\ell k)$ is unitary for real k.

B - If S has a pole at k it has poles at $-k^*$ and zeroes at $+k^*$ and $-k$

C - Poles of k on the imaginary axis represent bound states.

D - If a pole is in the upper half of the k plane it must lie on the imaginary axis.

E - Poles in the lower half are symmetrical with respect to the imaginary axis.

The cross section is proved to have the approximate form

$$\sigma_\ell(k^2) \approx \frac{4(2\ell+1)}{k \quad \ell n^2} \qquad \frac{\Gamma_\ell \quad n^2}{(E - E_{\ell_n})^2 + \frac{1}{4}\Gamma^2_{\ell_n}} \tag{1.39}$$

where $\frac{1}{2}\Gamma$ is the imaginary part of k^2 at a pole. If $E = E_{\ell_n}$ and the pole is close to the real axis, the cross section becomes very large. This resonance can be seen from

$$\delta_\ell(k^2) = \delta^{NR} + \sum_n \text{arc tan} \frac{\frac{1}{2}\Gamma_{\ell n}}{F_{\ell_n} - E} \tag{1.40}$$

where the second term goes through π .

Let us consider the two-channel generalization. We introduce two branch points for the s-matrix at

$$k_1 = \pm \sqrt{a} \tag{1.41}$$

which is accomplished by the transformation

$$k_1^2 = k_2^2 + a \tag{1.42}$$

In order to keep the s-matrix single valued in the k plane we imagine a cut from $\sqrt{a}$ to $-\sqrt{a}$. When there is no coupling we have two diagonal elements for the s-matrix. The bound state poles of the second channel which lie on the imaginary axis in the k_2 plane by transformation (1.42), lie in k_1 between the two branch points on the real axis. When coupling occurs, these bound state poles move off the real axis downwards. This gives rise to resonances provided the coupling is small, i.e. Γ is small. This is the condition mentioned after equation (1.39).

CHAPTER TWO

Polarization

It has long been recognized that if a charged particle is scattered at low energy by an atom, the atom distorts slightly in the electric field of the particle. The induced multipoles produce an attractive potential referred to as the polarization potential.

If the polarization potential is ignored, the total wave function takes the form:

$$\psi(1,\ldots\ldots,N) = u_0(1)\phi_0(2,\ldots\ldots,N) \qquad (2.1)$$

where 1 stands for the set of co-ordinates of the scattered particle, and 2,......,N stand for the co-ordinates of the atomic electrons. ϕ_0 is the eigen function of the unpreturbed atomic system.

One way of considering polarization is to expand the total wave function in terms of the atomic eigen functions. In this case equation (2.1) becomes

$$\psi(1,\ldots\ldots N) = U_0(1)\phi_0(2,\ldots\ldots,N) + \sum_{i=1} u_i(1)\ \phi_i(2,\ldots\ldots,N) \qquad (2.2)$$

where ϕ_i are the eigen functions corresponding to all the other states of the atom. When this total wave function is substituted in the Schrodinger equation, we obtain a set of equations in $u_1(1)$. Unfortunately the method of using more terms than one in the expansion (2.2) leads to considerable difficulties.

In many cases the eigen functions of the atomic system are not always known. In order to avoid the difficulties one is restricted to a limited number of terms. By doing this all the other terms which are important in describing polarization are left out. Even when the number of terms is restricted to two the calculation of solving the coupled integro-differential equations is complicated and time consuming. This is not the only reason which prevents one from using this method. Keeping the complete set of terms in expansion (2.2) is the only way of getting the exact description of the collision. We do not know the relative importance of the different terms including the continuum. It has been found in some cases (Newstein 1955) that the states of the continuum are important in describing low-energy scattering. Apart from hydrogen there is no adequate approximation that uses the continuum states in expansion (2.2).

The eigen function expansion method for describing polarization therefore ignores the effect of the continuum, and all eigen functions beyond the trunction. Added to this is the difficulty associated with solving the equations obtained.

Relatively few successful calculations have been made for Quantitative evaluation of distortion. There are several techniques in practice. The earliest were rather primitive, and include ad. hoc. constants. Later development brought more sophisticated techniques to existence. They are the same in principle, and they use a perturbation method or variational methods.

2.1 Development of the Theory

One of the simplest ways of considering polarization was used by Holtsmark (1930) and Bates and Massey (1947). They used the potential

$$V_p = - \left[\frac{p}{(s^2+r^2)^2} \right] \tag{2.3}$$

where s is a cut off distance inserted for the purpose of preventing this term from diverging at the origin, p is a constant. The sign (-) is there to indicate the attractive nature of the polarization.

This parametric treatment of polarization enables one to employ it for both polarization and exchange (in the case of electron-atom scattering). The argument behind that is that both polarization and exchange are attractive. By exaggerating one of them, the other is automatically accounted for.

This potential is added to the static field potential in the static approximation or in the exchange approximation. Bransden (1958) has objected to including both exchange and polarization in this way arguing that the resulting equation cannot be derived from a variational treatment of the Schrodinger equation.

p and s have been determined by Klein and Brueckner (1958) for the scattering of electrons by oxygen atoms. Mittleman and Watson (1959) have used variational methods together with model calculations to find the best values of the constants.

Better methods of including polarization have developed for small systems. The first of these was derived by Bethe (1943) in studies of core polarization in the excited states of helium. Modifications of this method have been used by Bransden and Dalgarno (1953), Martin et. al. (1958) and Temkin (1957). The method now is referred to as the "Polarized orbitals" approach.

Later attempts aimed to represent the distortion by an effective potential. Watson et. al. (1959) developed such an approach for the calculation of electron and ion scattering. The weak point of their method is that it requires a high order perturbation method. That is because of the lack of orthogonality between the unperturbed wave-functions and the correction functions.

2.2 The Method of Polarized Orbitals

Dalgarno and Lewis (1957) have devised a method in which the distortion is considered as the result of the perturbation in the Hamiltonian due to the presence of the scattered particle. For the case of electron-hydrogen scattering, this perturbation is

$$V\ (r_1,r_{12}) = \frac{2}{r_{12}} - \frac{2}{r_1} \tag{2.4}$$

where r_1 is the distance between the proton and the scattered electron and r_{12} is the distance between the two electrons. In the positron-hydrogen case the corresponding potential is $-V$. For sufficiently large r_1, V can be expanded in terms of Legendre polynomials according to the following equation:

$$V \sim 2 \sum_{n=1}^{\infty} \frac{r_{12}^{\ n}}{r_1^{\ n+1}} P_n(\cos \theta) \tag{2.5}$$

where $P_n(\cos \theta)$ is the nth order Legendre polynomial, and θ is the angle between r_1 and r_{12}. The perturbation method provides us with first and second order corrections to the unperturbed Hamiltonian. Since the eigenfunctions of this operator are the functions $\psi(r_2)$ of the atomic electron, then the corrections calculated in this way are independent of r_2, and hence the perturbing potential is dependent on r_1. Here the three-body problem is reduced to a two-body problem.

The corrections of the first and second order are

$$E_1 = (0|V|0) = \int \overset{*}{\psi}(r_2)\ V\ \psi\ (r_2)\ d\underset{\sim}{r}_2 \tag{2.6}$$

$$E_2 = \sum_{m\neq 1} \frac{(0|V|m)\,(m|V|0)}{E - \varepsilon_m} \tag{2.7}$$

where

$$(p|V|9) = \int \psi_p{}^{*}\ V\ \psi_9\ dr \tag{2.8}$$

and $\psi_n(r_2)$ is the nth orbital of the atom. The summation includes integration over the continuum. If we substitute (2.5) into (2.7) we obtain a series expansion in inverse powers of r_1 which represent the long range forces between the atom and the scattered particle. E_1 is the static field potential. E_2 is the correction we are interested in. If all of the terms are retained E_2 gives a second order correction. Dalgarno and Lewis (1957) used the rule

$$\sum_{m\neq 1} \frac{(0|g|m)\,(m|g|0)}{E - \varepsilon_n} = (0|fg|0) - (0|f|0)\,(0|g|0) \tag{2.9}$$

where f satisfies the equation

$$2\nabla f.\nabla\psi_0 + \psi_0\nabla^2 f = V\psi_0 - (0|V|0)\,\psi_0 \tag{2.10}$$

By that they could obtain an expression for the complete long range forces E_2. Unfortunately it will be shown later that it if not the complete polarization potential that we are interested in, because the monopole part of this potential needs suppressing, in which case the different parts of the potential need to be calculated separately. The expression obtained by Dalgarno and Lewis for the complete polarization is

$$
\begin{aligned}
E_2 = {} & \frac{1}{r^2}\ \{5-(4r^2+8r+10)\ \exp(-2r)\ + \\
& (4r^3+7r+5)\ \exp(-4r)\,\} - \frac{2}{r^2}\{(r+1)^2 \\
& \exp(-2r)\,(1+\exp(-2r)E_i(2r)) +\ (r-1)^2 \exp(2r) \\
& +(r^2+2r-3)\ +\ (4r+4)\exp(-2r)E_i\ -2r \\
& -2(r+1)^2 \exp\ -2r\ \ (1+\exp\ -2r\ ) \\
& (\sigma+\mathrm{Log}\ 2r)\,\}
\end{aligned}
\qquad (2.11)
$$

where σ is Euler's constant 0.5772157 and

$$E_i(x)\ =\ -\int_{-x}^{\infty} S^{-1}\exp(-S)\,dS \qquad (2.12)$$

At the same time Temkin (1957) followed slightly different lines in obtaining his polarization. In the following we shall describe briefly his method. The total wave function of the atom plus scattered particle can be written in the form

$$\psi(1,\ldots,N)\ =\ u_0(1)\ \phi_0(1,\ldots,N)+\phi^{p}(1,\ldots,N)$$

where the atom has (N-1) electrons, ϕ_0 is the wave function of the unperturbed atom. ϕ^p is the correction to be determined. It describes the distortion in the atomic system since $u_0(1)$ is outside of the brackets. But it is dependent on 1 (the scattered particle co-ordinates). This is the basic idea of the polarized orbitals method.

Let H_0 be the unperturbed Hamiltonian of the target. It can be written in the form

$$H_0 = \sum_{i=2}^{N} - \nabla_i^2 + \sum_{i=2}^{N} \frac{2(N-1)}{r_i} - \sum_{i>j}^{N} \sum_{j=2} \frac{2}{r_{ij}} \qquad (2.14)$$

The atomic wave functions $\phi_0(2,\ldots,N)$ are the eigen functions of H_0, and they are supposed to be known before hand. The total Hamilton H has the form

$$H = H_0 + \quad - \nabla_1^2 + \frac{2(N-1)}{r_1} - \sum_{i=2}^{N} \frac{2}{r_{ij}} \qquad (2.15)$$

In some approximations the scattered particle is assumed to be static at distance r_1, in which case the kinetic energy operator is neglected. Here the co-ordinates r_1 of the scattered particle are treated as parameters. The solution of this problem will be a function of the co-ordinates 2,...,N. Therefore ϕ^{pol} is similar to ϕ_0 in this respect. This is the adiabatic approximation. The distortion of the atomic orbitals from their unperturbed form is represented by the function ϕ^{pol}. Having obtained the total wave function for the system we can treat it in the same was as in the no-polarization case. That is, to substitute it in the Schrodinger equation

$$(H - E)\ \psi = 0 \tag{2.16}$$

which can easily be reduced to an integro-differential equation. The difference between this equation and the no-polarization one is the existence of additional terms.

The other approximation apart from the adiabaticity in Temkin's method is done after noticing that polarization effects arise at distances of the scattered particle which are greater than the average radius of the electron clouds of the atom. This enables us to neglect terms like $1/r^n$ whenever n is larger than two. If the perturbing potential is expanded in terms of Legendre polynomials as in the equation

$$\frac{2(N-1)}{r_1} - \sum_{j=2}^{N} \frac{2}{r_{1j}} = \frac{2(N-1)}{r_1} - \sum_{j=2}^{N} \sum_{n=1}^{\infty} \frac{2r_<^{\,n}}{r_>^{\,n+1}}\, p_n(\cos \theta_{ij}) \tag{2.17}$$

where $p_n(\cos \theta_{ij})$ is the nth order Legendre polynomial and θ_{ij} is the angle between r_i and r_j, then it is a reasonable approximation to replace $\frac{r_<^{\,n}}{r_>^{\,n+1}}$ by $\frac{r_j^n}{r_1^{\,n+1}}$ and hence neglect all but the first two terms in the summation. The perturbing potential now becomes:

$$V = \sum_{j=2}^{N} \frac{2r_j}{r_1^{\,2}} \cos \theta_{ij} \tag{2.18}$$

This is referred to as the dipole approximation. In order to justify this approximation we recall the fact that due to the boundary condition at the origin, the multiplication of r_1 by the scattered particle wave function is necessarily small. Because of that it is expected that the main interaction near the origin is the nuclear coulombic interaction. The coulombic interaction of the orbital electrons is small in comparison.

In this approximation, summation (2.18) is added to the Hamiltonian H_0 of the unperturbed atom. H, the total Hamiltonian, becomes

$$H = H_0 + \sum_{j=2}^{N} \frac{2r_j}{r_1^2} \cos \theta_{1j} \qquad (2.19)$$

The same assumption, namely $r_1 > r_j$, is used again to enable us to consider the deviation of the Hamiltonian relatively small, which is what the perturbation method requires. In this case the unperturbed wave function ϕ_0 goes over to ϕ and can be determined either by the perturbation method or variational methods.

2.3 The Adiabatic Approximation

The adiabatic method has been considered for some time. Its advantage is its simplicity. Its incompleteness, however, has been also recognised, and consequently prevented one from taking it quite seriously.

The adiabatic approximation employs the assumption that the scattering particle wave function in the perturbed atomic orbital equation is stationary. This reduces the exact equation to one similar to the unperturbedequation.

The error produced by the adiabatic approximation is expected to increase with the velocity of the scattered particle. This may also be seen from the following analysis. For very low velocity of the incident particle, the atomic electrons move sufficiently fast to adjust themselves to the slow changes in position of the incident particle. However, as the velocity of the incident particle increases, either by increasing the initial velocity with which that particle starts its motion towards the target, or under the effect of accelaration caused by the attractive polarization potential, the point is soon reached where the changes in position of the incident particle are too large for the atomic electrons to follow. When this occurs, the statically derived perturbed orbitals give essentially an over-estimate of the attractive polarization potential.

The excess of attraction introduced by the adiabatic second order potential can be traced to the monopole or short-range part (Drachman 1965).

Higher-order adiabatic calculation should naturally improve the qualitative situation. One may then rely on the adiabatic approximation. In particular, E. A. Hyllaraas (1931) has used the complete adiabatic potential for the H_2 ion. The complete adiabatic problem assumes two fixed positive particles in whose field an electron moves within the frame work of quantum mechanics. Adiabaticity is more justifiable for heavier incident particles in which case rearrangement is more probable. The reason for this is that the adiabatic approximation is based on emphasizing the movement of the atomic electrons compared with that of the incident particle, and this is more so for heavy incident particles. The mass centre of the heavy incident particle plus atomic electron is nearer to the incident particle. The atomic electron does most of the movement induced by the mutual interaction as well as the nuclear interaction.

The adiabatic theory is correct in the limit when the distance between the target and the scattered particle is large and when an inelastic collision is energetically impossible. At large separations the dipole moment has a large effect on attracting the colliding particle. This particle is subject to a potential

$$V_p \sim - \frac{\alpha}{2r^4} \tag{2.20}$$

which is the dipole moment induced in the target atom, x being its polarizability.

One consequence of the adiabatic approximation is that by approaching the nucleus, the incident particle reaches a situation in which it can exchange with the atomic electron if it is an electron or pick it up if it is a positron. Thus, the adiabatic approximation partly includes exchange (or partly includes pick-up).

2.4 Corrections to the Adiabatic Approximation

The adiabatic approximation consists of including only the static polarization potential part of the distortion effects through second order in the interaction of the atom with the scattered particle. Thus, all the velocity dependent interactions are neglected in this approximation.

Allowance for non-zero velocities of the scattered particle is made by coupling the wave function representing the motion of the scattered particle into the equation for the perturbed atomic orbitals. This polarization of the atomic orbitals is consistent with the motion of the scattered particles for all velocities. The interaction results from the operation of the kinetic energy operator of the scattered particle obtained in the adiabatic atomic orbitals (Labahn and Callaway 1966). The effect of this interaction, thus, tends to correct the error produced by the use of perturbed orbitals to describe polarization when the incident particle has a large wave number,.

The wave function of the atom, being dependent on the co-ordinates of the incident particle means that there is a contribution to the kinetic energy of the system from the action of the kinetic energy operator of the scattered particle on the atomic wave function. This contribution depends on r_1 (the co-ordinates of the incident particle), and it contributes to the effective potential experienced by the scattered particle. This effect is repulsive. That is, it tends to counterbalance the attractive polarization potential. It is given the name "Distortion potential" by Laban and Gallaway (1966). They have added it to the adiabatic potential in the calculation of electron-helium, electron-hydrogen, positron-helium, and positron-hydrogen scattering. Their work yielded fairly good agreement with assumed exact results of rigorous variational calculations. The monopole polarization which over-estimates the attraction has been successfully suppressed.

CHAPTER 3

Rearrangement Collisions

General Theory

3.1 Formal expressions for the scattering amplitude:

Let us consider the following processes: electron capture by ions or atoms from atoms, exchange in electron-atom scattering, and the formation of positronium by positron impact on atoms. During the collision between the two systems of particles in these processes one or more particles are exchanged between the two systems. We refer to these processes as rearrangement collisions.

Let the number of interacting particles be three. Let particles (2) and (3) be initially bound in a state (2+3). As a result of the collision there is a certain probability that particle (1) and (2) will be bound in a state (2+1) and particle 3 set free. Let the Hamiltonian be

$$H = K + V_1 + V_2 + V_3 \tag{3.1}$$

where K is the kinetic energy operator of the whole system. V_1,V_2 and V_3 are the potentials acting between particles (2) and (3), (3) and (1), and (1) and (2) respectively. We define the resolvents (Green's functions) $G(\eta)$ and, $G_\alpha(\eta)$ as the following:

$$G(\eta) = (\eta - H)^{-1} \tag{3.2}$$

$$G_\alpha(\eta) = (\eta - K - V_\alpha)^{-1} \qquad \alpha=0,1,2,3 \tag{3.3}$$

where $V_0 \equiv 0$. We note that G_1 and G_3 are the appropriate resolvents to the initial and final states respectively.

Initially V_2 and V_3 are zero. The Schrodinger equation is

$$(K + V_1 - E_n)\emptyset_n^{(1)}(E_n) = 0 \tag{3.4}$$

where $\emptyset_n^{(1)}(E_n)$ is the nth state of the system. It represents a bound-state and a plane wave. The Schrodinger equation of the complete system is

$$(H - E_i)\psi_i^{(+)}(E_i) = 0 \tag{3.5}$$

where (+) stands for the out-going wave, in which (2+3) are initially bound and (1+2) finally bound. From (3.3),(3.4) and (3.5) we have

$$\psi_i^{(+)}(E_i) = \mathrm{Lim}_{\varepsilon \to 0}\psi_i^{(+)}(E_i + i\varepsilon) \tag{3.6}$$

where

$$\psi_i^{(+)}(E_i + i\varepsilon) = \emptyset_i^{(1)}(E_i) + G_1(E_i + i\varepsilon)(V_2 + V_3) \times \psi_i^{(+)}(E_i + i\varepsilon) \tag{3.7}$$

and

$$(H - E_i - i\varepsilon)\psi_i^{(+)}(E_i+i\varepsilon) = -i\varepsilon\emptyset_i^{(1)}(E_i) \tag{3.8}$$

If we operate on (3.2) on the left and right by (n-k) we obtain -the following equations for G.

$$G = G_0(\left[1+(V_1+V_2+V_3)G\right] = \left[1+G(V_1+V_2+V_3)\right]G_0 \tag{3.9}$$

and

$$G = G_1\left[1+(V_2+V_3)G\right] = \left[1+G(V_2+V_3)\right]G_1 \tag{3.10}$$

From (3.10) and (3.2) we have

$$\left[1-G_1(V_2+V_3)\right]\left[1+G(V_2+V_3)\right] = 1 \tag{3.11}$$

From (3.7) and (3.11) we have

$$\psi^{(+)}(E_i+i\varepsilon) = \left[1+G(E_i+i\varepsilon)(V_2+V_3)\right]\emptyset_i^{(1)}(E_i) \tag{3.12}$$

By operating on (3.11) by $(E+i\varepsilon-K-V_1)$, then by G_3, and rearranging we obtain

$$\left[1-G_3(V_1+V_3)\right]\left[1+G(V_2+V_3)\right] = 1+G_3(V_3-V_1) \tag{3.13}$$

This leads to

$$\begin{aligned}\left[1-G_3(V_1+V_2)\right]\psi_i^{(+)}(E_i+i\varepsilon) &= \left[1+G_3(V_3-V_1)\right]\emptyset_i^{(+)}(E_i)\\ &= i\varepsilon G_3\emptyset_i^{(1)}(E_i)\end{aligned} \tag{3.14}$$

and consequently

$$\psi_i(E_i+i\varepsilon) = G_3(E_i+i\varepsilon)\left[i\varepsilon\phi_i^{(1)}(E_i)+(V_1+V_2)\psi_i^{(+)}(E_i+i\varepsilon)\right] \quad (3.15)$$

Lippmann (1956) has shown that the first term on the right-hand side of (3.14) contains no singularity and hence, vanishes with $\varepsilon\rightarrow 0$ except for the case when all three particles are unbound initially and finally. Equations (3.17) and (3.15) may be written in the form:

$$\psi_i^{(+)}(E_i) = \phi_i^{(1)}(E_i)+\left[\mathrm{Lim}_{\varepsilon\rightarrow 0}G_1(E_i+i\varepsilon)\right](V_2+V_3)\psi_i^{(+)}(E_i) \quad (3.16)$$

$$\psi_i^{(+)}(E_i) = \left[\mathrm{lim}_{\varepsilon\rightarrow 0}G_3(E_i+i\varepsilon)\right](V_1+V_2)\psi_i^{(+)}(E_i) \quad (3.17)$$

(3.16) represents the case where no rearrangement occurs. (3.17) represents the case where rearrangement occurs. The final state of the rearrangement collision satisfies

$$(K+V_3-E_m)\phi_m^{(3)}(E_m) = 0 \quad (3.18)$$

From (3.15) it is easily shown that the transition rate W_{if} is

$$W_{if} = \frac{\partial}{\partial t}\ |<\phi_f^{(3)}|\psi i^{(+)}>|^2 = \mathrm{Lim}_{\varepsilon\rightarrow 0}\frac{2\varepsilon}{\hbar}\ \frac{|T_{if}|^2}{(E_i-E_f)^2+\varepsilon^2} \quad (3.19)$$

where

$$T_{if} = (\phi_f^{(3)}(E_f)|V_1+V_2|\psi_i^{(+)}(E_i)) \quad (3.20)$$

but since

$$\lim_{\varepsilon\to 0} \frac{\varepsilon}{X^2+\ ^2} = i\pi\delta(x) \tag{3.21}$$

W_{if} becomes

$$W_{if} = \delta(E_i - E_f)\,\frac{2\pi}{\hbar}|T_{if}|^2 \tag{3.22}$$

In the same way it can be shown that

$$T_{fi} = (\psi_f^{-}(E_f)\,|V_2+V_3|\,\phi_i^{(1)}(E_i)) \tag{3.23}$$

where here the process is reversed. The wave function $\psi_f^{(-)}$ satisifies

$$\psi^{(-)}(E_f - i\varepsilon) = \phi_f^{(3)}(E_f) + G_3(E_f - i\varepsilon)(V_1+V_2)\psi_f^{(-)}(E_f - i\varepsilon) \tag{3.24}$$

Castillejo et. al (1960) have used an explicit configuration space treatment and obtained the same results for the electron-hydrogen atom scattering.

3.2 Eigenfunction Expansions

This method has its major application for low-energy scattering, although it is by no means confined to that situation. Instead of using the usual expansion

$$\psi_i^{(+)}(E_i) = \sum_n \psi_n^{(1)}(R_1)F_n^{(1)}(r_1) \qquad (3.25)$$

where R_1 is the relative position vector of particles 2 and 3 (R_2 and R_3 are defined in a similar way), in rearrangement problems we use

$$\psi_i^{(+)}(E_i) = \sum_n^{(1)} \psi_n^{(1)}(R_1)F_n(r_1) + \sum_m \psi_m^{(3)}(R_3)G_m(r_3) \qquad (3.26)$$

where $\psi_m^{(3)}$ is the mth orbital of the system (1+2), and F_0 and G_0 have the asymptotic forms

$$F_0(r_1) \sim \exp(ik_i,r_1) + r_1^{-1}\exp(ik_i,r_1)f(\theta_1,\phi_1) \qquad (3.27)$$

$$G_0(r_3) \sim r_3^{-1}\exp(ik_f\ r_3)g(\theta_3,\phi_3) \qquad (3.28)$$

where f and g are the scattering amplitudes for the direct and rearrangement collisions respectively.

It should be noted that the terms at the first summation are not orthogonal to the terms of the second summation, but the whole expansion is complete. It is common to avoid the calculational difficulties to take the first term of each summation. This corresponds to considering the initial state and the final state of the rearrangement collision.

Proceeding according to the Hartree-Fock method we form the quantity

$$I = \quad d\tau\{\psi_i^{*}(H-E)\psi_i\} \tag{3.29}$$

where ψ_i is substituted from (3.26). If we use the property that I is stationary under the independent variations of F_n and G_n we obtain the Euler equations of I which on using the Schrodinger equations for $\psi_0^{(1)}$ and $\psi_0^{(3)}$ become

$$\left[\nabla_{r_1}^{2}+k_i^{2}+U_{11}(r_1)\right]F_0(r_1) = \frac{\mu_1}{\mu_3}\int dr_1\{\psi_0^{(1)*}(R_1)$$

$$\psi_0^{(3)}(R_3)\left[-\nabla_{r_3}^{2}-k_f^{2}+\frac{2\mu_3}{\hbar^2}(V_1+V_2)\right]G_0(r_3)\} \tag{3.30}$$

$$\left[\nabla_{r_3}^{2}+k_f^{2}+U_{33}(r_3)\right]G_0(r_3) = \frac{\mu_3}{\mu_1}\int dR_3\{\psi_0^{(3)}(R_3)$$

$$\psi_0^{(1)}(R_1)\left[-\nabla_{r_1}^{2}-k_1^{2}+\frac{2\mu_1}{\hbar^2}(V_3+V_2)\right]F_0(r_1) \tag{3.31}$$

where $\hbar k_i$ and $\hbar k_f$ are the initial and final relative momenta of the colliding particles respectively. U_{11} and U_{33} are the static potentials in the initial and final states respectively. They satisfy the following equations:

$$U_{11}(r_1) = \frac{-2\mu_1}{\hbar^2}\int dR_1\{\psi_0^{(1)*}(R_1)\psi_0^{(1)}(R_1)(V_2+V_3)\} \tag{3.32}$$

$$U_{33}(r_3) = \frac{-2\mu_3}{\hbar^2}\int dR_3\{\psi_0^{(3)*}(R_3)\psi_0^{(3)}(R_3)(V_1+V_2)\} \tag{3.33}$$

Equations (3.30) and (3.31) can be reduced in different ways according to the type of systems in hand. For example, for low-energy electron-atom or positron atom scattering F_i and G_i are expanded in partial waves. If, on the other hand, the bound system is much heavier than the colliding particle, then the system of equations is converted to coupled differential equations rather than integro-differential equations (Bates (1958).

3.3 Charge exchange reactions:

We define charge exchange reactions as those in which one or more electrons bound to one system are picked up or captured by another. Let ion B be incident on ion (A+e). Then the interaction is described by the following equation:

$$B + (A+e) \rightarrow (B+e) + A \tag{3.34}$$

An example of this reaction is the case of a proton scattered by a hydrogen atom in the ground state. The result of the interaction is that the electron is picked-up by the incident proton to form a new hydrogen atom (not necessarily in the ground state). We can describe this in the following equation:

$$H^+ + H_0 \rightarrow H_\alpha + H^+ \tag{3.35}$$

where 0 and α are the ground state and the αth state of the hydrogen atom respectively. In this case T_{if} defined in equation (3.20) takes the form

$$T_{if} = \int dr_3 \int dR_3 \{\psi_\alpha^*(R_3)\exp(-ikf.r)\left[V_2(R_2)+V_1(R_1)\right]\psi_i(r_1,R_1)\} \tag{3.36}$$

where $\psi_\alpha(R_3)$ is the αth state of the hydrogen atom. From T_{if} it is easy to obtain the total cross section for the scattering

$$Q_{i\to f} = 2\pi \int_{1}^{+1} |g(\theta)|^2 \, d \cos \theta \qquad (3.37)$$

where

$$g(\theta) = \frac{M}{2\pi} T_{if} \qquad (3.38)$$

Here we have taken the mass of the electron equal to one and that of the proton equal to M. and $\cos \theta = (-\vec{ki} \cdot \vec{kf}/k_i k_f)$ and $V_1(X) = V_3(X) = -V_2(X) = -\frac{1}{X}$ the solution of this problem can be simplified by considering the fact that the potential between the two protons should not contribute to the scattering amplitude. This has been indicated by Oppenheimer (1928) and Brinkman and Kramers (1930). The reason for this is that r_3 satisfies

$$r_3 = -R_2 + \left[1 | (M+1)\right] R_3 \qquad (3.39)$$

and the mass M of the proton is much greater than that of the electron. Hence $r_3 \approx -R_2$ to the order of 1/M and $V_2(R_2)$ can be replaced by $V(r_3)$. But since any potential which is a function of the distance between the centre of masses of the two colliding particles does not contribute to rearrangement or excitation we can ignore $V_2(r_3)$. i.e. $V_2(r_3)$ in equation (3.36) should be neglected. Another way of justifying this is by considering the fact that due to the great incident energy of the proton, the de-Broglie wave length is negligible compared with the atomic dimensions.

Consequently, we can treat the relative motion classically. It follows that direct and exchange scattering amplitudes can be obtained separately, even if A and B were identical. The trajectories of the protons are affected negligibly from the classical ones, which are straight lines defined by an impact parameter. In this case v_2 does not contribute to the scattering amplitude. This is true unless the stage of close distances plays the most important role in determining the scattering (Fennema 1963).

3.4 The Born Approximation

When the incident particle has a large velocity compared with that of the orbital electron, a plane wave approximation may be used (Brinkman and Kramers (1930)). The incident wave is seriously distorted. The energy of the incident particle should be considerably above 25 k.e.v.

Bates and Dalgarno (1952) have used the cross section calculated by Brinkman and Kramers using plane waves and omitting the internuclear potential for electron capture by protons in helium. They used the simple variational wave function for the helium atom

$$\psi(X,y) = \frac{X^3}{\pi} \exp\{-\lambda(X+y)\}, \qquad \lambda = 1.6875 \tag{3.40}$$

They found out that the Brinkman-Kramers cross section is several times too large.

The potential which acts between the two nuclei should not be dropped as has been suggested in the preceding approximation. For better results one would look for higher-order terms in the Born series. The second term in this series is retained. Unfortunately the second Born approximation has so far resisted complete evaluation, but Drisko (1955) has examined the high energy behaviour of this approximation and obtained some interesting results. For electron capture by protons in hydrogen,

$$T_{if}^{B_2} = (\phi_f^{(3)} | (V_1+V_2)+(V_1+V_2)G_0(V_2+V_3) | \phi_i^{(1)}) \tag{3.41}$$

where G_0 is given by

$$G_0(r_3, R_3, r_3^1, R_3^1) =$$

$$(2\pi)^{-6} \int dq_3 \int dp_3 \frac{\exp i\{q_3 \cdot (r_3-r_3^1)+P_3(R_3-R_3^1)\}}{k^2_f k_{p_3}+E_B+i -E_{q_3}-E_{P_3}}$$

where it has been represented in configuration space. E_B is the energy at the (1s) ground state of hydrogen and P_3 is the relative momentum of particles of 2 and 1. q_3 is the momentum of 3 relative to the center of mass of (2+3). P_3 and q_3 are given by

$$P_3 = \left(\frac{1}{M_2+m_1}\right) \left[m_1 k_2 - m_2 k_1\right] , \tag{3.43}$$

$$q_3 = \left(\frac{1}{m_1+m_2+m_3}\right) \left[m_3(k_2+k_1)-(m_2+m_1)k_3\right] \tag{3.44}$$

and the reduced mass μ is given by

$$\mu_3 = \frac{m_3(m_1+m_2)}{m_3+m_2+m_1} \tag{3.45}$$

The crosssection in the high-energy limit becomes

$$Q^{B2} \sim \frac{1}{4\pi v^2} \int_{v^2/4}^{\infty} \left| \frac{-32\pi}{(1+\alpha^2)^3} + \frac{16\pi}{\alpha^2 (V^2/2- \alpha^2/2+4iV} \right|^2$$

$$= \{0.2946 + \frac{5\pi\nu}{2^{12}} \} Q_{BK} \tag{3.46}$$

where Q_{BK} stands for the Brinkman-Kramers cross section. These results are interesting. It has been shown that the internuclear potential is cancelled by the second order term. No matter how high the energy, the Born series does not converge to its first term. The second term in (3.46), which dominates the cross section, changes the velocity dependence from V^{-12} to V^{-11} if the energy is high enough.

CHAPTER 4

Review of previous work

Electron-atom scattering is closely connected with positron-atom scattering. The electron and positron have the same mass and the same magnitude of change (one negative and the other positive). In most calculations one can obtain the equations of one of the two problems from those at the other by simply altering some signs. One can learn about various effects by comparing the two problems. Therefore it is interesting to review the previous work done for electron-atom scattering as a stage leading to positron-atom scattering calculations, especially since most approximations have been originally devised for electron-atom scattering.

4.1 Electron-atom scattering

One of the earliest works on electron-atom scattering was done by MacDaugall (1933) on electron-helium scattering. He attempted to determine the atomic wave function using the Hartree approximation. Morse and Allis (1933) emphasised the importance of exchange and used antisymmetrical wave functions to describe the scattering. Later, various works completed the treatment of the problem by considering polarization and correlation as well as exchange. Among various collision problems, those of electron-hydrogen and electron-helium have received the most attention.

It is natural to include exchange and distortion in the electron-helium scattering problems. Moiseiwitsch (1960) has found good agreement between his results and experiment. The relative error was (± 15%). This led him to conclude that the most important affects in this scattering are exchange and distortion, and that all other effects lead to small corrections. In his calculations which involved both solving the integro-differential equations and the use of variational methods, the scattering length was (1.442) atomic units.

O'Malley on the other hand (1963) extrapolated his scattering length and it was (1.19) atomic units. These two figures are to be compared with the experimental figure which is (1.32). It is quite reasonable to believe that the difference is caused by neglecting polarization.

Total elastic cross sections for the scattering of electrons from hydrogen in its (1s) state have been calculated by Burke and Smith (1962), allowing for virtual excitation to the (2s) and (2p) states and for incident energies below (10.2) electron volts. They showed that the virtual states are important.

Massey and Moiseiwitsch (1951) have applied the Hulthen and Kohn variational methods for electron-hydrogen scattering allowing for exchange and polarization. They have shown that exchange is more important than polarization.

4.2 Positron-Hydrogen Scattering

Although no experimental results exist for positron-hydrogen scattering, comparison can be made between the results of various approximations to learn more about the physics of the process.

It has been realized that, to some extent, the calculation of the positron-hydrogen atom phase shift is not reliable. There is some doubt about the rigorous upper bounds for the scattering length (Spruch and Rosenberg 1960, Schwartz 1961). For although Schwartz has used as many as fifty variational parameters in obtaining his scattering length and phase shifts, Rotenberg (1962) using Sturmian functions has obtained phase shifts considerably larger than those of Schwartz.

Since the positron and the atomic electron are distinguishable, then the problem of antisymmetrization does not exist. However, the possibility of the formation of positronium produces the necessity of adding terms similar to those for electron atom scattering.

Virtual positronium formation produces an attractive potential which has the effect of reducing the absolute value of the negative phase shift given by the mean static approximation. It is not enough, though, to change the sign form negative to positive. The reduction is consistant with Percival's theorem (1960). This theorem states that any further allowance for distortion of the atomic wave function will appear as an effective attraction tending to reduce the magnitude of the negative phase shift.

There are two points which play a basic role in positron hydrogen scattering. The first point is that at close distances the positron feels the repulsion of the positive proton. The second point is that at far distances it feels the attraction of the induced dipole moment of the hydrogen atom. Solving the problem of positron-hydrogen scattering then determines the combination of those two extreme cases.

The importance of the study of positron reactions was emphasised by Massey and Mohr (1954), who calculated the cross-section for the positronium formation reaction (1) from threshold (6.75 ev) to 32 ev in the first Born approximation. They also calculated the cross-section at 13.5 ev. in a distorted wave approximation in which the $l = 0$ partial cross-section was corrected by employing the wavefunction of a positron moving in the static field of a hydrogen atom, in place of a plane wave. The cross-sections obtained by the two methods disagreed (see figure 1), showing that a plane wave approximation was not adequate. To go beyond first order methods, Cheshire (1964) applied a version of the impulse approximation, but as multiple scattering could not be included this procedure is difficult to justify. The results he obtained are also shown in fig. 1 and are within a factor of two of those of the Born approximation.

Massey and Moussa (1958) have used the static approximation for 1 = 0 for k = 0.2, 0.5 and 1.0 Smith et al (1960) have checked these results and solved the problem for k = 1.0, 1.2, 1.5 and 2.0 for all significant partial wave contributions to the elastic scattering cross section.

Smith et. al (1960) have used the strong coupling approximation for k = 1.0, 1.2, 1.5 and 2.0 for all significant partial waves.

Moussa (1959) has applied the Hulthen and Kohn variational methods in which he took polarization into account. The results supported the idea that polarization is attractive.

Smith and Burke (1961) have calculated the S and P and D waves by the strong coupling approximation including excitation to the 2s state.

C. Schwartz (1961) has calculated the phase shifts for 1 = 0 using Kohn's variational principle with 50 trial functions of the type introduced by Hylleraas. He calculated the phase shift for energies up to 10 e.v. The solution did not converge as rapidly as in the case of electron-hydrogen scattering. The results were of probable error of about ± 0.001 radians. For the scattering length he found the upper bound $a_+ \leq -2.17$.

Bransden (1961) has estimated the effect of real or virtual positronium formation by a perturbation method. In this method the effect of the static field potential of the hydrogen atom is automatically allowed for. The results support the fact that the positron is attracted to the atom at low energies.

Cody et. al (1964) have included polarization and found that it does change the sign of the phase shift for $k^2 < 0.16$ showing that for low energies of impact, the positron experience an effective attraction. When they combined both polarization and positronium formation the phaseshift remained positive up to the threshold for positronium formation. From these results it is concluded that positronium formation is an important effect of an attractive affective potential. Recalling that it could not alone change the sign of the phase shift, while polarization could, we conclude that it is less important than polarization. In the electron-hydrogen scattering in contrast, exchange plays the most important role rather than polarization.

Drachman (1965) has used the complete Dalgarno-Lunn second order adiabatic potential to calculate the s-wave elastic scattering below the threshold of positronium formation. He showed that the potential is too attractive, and proposed a simple one parameter modification related to the monopole term of the polarization which leads to exact agreement with Schwartz's value for the scattering length.

Kleinman et. al. (1965) have applied the minimum principle formalism for a number of incident energies below the threshold of positronium formation. They obtained rigorous lower bounds for the phase shifts in the s-wave and P-wave scattering. Because their trial function has not included a positronium channel the convergence was slow for obtaining the solution.

Drachman (1967) has used a trial function of the form

$$\psi(X,r) = \left[\psi(r) + F(X)G(X,r)\right]\phi(r) \qquad (4.1)$$

where $\phi(r)$ is the atomic ground state function and $G(X,r)$ is the adiabatic correlation function satisfying the equation

$$\left[G,H_0\right]\phi(r) = \left[V - V_1\right]\phi(r) \qquad (4.2)$$

His coupled equations gave 80% of the difference between the unpolarized results $G \to 0$ and those of Schwartz (1961).

CHAPTER 5

The present calculations

5.1 The co-ordinate system

Let the positron (e^+) of wave number k_0 be scattered by a hydrogen atom in the ground state. Let (P) be the proton and (e^-) be the electron of the hydrogen atom. The result of the collision will be the elastic scattering of the positron or the formation of positronium (e^{+-}). The two alternatives are described by the following two equations.

$$e^+ + H \xrightarrow{\qquad} e^+ + H \tag{5.1}$$

$$e^+ + H \xrightarrow{\qquad} e^{+-} + P \tag{5.2}$$

Because the proton is much heavier than the other two particles we may consider it stationary, and we may consider it the centre of mass of the system. Consequently the co-ordinate system of the centre of mass coincides with that of the Laboratory. P will be the origin of co-ordinates.

Let $\underline{s}$ be the co-ordinate of the electron, and $\underline{r}$ the co-ordinate of the positron. It will be convenient to change the co-ordinates for the positronium channel. In that channel the formed positronium atom travels away from the proton. So we want one vector to describe its centre-of -mass motion, and an other vector to describe its internal motion. Let $\underset{\sim}{R}$ be the co-ordinate of the positronium centre-of-mass, and $\underset{\sim}{t}$ the vector joining the positron to the electron. The relations between the two co-ordinate systems are shown in the following equations

$$r + \tfrac{1}{2}\, t = R \tag{5.3}$$

$$s - \tfrac{1}{2}\, t = R \tag{5.4}$$

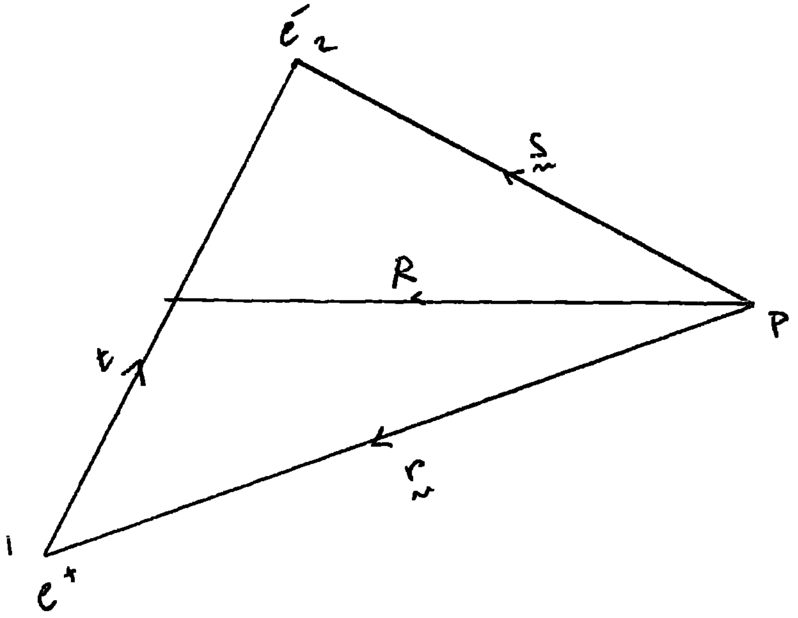
hence

$$R = \tfrac{1}{2}\, (r + s),\ r = s - 2t/2 \tag{5.5}$$

From these it is possible to obtain s and t in terms of R and r

$$s = 2R - r \tag{5.6}$$

$$t = 2R - 2r \tag{5.7}$$



5.2 The scattering equations

The solution of this problem will consist of two parts. In the first part we solve the equations for a particular trial wave function. In the second part we add variational corrections. On the other hand we can divide the calculations into those of the one-channel treatment and the two-channel treatment. We shall find that the one-channel calculations are a special case of the two-channel calculations. Therefore, we proceed by doing the formulation of the general case. Let us start with the following trial function.

$$\psi(1,2) = \psi_0(\underset{\sim}{s})F_0(\underset{\sim}{r}) + \phi_0(\underset{\sim}{t})G_0(\underset{\sim}{R}) \tag{5.8}$$

where 1 and 2 stand for e^+ and e^- respectively, and $\psi_0(s)$ is the ground state wave function of the hydrogen atom, and $\phi_0(t)$ the ground state function of positronium. $F_0(r)$ and $G_0(r)$ are the wave functions of the relative motion. Determining them is the purpose of these calculations. The two terms on the right-hand side of equation (5.8) are the first terms in the summation of equation (3.26).

The Hamiltonian with its kinetic energy part and potential energy part can be written as

$$H = T + V_{1p} + V_{2p} + V_{12} \tag{5.9}$$

where

$$T = -\tfrac{1}{2}\nabla_1^{\,2} - \tfrac{1}{2}\nabla_2^{\,2} = -\nabla_t^{\,2} - \tfrac{1}{4}\nabla_R^{\,2} \tag{5.10}$$

and where V_{ij} is the potential acting between particles i and j, with i and j taking the values 1, 2, and 3.

If we substitute our wave function in the Schrodinger equation as a first step in the eigen function expansion method we obtain the equation

$$(T+V-E)\left[\psi_0(s)F(r)+\phi_0(t)\cdot G_0(R)\right] = 0 \tag{5.11}$$

where we have written V to stand for the three potentials. If we multiply on the left by $\psi_0^{\,*}(s)$ and integrate over $\underset{\sim}{s}$, then repeat by multiplying on the left by $\phi_0^{\,*}(t)$ and integrate over $\underset{\sim}{t}$ we obtain the following coupled integro-differential equations

$$\int \psi_0^{\,*}(s)\,(T-V-E)\,\Psi d\underset{\sim}{s} = 0 \tag{5.12}$$

$$\int \phi_0^{\,*}(t)\,(T-V-E)\,\Psi d\underset{\sim}{t} = 0 \tag{5.13}$$

These two equations are what one gets from applying independent variations to I defined by

$$I = \int \Psi^{*}\,(T+V-E)\,\Psi d\tau \tag{5.14}$$

If we substitute for Ψ in equations (5.12) and (5.13) from (3.8) we obtain

$$(-\tfrac{1}{2}\nabla_r^{\,2}-\tfrac{1}{2}k^2)F_0(\underset{\sim}{r}) = -\int d\underset{\sim}{s}\,\psi_0^{*}(s)\Big[(T-E+V)\emptyset(t) \times G_0(R)+(V_{1p}+V_{12})\psi_0(s)F_0(r)\Big] \tag{5.15}$$

$$(-\tfrac{1}{4}\nabla_R^{\,2}-\tfrac{1}{2}K^2)G_0(\underset{\sim}{R}) = -\int d\underset{\sim}{t}\;\emptyset_0(t)\Big[(T-E+V)\psi_0(s)\;\times F_0(r)+(V_{1p}+V_{2p}) \times \emptyset_0(t)G_0(R)\Big] \tag{5.16}$$

Here we have split the total energy E into two parts. One part is the energy of the incident particle and the other is the energy of the atom which is a known constant. This is seen in the equation

$$E = \tfrac{1}{2}k^2 + \varepsilon_0 = \tfrac{1}{4}K^2 + \eta_0 \tag{5.17}$$

where k is the wave number of the positron and K is the wave number of the positronium in its motion relative to the proton. ε_0 is the ground state energy of the hydrogen atom and η_0 is the ground state energy of the positronium atom. Hence the two equations (5.15) and (5.16) take the form

$$(-\tfrac{1}{2}\nabla_r^{\,2}-\tfrac{1}{2}k^2)F_0(r) = -\int d\underset{\sim}{s}\,\psi_0^{*}(s)(-\tfrac{1}{4}\nabla_R^{\,2}-\tfrac{1}{4}K^2)\emptyset(t)G_0(R)$$

$$-U_{00}(r)F(r)-\int ds\,\psi_0^{*}(s)\{V_{1p}+V_{2p}\}\emptyset(t)G_0(R) \tag{5.18}$$

$$(-\tfrac{1}{4}\nabla_R^{\,2}-\tfrac{1}{4}K^2)G_0(R) = -\int d\underset{\sim}{t}\,\phi_0^{\,*}(t)(-\tfrac{1}{2}\nabla_r^{\,2}-\tfrac{1}{2}k^2)\psi_0(s)F_0(r)$$

$$-\int dt\,\phi(t)(V_{1p}+V_{12})\psi_0(s)F_0(r) \tag{5.19}$$

where

$$U_{00}(r) = \int\psi^{*}(\underset{\sim}{s})(V_{1p}+V_{12})\psi_0(s)\,ds \tag{5.20}$$

which is the repulsive static field potential acting by the hydrogen atom on the positron. It has the value

$$U_{00}(r) = (1+\frac{1}{r})\;e^{-2r} \tag{5.21}$$

In equation (5.19) we have used the symmetry of the situation in the positronium channel which yields

$$\int\phi_0^{\,*}(t)(V_{1p}+V_{2p})\phi(t)\,d\underset{\sim}{t} = 0 \tag{5.22}$$

Here the need arises for using the other set of co-ordinates. According to the transformation of equations (5.6) and (5.7) the integrals are transformed to the form

$$\int d\underset{\sim}{s}\;f(r,s) = 8\int d\underset{\sim}{R}\;f'(r,R) \tag{5.23}$$

$$\int d\underset{\sim}{t}\,f(t,R) = 8\int dr\;f'(r,R) \tag{5.24}$$

which, when applied to equations (5.18) and 5.19), yields

$$(-\tfrac{1}{2}\nabla_r^{\,2}-\tfrac{1}{2}k^2)F_0(r) = -8\int d\underset{\sim}{R}\; G(R)\left(-\frac{\nabla_R^{\,2}}{4}-\frac{k^2}{4}\right)$$

$$x\ \{\psi_0(s)\phi_0(t)\} - U_{00}(r)F_0(r)$$

$$-8\int d\underset{\sim}{R}\psi_0(s)\phi_0(t)(V_{1p}+V_{2p})G_0(R) \qquad (5.25)$$

$$(-\tfrac{1}{4}\nabla_R^{\,2} - \tfrac{1}{4}K^2)G_0(R) = -8\int dr\; F_0(r)(-\tfrac{1}{2}\nabla_r^{\,2}-\tfrac{1}{2}k^2)$$

$$\{\phi_0(t)\psi_0(s)-8\int dr\psi_0(s)\phi_0(t)$$

$$x\ (V_{1p}+V_{12})F_0(\underset{\sim}{r}) \qquad (5.26)$$

In equation (5.25) we have used integration by parts to interchange $G_0(R)$ and $\psi_0(s)$. On the right-hand side of these equations the kinetic energy operators $\nabla_R^{\,2}$ and $\nabla_r^{\,2}$ are acting on $\phi_0(t)\psi_0(s)$. We want to replace these two operators by other ones which are in terms of s and t instead of R and r. Using the transformation equations and the property of a Laplacian operating on a physical system (Schrodinger equation) for the case of hydrogen and positronium we obtain

$$\nabla_R 2\{\psi_0(s)\phi(t)\} = (4\nabla_s^{\,2}-4\nabla_t^{\,2}+8\nabla_s.\nabla_t)\psi(s)\phi(t) \qquad (5.27)$$

$$\nabla_r^{\,2}\{\psi_0(s)\phi(t)\} = (\nabla_s^{\,2}+4\nabla_t^{\,2}+4\nabla_s.\nabla_t)\psi(s)\phi(t) \qquad (5.28)$$

$$\nabla_s^{\,2}\psi(s) = (2V_{2p}-2\varepsilon_0)\psi(s) \qquad (5.29)$$

$$\nabla_t^2 \emptyset(t) = (V_{12} - \eta_0)\emptyset(t) \quad (5.30)$$

substituting (5.27) and (5.28) in (5.25) and (5.26) we have

$$\nabla_R^2 \{\psi_0(s)\emptyset(t)\} = (8V_{2p}+4V_{12}-8\varepsilon_0+4\eta_0)$$

$$\times \quad \psi_0(s)\emptyset_0(t)+8(\frac{s.t}{st})\psi'(s)\emptyset'(t) \quad (5.31)$$

$$\nabla_r^2 \{\psi_0(s)\emptyset_0(t)\} = (2V_{2p}+4V_{12}-2\varepsilon_0+4\eta_0)$$

$$\times \quad \psi_0(s)\emptyset(t)+4(\frac{s.t}{st})\psi'(s)\emptyset'(t) \quad (5.32)$$

where $\psi'(s)$ and $\emptyset'(t)$ are the first derivatives of $\psi(s)$ and $\emptyset(t)$ with respect to s and t respectively. Now we substitute these kinetic energy operators into equations (5.25) and (5.26) to obtain

$$(\nabla_r^2+k^2)F(r) = 2U_{00}F(r)+16\int d\underset{\sim}{R}\ K_{01}(\underset{\sim}{r},R) \times G(R)$$

$$(\nabla_R^2+K^2)G(R) = 32\int d\underset{\sim}{r}\ K_{10}(R,r)F(r) \quad (5.34)$$

where

$$K_{01}(r,R) = -2(\frac{s.t}{st})\ \psi'(s)\emptyset'(t) \quad (5.35)$$

$$+\{-E+2\varepsilon_0+2\eta_0+V_{1p}+V_{2p}-V_{12}\}\psi(s)\emptyset(t)$$

and

$$K_{10}(R,r) = -2(\frac{s.t}{st})\ \psi'(s)\emptyset'(t) \quad (5.36)$$

$$+\{-E-V_{2p}+V_{1p}-V_{12}-V_{2p}+2\eta_0+2\varepsilon_0\}\psi(s)\emptyset(t)$$

The kernels thus defined are identical, and this can be expressed by the symmetry

$$K_{10}(R,r) = K_{01}(r,R) \tag{5.37}$$

The usual way of dealing with equations (5.33) and (5.34) is to reduce them to radial equations by expanding F and G in Legendre polynomials.

$$F(r) = \sum_{\ell=0}^{\infty} \frac{f_\ell(r)}{r} (2\ell+1) i^\ell P_\ell(\cos \theta_r) \tag{5.38}$$

$$G(R) = \sum_{\ell=0}^{\infty} \frac{g_\ell(R)}{R} (2\ell+1) i^\ell P_\ell(\cos \theta_{R_1}) \tag{5.39}$$

where θ_r is the angle between the incident beam and the scattered particle in the first channel and θ_{R_1} is the corresponding angle for the second channel.

$$\theta_r = \underset{\sim}{k}_0 {}^\wedge \underset{\sim}{r} \qquad \text{and} \qquad \theta_{R_1} = \underset{\sim}{k}_0 {}^\wedge \underset{\sim}{R} \tag{5.40}$$

By sutstituting (5.38) and (5.39) into (5.33) and (5.34) an infinite set of integro-differential equations are obtained. Each pair corresponding to a particular ℓ are coupled.

$$\left(\frac{d_2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right) f_n(r) = r \int_{-1}^{+1} d\mu \;\; P_\ell(\mu) \frac{i}{2}^{-\ell}$$

$$\times \left[2U_{00}(r) F_0(r) + 16 \int d\underset{\sim}{R} K_{01}(r,R) G(R)\right] \tag{5.41}$$

$$\left(\frac{d2}{dR^2}{}_2 - \frac{\ell(\ell+1)}{R^2} + K^2\right) g(R) = R \int_{-1}^{+1} d\mu \; P_\ell(\mu') \frac{i}{2}^{-\ell}$$

$$\times \quad 32 \int d\underset{\sim}{r} \; K_{10}(R,r) F(r) \tag{5.42}$$

These are the equations we want to solve in order to obtain f_n and g_n. At this stage we know that they must have the asymptotic forms

$$f_n(r) \sim A^0 \sin(k_r - \frac{\ell\pi}{2}) + B^0 \cos(k_r - \tfrac{1}{2}\ell\pi) \tag{5.43}$$

$$g_n(R) \sim A^1 \sin(KR - \frac{\ell\pi}{2}) + B^1 \cos(KR - \frac{\ell\pi}{2}) \tag{5.44}$$

5.3 The adiabatic potential

Polarization can be considered as a correction to the trial wave function which determines the distortion in the orbitals. It can be considered also as an effective potential, which is to be added to the static potential. The polarization potentials in the two channels can be shown to have a simple relation with each other. One is eight times the other. Therefore it is sufficient to calculate one, then multiply by eight to get the other. Let us consider the interaction governed by the equation.

$$(H_O+V-E)\psi = 0 \tag{5.45}$$

where ψ is the total wave function of the system. $V = -(\frac{1}{F}-\frac{1}{R})$ is the potential which causes the distortion and which is assumed to be small enough to be treated as a perturbation. In the adiabatic approximation the incident particle is assumed to be stationary. Hence r is a fixed parameter. If we apply first order perturbation theory we obtain the static potential. The second order perturbation is what we are interested in. The different energy terms are

$$E = \varepsilon_O+E^{(1)}+E^{(2)}+\ldots \tag{5.46}$$

k is dropped as implied by the adiabatic approximation. $E^{(2)}$ is given by

$$E^{(2)} = \sum_{n\neq 0}\left[\frac{|\int d_s\psi_n^*(s)V\psi_0(s)|^2}{\varepsilon_0 - \varepsilon_n} \right] \tag{5.47}$$

If we use equation (2.9) this becomes

$$\begin{aligned} E^{(2)} &= \int\psi_0^*(s)\left[V-E^{(1)}\right]\psi^{(1)}(s)ds \\ &= \int\psi_0(s)\ V\psi^{(1)}(s)ds \end{aligned} \tag{5.48}$$

if ψ_0, $\psi^{(1)}$ are orthogonal where $\psi'(s)$ satisfies

$$(H_0-\varepsilon_0)\psi^{(1)} = E^{(1)}\psi_0 - V\psi_0 \tag{5.49}$$

It has been usual to expand V in terms of Legendre polynomials as

$$V = \sum_{\ell} \gamma_\ell(r,s)\ P_\ell(\cos\theta_{rs}) \tag{5.50}$$

If we expand the correction $\psi'(s)$ in spherical harmonies and substitute it together with V of (5.50) in (5.47) the evaluation of $E^{(2)}$ is reduced to the evaluation of the various terms of the expansion

$$E^{(2)} = \sum_{n=0}^{\infty} E_n^{(2)} \tag{5.51}$$

The term corresponding to n = 0 is called the monopole, that corresponding to n = 1 the dipole and that corresponding to n = 2 the quardupole. It is known that the dipole potential is the most important one and all the terms of $n>2$ are negligible. The other terms have been calculated by Reeh (1960). We have carried out the calculation and found agreement with Reeh's calculations. $E_1^{(2)}$ has the form

$$E_\ell^{(2)} = \int_0^\infty s^2 ds\ V_\ell(r,s)\,\psi_0(s)\,\psi'_{\ell_{10}}(s,r)\sqrt{\frac{2\ell+1}{4\pi}}\ \frac{4\pi}{2\ell+1}$$

$$= \sqrt{\frac{4\pi}{2\ell+1}}\int_0^\infty s^2 ds\ V_\ell(r,s)\,\psi_0\psi_{\ell 0}^{(1)}(s,r) \tag{5.52}$$

and

$$\psi'(s,r) = \sum_{\ell=0}^{\infty}\ \sum_m \psi_{\ell m}^{(1)}(s)\ Y_{\ell,m}(\theta,\emptyset)$$

$\psi_{\ell,0}^{(1)}(s,r)$ satisfies

$$\left[-\frac{1}{2S^2}\ \frac{\partial}{\partial s}\ s^2\ \frac{\partial}{\partial s} + \frac{\ell(\ell+1)}{2S^2} - \frac{1}{5} - \varepsilon_0\right]\psi^{(1)}(s,r)$$

$$= \delta_{\ell 0}E^{(1)} - V_\ell(r,s)\,\psi(s)\sqrt{\frac{4\pi}{2\ell+1}} \tag{5.53}$$

This equation is solved and the following solution is obtained. For $1>0$ we have

$$s>r \qquad \psi_{\ell,0}^{(1)}(r,s) = \beta\ F_1 + Y_2 \tag{5.54}$$

$$s<r \qquad \psi_{\ell,0}^{(1)}(r,s) = \alpha(F_1-F_2)+Y_1 \tag{5.55}$$

where F_1 and F_2 are determined according to 1. In the case 1 = 1 they are

$$F_1(s) = \left[\frac{1}{S} + \frac{2}{S} + 2\right] e^{-s} \tag{5.56}$$

$$F_2(S) = \frac{1}{S}2\ e^{+s},\ F_1 - F_2 \xrightarrow{\qquad} \text{limit as } S \to 0 \tag{5.57}$$

In the case 1 = 2 they are

$$F_1(S) = \left[\frac{1}{S^3} + \frac{3}{2S^2} + \frac{1}{S} + \frac{1}{3}\right] e^{-s} \tag{5.58}$$

$$F_2(s) = \left[\frac{1}{S^3} - \frac{1}{2S^2}\right] e^{+s} \tag{5.59}$$

y_1 and y_2 are given by

$$y_1 = \frac{-S^{\ell}}{p^{\ell+1}}\, C\, e^{-s}\left(\frac{1}{2\ell} + \frac{S}{2(\ell+1)}\right) \tag{5.60}$$

$$y_2 = \frac{r^{\ell}}{S^{\ell+1}}\, C\, e^{-s}\left(\frac{1}{2(\ell+1)} + \frac{S}{2\ell}\right) \tag{5.61}$$

for 1 = 1, β and α are given by

$$\alpha = -\left(\frac{3}{8}\right) e^{-2r}\left(1+\frac{1}{r}\right)^2 C \tag{5.62}$$

$$\beta = \alpha - \frac{3}{8}\left(1 - \frac{1}{r^2}\right) C \tag{5.63}$$

for 1 = 2, α and β are given by

$$\alpha = \frac{5}{4}\, e^{-2r}\left(1+\frac{1}{r}\right)\left(1+\frac{3}{r}+\frac{3}{r^2}\right). C \tag{5.64}$$

$$\beta = \alpha - \frac{5}{4}\left(1+\frac{1}{r}\right)\left(\frac{3}{r^2} - \frac{3}{r} + 1\right) C \qquad (5.65)$$

where $C = \frac{4}{2l+1}$

In the case of l = 0 we have different solutions is given by

$$\psi_{00}^{(1)}(r,s) = y_1 + \left(\frac{1}{r} - \alpha\right)\frac{F_2}{4} + \alpha F_1 \qquad s<r \qquad (5.66)$$

$$\psi_{00}^{(1)}(r,s) = y_2 + \beta\ F_1 \qquad s>r \qquad (5.67)$$

with

$$\alpha = -\left(1+\frac{1}{r}\right) e^{-2r}(\log 2 + a + \tfrac{1}{2}\log r) + \tfrac{1}{2}\left(\frac{1}{r} - 1\right)$$

$$\times\ E_i(-2r) + e^{-2r}\left(\frac{1}{4r} + \tfrac{1}{2} - \tfrac{1}{2}r\right) \qquad (5.68)$$

$$\beta = \left(1+\frac{1}{r}\right)\Big[e^{-2r}(\tfrac{1}{2}\overline{E}_i(2r) - \tfrac{1}{2}\log r - \log 2 - a)$$

$$-\tfrac{1}{4}\Big] + \tfrac{1}{2}\left(\frac{1}{r} - 1\right)\{E_i(-2r) - \log r\} + e^{-2r}$$

$$\times\ \left(\frac{1}{4r} + \tfrac{1}{2} - \tfrac{1}{2}r\right) \qquad (5.69)$$

$$F_1(S) = C\ e^{-S} \qquad (5.70)$$

$$F_2(S) = -\frac{C\ e^{+S}}{S} + 2C\ \overline{E}_i\ (2S)e^{-S} \qquad (5.71)$$

where

$$\overline{E}_i(x) = \int_{-\infty}^{x} \frac{e^t}{t}\,dt = E_i^{*}(x) \qquad (5.72)$$

$$E_i(-x) = -\int_x^\infty \frac{e^{-t}}{t}dt \tag{5.72}$$

when we substitute these solutions in equation (5.52) we get the required polarization potential. The dipole is given by

$$V_p^{(1)}(r) = \frac{-9}{4}\frac{1}{r^4}\left[1-\frac{e^{-2r}}{3}(1+2r+6r^2+\frac{20}{3}r^3 \right.$$

$$\left. +\frac{4}{3}r^4 - \frac{2}{3}e^{-4r}(1+r)^4\right] \tag{5.73}$$

In the asymptotic region it behaves like $-9/4 \cdot r^4$. Near the origin it behaves like $-(2/3)r^2$. The quadrupole is given by

$$V_p^{(2)}(r) = \frac{-15}{2}\frac{1}{r^6}\{1-2e^{-2r}(1+2r+\frac{4}{3}r^2+\frac{1}{3}r^3+\frac{2}{9}r^4$$

$$+\frac{2}{9}r^5+\frac{1}{18}r^6 - \frac{1}{9x15}r^7+\frac{1}{9x15}r^8-\frac{2}{9x15}r^9)+\frac{8}{9x15}r^{10}$$

$$x\ (E_i(-2r)+e^{-4r}(1+4r+\frac{20}{3}r^2+6r^3+\frac{28}{9}r^4+\frac{8}{9}r^5+\frac{r^6}{9}))\} \tag{5.74}$$

Asymptotically it behaves like $\frac{15}{2}r^6$ and near the origin it goes to zero faster than r^2. The monopole has the form

$$V_p^{(0)}(r) = e^{-2r}\{-\frac{2}{r^2}+\frac{1}{2}\frac{1}{r}+\frac{5}{2}+r+2(\log r + \gamma)(\frac{1}{r}+\frac{1}{r})+$$

$$+E_i(-2r)(1-\frac{1}{r^2}) + \log r\ (-2r+1+\frac{2}{r}+\frac{1}{r^2})$$

$$-\ \alpha\ (\frac{2}{r}+4+4r)+\beta(2+4r)\}+\frac{2\alpha}{r}+(1-\frac{1}{r})$$

$$\times\, E_i(-2r)+e^{-r}\{\frac{2}{r^2}+\frac{7}{2}\frac{1}{r}+\frac{5}{2}+r-\overline{E}_i(2r)$$

$$\times\,(\frac{1}{r^2}+\frac{3}{r}+4+2r)+(\frac{1}{r^2}+\frac{2}{r}+1)\log r \qquad (5.75)$$

where α and β are defined in equation S (5.68) and (5.69) and $C = 0.577215665..$).

5.4 Variational Corrections

In this section we shall add corrections to the trial function (5.8), and see the effect of that on the scattering parameters. This can be done in different ways. The first is to insert these corrections in the scattering equations, and then solve them. The second is to use a minimum principle which provides a bound on some scattering parameter using the results of the unperturbed equations. In both of these methods we are going to use projection operator techniques.

Let us take the total wave function Ψ. It consists of the original part (5.8) and the correction part. It is very natural to use the adiabatic corrections calculated in the previous section as the correction part in this variational treatment. The wave function has the form

$$\Psi = \chi(1,2) + \psi_0(s)F_0(r) + \phi_0(t)G_0(R) \tag{5.76}$$

where $\chi(1,2)$ is defined by

$$\chi(1,2) = \sum_{\ell\neq 0} \alpha\psi_{\ell 0}{}^{(1)}(s,r)F_0(r)Y_{\ell 0}(\cos\theta_{rs}) + \beta\phi_0{}^{(1)}(t,R)G_0(R)Y_{\ell,0}(\cos\theta_{t,R}) \tag{5.77}$$

where $\psi_{\ell 0}{}^{(1)}$ and $\phi_{\ell 0}{}^{(1)}$ are defined in (5.54) and (5.55). Until recently, the fact that $\phi_0(t)F_0(r)$ and $\psi_0(s)\ G_0(R)$ are not orthogonal has produced a difficulty for obtaining minimum principles. This has been solved by Hahn (1966) by constructing a simple form of projection operators applicable in general rearrangement and exchange processes. According to Hahn's method, each of the two open channel configurations will be associated with a component of a two dimensional wave function. This is written in the form

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{5.78}$$

where

$$\psi_1 \sim \psi_0(s)\, F_0(\underset{\sim}{r}) \qquad \text{for large } r \tag{5.79}$$

$$\psi_1 \sim 0 \qquad \text{for large } R$$

$$\psi_2 \sim 0 \qquad \text{for large } r$$

$$\psi_2 \sim \phi_0(t) G(R) \qquad \text{for large } R$$

By using the matrix form for H and E, the Schrodinger equation becomes

$$\begin{pmatrix} H - E & H - E \\ H - E & H - E \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0 \tag{5.80}$$

We define two projection operators in the following

$$P_1(r,s,r',s') = \psi_0(s) \int d\underset{\sim}{s}'\, \psi_0(s') \int d\underset{\sim}{r}'\, \delta(r-r') \tag{5.81}$$

$$P_2(t,R,t'.R') = \phi_0(t)\int d\underset{\sim}{t}'\phi_0(t')\int dR'\delta(\underset{\sim}{R}-\underset{\sim}{R}') \tag{5.82}$$

Then $P_1^{\,2} = P_1, \quad P_2^{\,2} = P_2$

We can define a two dimensional matrix operator P as

$$P = \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix} \tag{5.83}$$

Let Q be the projection operator which projects into the closed channels. It must satisfy

$$Q = 1 - P \tag{5.84}$$

so that $Q^2 = Q$ and $PQ = QP = 0$. In the matrix representation the scattering equations are

$$P(\underset{\sim}{H} - E)P\,\Psi = -P(\underset{\sim}{H} - \underset{\sim}{E})Q\,\Psi \tag{5.85}$$

which can be written in the form

$$P_1(H - E)P_1\psi_1+P_1(H - E)P_2\psi_1 = -P_1H_1Q_1\psi_1-P_1(H - E)Q_2\psi_2 \tag{5.86}$$

$$P_2(H - E)P_2\psi_2+P_2(H - E)P_1\psi_1 = -P_2HQ_2\psi_1-P_2(H - E)\phi_1\psi_1 \tag{5.87}$$

where

$$Q_2\psi_2 = \phi_{\ell'}^{(1)}(t,R)Y_{\ell',0}(\cos\theta_{tR})(2\ell+1)i^{\ell}P_{\ell}(\cos\theta_{tR})\frac{g\ell(R)}{R} \tag{5.88}$$

and

$$Q_1\psi_1 = \psi_{\ell}^{(1)}(r,s)Y'_{\ell,0}(\cos\theta_{rs})(2\ell+1)i^{\ell}P_{\ell}(\cos\theta_{rs})\frac{f\ell(r)}{r} \tag{5.89}$$

5.5 The perturbed coupled equations

The left-hand sides of equations (5.86) and (5.87) are the same equations (5.33) and (5.34). The first terms on the right are the polarization terms. The second terms are to be calculated and then substituted in the equations. We start by $P_1(H - E)Q_2\psi_2$. It must be multiplied by Legendre polynomials as in equation (5.41), then integrated over $\theta_r = \underset{\sim}{k}_0 \hat{\underset{\sim}{r}}$ and multiplied by r. Let us call what we obtain A. Then we have

$$A = 16\pi \int_0^\infty dR \int d\omega_r \int d\omega_r \Big[\psi_0(s') P_\ell(\cos\theta_R) P_\ell(\cos\theta_r) \tag{5.90}$$

$$g_\ell(R)(2\ell+1)(r\chi R)\{V(t,R)\emptyset'_{\ell'}(t,R)Y_{\ell';0}(\hat{t}R)$$

$$-V_{\ell'}(t,R)\emptyset_0(t)Y_{\ell',0}(t,R)\sqrt{\frac{4}{2\ell'+1}}\ \Big\}\Big]$$

Let

$$K(r,R) = \sum_\ell P_\ell(\cos\theta_{Rr})k_n(r,R)\frac{(2\ell+1)}{2}$$

Then

$$K_\ell = \int_{-1}^{+1} d\cos\theta_{rR}\, P_\ell(\cos\theta_{rR})\{V(t,R)\emptyset_{\ell'}^{(1)}(t,R)$$

$$Y_{\ell',0}(t,\hat{R}) - V_{\ell'}(t,R)\emptyset_0(t)Y_{\ell'0}\sqrt{\frac{4\pi}{2\ell+1}}\ \}\times\ \psi_0(s) \tag{5.91}$$

A can be expanded in the form $A = \sum_\ell A_\ell$ where A_ℓ is

$$A_\ell(r) = \int_0^\infty \bar{k}_\ell(r,R)g_\ell(R) \tag{5.92}$$

with

$$\bar{k}_\ell = 32\pi (r.R) \int_{-1}^{+1} d\cos\theta_{rR}\, P_\ell(\cos\theta_{rR}) \{V(t,R)$$

$$\phi'(t,R) Y_{\ell'}(t\hat{R}) - V_{\ell'}\, \phi(t) Y_{\ell'}(t,\hat{R})\} \psi_0(s) \qquad (5.92)$$

which in terms of r and R becomes

$$\bar{K}_\ell(r,R) = 32 \int_{-1}^{+1} P_\ell(\mu) d\mu . e^{-B} (\frac{R-r\mu}{BA}) \{ (\frac{1}{r} - \frac{1}{B})$$

$$\phi^{(1)} (\frac{t}{2},R) (\frac{\sqrt{3}}{2}) - 2\gamma_1 (\frac{tR}{2}) \frac{1}{\sqrt{8}}\, e^{-A} \} (r.R) \qquad (5.93)$$

where A and B are defined in (6.17) and (6.17'). We have two regions in which $\phi^{(1)}$ and γ_1 have different values. In region

(1) A>R

$$\gamma_1(A,R) = \frac{R}{A^2}$$

$$\phi_>^{(1)}(A,R) = \frac{4}{\sqrt{3}}\, e^{-A} \{ \frac{R}{2A^2} (\tfrac{1}{2}+A) - \frac{3}{8} (\frac{1}{A^2} + \frac{2}{A} + 2)$$

$$x \left[e^{-2R} (1+\frac{1}{r})^2 + (1- \frac{1}{R^2}) \right] \} \qquad (5.94)$$

(2) A<R

$$\gamma_1(A,R) = \frac{A}{R^2}$$

$$\phi_<^{(1)}(A,R) = \frac{4}{\sqrt{3}} \left[\frac{-A}{R^2}\, e^{-A} (\tfrac{1}{2}+\frac{A}{4})\ \frac{3}{8}\, e^{-2R} (1+\frac{1}{R})^2 \right.$$

$$\left. x\ \{ (\frac{1}{A^2} + \frac{2}{A} + 2) e^{-A} - \frac{1}{A^2}\, e^{+A} \} \right] \qquad (5.95)$$

In region (1) both γ_1 and $\phi_>^{(1)}$ αR as R goes to zero. Hence k goes to zero with R. In region (2) γ_1 and $\phi_<$ αA so that the integrand is finite in (5.93) at A = 0. At B = 0 there is a singularity.

In the same way we can calculate $P_1(H - E)Q_1\psi_1$. The corresponding kernel is

$$\overline{k}(R,r) = 64\pi(r.R)\frac{1}{\sqrt{8}} \int_{-1}^{+1} d\mu\, P_\ell(\mu)\ e^{-A}$$

$$x\left[\frac{2R\mu-r}{B}\right]\left[\left(\frac{1}{R} - \frac{1}{2A}\right)\psi_{\gtrless}^{(1)}(r,R)\left(\frac{\sqrt{3}}{4}\right) - \nu_1(B,r)e^{-B}\right] \tag{5.96}$$

(1) B>r

$$\gamma_1 = \frac{r}{B^2}$$

$$\psi_>^{(1)}(r,R) = \frac{4}{\sqrt{3}}\ e^{-B}\left\{\frac{r}{2B^2}(\tfrac{1}{2}+B) - \frac{3}{8}\left(\frac{1}{B^2} + \frac{2}{B} + 2\right)\right.$$

$$\left. x\left[e^{-2r}\left(\frac{1}{r} + 1\right) + \left(1 - \frac{1}{r^2}\right)\right]\right\} \tag{5.97}$$

(2) B<r

$$\gamma = \frac{B}{r^2}$$

$$\psi_<^{(1)} = \frac{4}{\sqrt{3}}\left[\frac{B}{r^2}\ \left(\tfrac{1}{2}+\frac{B}{4}\right)e^{-B} - \frac{3}{8}\ e^{-2r}\left(1+\frac{1}{r}\right)^2\right.$$

$$\left. x\left\{\left(\frac{1}{B^2} + \frac{2}{B} + 2\right)\ e^{-B} - \frac{1}{B^2}\ e^{-B}\right\}\right] \tag{5.98}$$

at A = 0 there is a singularity for k(r,R).

This way of forming $P_1(H - E)Q_2\psi_2$ and $P_2(H - E)Q_1\psi_1$ enables us to add them to the scattering equations (5.33) (5.34) in a way such that all that is needed to be done is to have a new kernel in each channel. Each kernel is the sum of the original kernel (5.35) and the new one. The new equations are solved as in the first time.

5.6 The variational principle

Hahn (1965) has obtained a variational principle for the scattering phase shift. If tan δ_ℓ^A is the ℓth partial wave phase shift obtained in the exact solution of equation (6.24) then

$$\tan\ \delta_\ell \geq \tan\ \delta_\ell{}^A - (2\pi k)^{-1}(Q\psi_{A_\ell}, (H - E)\psi_{A_\ell}) \tag{5.99}$$

where A stands for the trial wave function and ℓ for the particular partial wave. The second term in (5.99) is written in the form

$$I = \int\int \frac{F_\ell(r)}{r}\ \phi^{(1)}(r,s)\Big[H - E\Big]\{\phi^{(1)}(r,s) + \psi(s)\}$$

$$\times\ \frac{F(r)}{r} d\underset{\sim}{s}\ d\underset{\sim}{r} = I_1 + I_2 \tag{5.99'}$$

where I_1 and I_2 correspond to the first and second terms in the brackets { } respectively. By using the Schrodinger equation for hydrogen and the orthogonality of $\psi_0(s)$ and $\phi^{(1)}(r,s)$ we obtain

$$I_2 = \int\frac{F^2(r)}{r^2} d\underset{\sim}{r} \int\phi^p(r,s)\left(\frac{1}{r} - \frac{1}{t}\right)\psi_0(s)\,d\underset{\sim}{s} \tag{5.100}$$

and by using the property

$$(H_0 - \varepsilon_0)\emptyset_\ell(r,s) = E^{(1)}\psi_0(s)\delta_{\ell 0} - V\psi_0(s)$$

I_1 becomes

$$I_1 = I_{11} + I_{12} + I_{13} + I_{14} \qquad (5.101)$$

where

$$I_{11} = \int\int \frac{F^2(\underset{\sim}{r})}{r^2} |\emptyset^p(r,s)|^2 \left(\frac{-k^2}{2} + \frac{1}{r} + \frac{1}{t}\right) d\underset{\sim}{r}d\underset{\sim}{s} \qquad (5.102)$$

$$I_{12} = -\int\int \frac{F^2(\underset{\sim}{r})}{r^2} |\emptyset^p(r,s) \left(\frac{1}{r} - \frac{1}{t}\right) \psi_0(s)\ d\underset{\sim}{r}\ d\underset{\sim}{s} \qquad (5.103)$$

$$I_{13} = -\int\int \frac{F^2(\underset{\sim}{r})}{r^2} \emptyset^p(r,s)\ \left(\frac{1}{r} + 1\right)\ e^{-2r}\psi_0(s)\ d\underset{\sim}{r}\ d\underset{\sim}{s} \qquad (5.104)$$

$$I_{14} = \int\int \frac{F(\underset{\sim}{r})}{r} \emptyset^p(r,s)\nabla_r^{\ 2}\ \emptyset^p(r,s)\frac{F(\underset{\sim}{r})}{r} d\underset{\sim}{r}\ d\underset{\sim}{s} \qquad (5.105)$$

when I_1 is added to I_2, I_{12} cancels out with I_2. What is left are the terms I_{11}, I_{13} and I_{14}.

CHAPTER SIX

Solution of the equations

6.1 The linear equations:

One of the methods of solving equations (5.33) and (5.34) is to reduce them to a set of simultaneous algebraic equations. We start by writing them in the form

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right) f_n(r) = \phi(r) \qquad (6.1)$$

$$\left(\frac{d^2}{dR^2} - \frac{\ell(\ell+1)}{R^2} + K^2\right) g_n(R) = \Phi(R) \qquad (6.2)$$

Mott and Massey (1949) have obtained the solutions to these equations. The solutions are

$$f_n(r) = A\, W_n(kr) + \frac{1}{k}\int_0^\infty dr' L_n^O(r,r')\phi(r')dr' \qquad (6.3)$$

$$g_n(R) = A' W_n(KR) + \frac{1}{K}\int_0^\infty dR' L'_n(R,R')\Phi(R')dR' \qquad (6.4)$$

where $W_n(x) = x\, j(x)$ and where

$$L_n(x,x') = xx'\, j_n(x_<)\, n_n(x>) \text{ with} \qquad (6.5)$$

$x = kr$ and $x' = kr'$

Here $j_n(x)$ and $n_n(x)$ are the nth order spherical Bessel functions and Neumann functions respectively. The signs $<$ and $>$ are there to indicate when x takes the value x'. In (6.4) it is meant that $j_n(x)$ takes the value $j_n(x)$ for $x<x'$ and the value $j_n(x')$ otherwise. The same is said about the Neumann function. The boundary conditions for f_n and g_n require that they both go to zero with r and R and in the asymptotic region they have the forms

$$f_n(r) \sim A_i^0 \sin(kr-\tfrac{1}{2}n\pi)+B_i^0 \cos(kr-\tfrac{1}{2}n\pi) \tag{6.6}$$

$$g_n(r) \sim A_i^1 \sin(KR-\tfrac{1}{2}n\pi)+B_i^1 \cos(KR-\tfrac{1}{2}n\pi) \tag{6.7}$$

with B satisfying

$$B = -k^{-1} \int_0^\infty (kr)\, j_n(kr)\emptyset(r)\, dr \tag{6.8}$$

We substitute for $\emptyset$ and Φ from equations (5.33) and (5.34). Equation (6.3) becomes

$$kf_n(r) = kA^0 W_n(kr) + \int_0^\infty dr' L_n(r,r') 2U_{00}(r') f_n(r')$$
$$+ \int_0^\infty dR\, \mathcal{K}_n(r,R)\, g_n(R) \tag{6.9}$$

with

$$h_n(r,R) = 16 \int_0^\infty dr^1 L_n(r,r^1) k_n(r^1,R) r^1 . R . 2\pi \qquad (6.10)$$

and

$$k_n(r^1,R) = \int_{-1}^{+1} d\mu K_{10}(r,R) P_n(\mu) \qquad \mu = \cos \theta_{r'R} \qquad (6.11)$$

Equation (6.4) becomes

$$Kg_n(R) = KA\ W_n(KR) + \int_0^\infty dr\ \bar{h}_n(R,r) f_n(r) \qquad (6.12)$$

with

$$\bar{h}_n(R,r) = 32 \int_0^\infty dR' L_n(R',R) \bar{k}_n(R',r).(R' \chi r) 2\pi (r) \qquad (6.13)$$

where

$$k_n(R',r) = \int_{-1}^{+1} d\mu\ K_{10}(R',r) P_n(\mu) \qquad (6.14)$$

Here μ is the cosine of the angle between R' and r. We notice that according to the definition of K_{10} and K_{01} they must satisfy the symmetry

$$K_{10}(R,r) = K_{01}(r,R) \qquad (6.15)$$

These kernels, as defined after equation (5.34), need to be expressed in terms of r and R only. Thus, they take the form

$$k(r,R) = \frac{1}{8}\frac{\sqrt{2}}{\pi^2}\left[\frac{-2C}{AB} - k^2 - 2 + \frac{2}{r} + \frac{1}{A} + \frac{2}{B}\right]e^{-A-B} \qquad (6.16)$$

where

$$A = \sqrt{R^2 + r^2 - 2rR\mu} \qquad B = \sqrt{4R^2 + r^2 - 4Rr\mu} \qquad (6.17)$$

and

$$C = 2R^2 + r^2 - 3Rr\mu \qquad (6.17)'$$

k(r,R) goes through a singularity for R = r and r = 2R. In equation (6.16) the wave functions of hydrogen and positronium have been written explicitly. The values -½ and -¼ have been assigned to ε_0 and η_0 respectively.

Our coupled equations are now (6.9) and (6.12). At this stage they can be reduced to a set of algebraic linear equations. That can be done by replacing the integration by a summation. With $f_n(r)$ and $g_n(R)$ the unknowns, the two equations are

$$A^{O}kW_n(kr) = kf_n(r) + \sum_{i}^{N} a_i(r)f(r_i) + \sum_{j}^{N} b_j(R)g(R_j) \qquad (6.18)$$

$$A'KW_n(KR) = Kg_n(R) + \sum_{i}^{N} c_i(r)f_n(r_i) \qquad (6.19)$$

We can have 2N equations by assigning to r and R all the N values taken in the summation. These are

$$A^{O}kW_n(kr_1) = kf_n(r_1) + a_{11}f_n(r_1) + a_{12}f_n(r_2) + \ldots + a_{1N}f_n(r_n)$$

$$\ldots + b_{11}g_n(R_1) + b_{12}g(R_2) + \ldots + b_{1N}g_n(R_N)$$

$$A^{O}kW_n(kr_2) = kf_n(r_2) + a_{21}f_n(r_1) + a_{22}f_n(r_2) + \ldots + a_{2N}f_n(r_N)$$

$$\ldots + b_{21}g_n(R_2) + b_{22}g(R_2) + \ldots + b_{2N}g_n(R_N)$$

$$A'KW_n(KR_1) = Kg_n(R_1) + C_{11}f_n(r_1) + \ldots$$

$$A'KW_n(KR_1) = Kg_n(R_2) + C_{21}f_n(r_1) + \ldots \qquad (6.20)$$

These equations with the 2N unknowns $f(r_1)$, $f(r_2)\ldots$ $g(R_1), g(R_2)\ldots$ have a matrix of coefficients which is 2N x 2N. It consists of four submatrices. Sub-matrix 11 is of elements a_{ij} except the diagonal to which k is added. Sub-matrix 12 is of elements b_{ij}. Sub-matrix 21 is of elements C_{ij}. The elements of sub-matrix 22 are all zeros or polarization if it is present except the diagonal where K is added. The left-hand side of the equations form a column matrix of length 2N. a_{ij}, b_{ij} and C_{ij} have the forms

$$a_{ij} = L_n(r_i, r_j) \quad 2U_{00}(r_j) \qquad (6.21)$$

$$b_{ij} = h_n(r_i, R_j) \quad C_{ij} = \bar{h}_n(R_i, r_j)$$

If we denote the submatrices by a, b and c the equations in matrix notation are

$$\left(\begin{array}{c|c} a & b \\ \hline c & 0 \end{array}\right) \begin{pmatrix} f_n(r) \\ g_n(R) \end{pmatrix} = \begin{pmatrix} W_1(r).k \\ W_2(R).K \end{pmatrix} \qquad (6.22)$$

Here $f_n(r)$, $g_n(R)$, W_1 and W_2 are all N long column matrices.

6.2 The one channel case:

As a special case we take b and c to be zero. This corresponds to the set of N linear equations

$$\text{(a)}\quad (f_n(r)) = (W(r) \times k) \tag{6.23}$$

In this case the kernels are equal to zero, which means that there is no coupling. Channel 1 alone is considered. Equation (6.23) is the solution of

$$\left[\frac{d2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2 + U_{00}(r)\right] f_n(r) = 0 \tag{6.24}$$

This is the static field approximation. By simply altering the sign of U_{00} we obtain the corresponding equation for the electron-hydrogen scattering. Equation (6.24) constitutes the basis of the single-channel calculation of our problem. The effective polarization potential can be inserted in it to study the different effects of the different multipoles of polarization. In this case a_{ij} becomes

$$a_{ij} = L_n(r_i, r_j) \times (2U_{00} + V_p) \tag{6.25}$$

Where V_p is the polarization potential considered. To check numerical work we have tried $(V_p=0)$ and compared the result with previous work of the static field approximation. If we take $A^0 = 1$ then B^0 gives cot η_h where η_h is the phase shift.

6.3 Two-channel case

Let us go back to equations (6.20). We want to determine b and c equations following (6.20). After substituting them, the set of linear equations are solved which yields two column matrices, the elements of which are all the various $f_n(r_i)$ and $g_n(R_i)$ with the asymptotic elements satisfying (5.43) and (5.44) with

$$\sqrt{V_i}\;B_j^{(i)} = \sum_k R_{jk}\,A_k^{(i)}\,\sqrt{V_k} \qquad (6.26)$$

where

$$V_1 = k \qquad\qquad V_2 = \tfrac{1}{2}K$$

In order to obtain the four elements of the reactance matrix from equation (6.26) we need two sets of A's and B's. This corresponds to solving the equations (6.22) twice. Each time, different values are assigned to the A's. In the special case when $A_1^{\,1} = 1$, $A_2^{\,1} = 0$ and then $A_1^{\,2} = 0$ and $A_2^{\,2} = 1$, R_{ij} have the values

$$\begin{aligned} R_{11} &= B_1^{(1)} & \qquad R_{12} &= B_1^{(2)}\sqrt{\frac{2k}{K}} \\ R_{22} &= B_2^{(2)} & \qquad R_{21} &= B_2^{(1)}\sqrt{\frac{K}{2k}} \end{aligned} \qquad (6.27)$$

This R matrix should be symmetric and real. It has the simple relation with the S matrix

$$S = \frac{1 + iR}{1 - iR} \qquad (6.28)$$

which in turn is related to the transition matrix T by

$$T = \frac{1}{2i}{}^{\kappa}\left[1 - S\right] \qquad (6.29)$$

hence

$$T = \left(\frac{R}{1 - iR}\right)$$

The cross section for the scattering from channel i to channel j is

$$\sigma_{i\to j} = \sum_{\ell=0}^{\infty} (k_i{}^2)\,|T_{ji}(\ell)|^2\, 4\pi(2\ell+1) \qquad (6.30)$$

where the values 1 and 2 are given to i in k_i which yields k and K respectively. The R matrix is the generalization of the phase shift. It can be diagonalized by the unitary matrix

$$U = \begin{pmatrix} \cos\varepsilon & \sin\varepsilon \\ -\sin\varepsilon & \cos\varepsilon \end{pmatrix} \qquad (6.31)$$

where ε is the mixing parameter. The relation between the R matrix and the diagonalized matrix is

$$R = U^{+} \tan\eta\; U \qquad (6.31)'$$

where tan η is given by

$$\tan\ \eta = \begin{pmatrix} \tan\ \delta(1) & 0 \\ 0 & \tan\ \delta(2) \end{pmatrix}$$

δ_1 and δ_2 are the eigen phase shifts. Equation (6.31) is written

$$\begin{pmatrix} \cos\ \varepsilon & -\sin\ \varepsilon \\ \sin\ \varepsilon & \cos\ \varepsilon \end{pmatrix} \times \begin{pmatrix} \tan\ \delta(1) & 0 \\ 0 & \tan\ \delta(2) \end{pmatrix}$$

$$\times \begin{pmatrix} \cos\ \varepsilon & \sin\varepsilon \\ -\sin\varepsilon & \cos\varepsilon \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \qquad (6.33)$$

This is equivalent to four algebraic equations in ε, $\tan\delta(1)$ and $\tan\delta(2)$. In terms of the R matrix elements the latter parameters are

$$\tan\ 2\varepsilon = \frac{R_{21} + R_{12}}{R_{11} - R_{22}} \qquad (6.34)$$

$$\tan\delta(1) = \tfrac{1}{2}\left[R_{11} + R_{22} + \frac{R_{12} + R_{21}}{\sin\ 2_{\varepsilon}}\right]$$

$$\tan\delta(2) = \tfrac{1}{2}\left[R_{11} + R_{22} - \frac{R_{12} + R_{21}}{\sin\ 2\varepsilon}\right]$$

6.4 Extrapolation

Since results exist only for energies below the threshold for positronium formation we had to extrapolate our results into the energy region below the threshold for the purpose of comparison with existing results. The reactance matrix is too sensitive to energy changes especially in the cases of resonance. We can use calculations based on the so called M matrix (Ross and Show (1961)) defined by

$$M_{ni} = k_i^{(n+\frac{1}{2})} \ (R^{-1})_{ij} k^{(n+\frac{1}{2})} \tag{6.35}$$

where no summation rule applies. The Matrix $(R^{-1})_{ij}$ (the inverse reactance matrix) has the elements

$$(R^{-1})_{11} = \frac{R_{22}}{R_{11}R_{22}-R_{12}R_{21}} \tag{6.36}$$

$$(R^{-1})_{12} = (R^{-1})_{12} = \frac{-R_{12}}{R_{11}R_{22}-R_{12}R_{21}} \tag{6.37}$$

$$(R^{-1})_{22} = \frac{R_{11}}{R_{11}R_{22}-R_{21}R_{12}} \tag{6.38}$$

For extrapolating the M matrix we use the expansion

$$M_{ij} = M_{0ij} + M_{1ij}k^2 + M_{2ij}k^4 + \ldots \tag{6.39}$$

The evaluation of the phase shift of the elastic scattering is based on the evaluation

$$k \text{ cat } \eta = R_e\left[\left(\frac{1}{M-ik}\right)_{11}\right]^{-1} \qquad (6.40)$$

where

$$\left(\frac{1}{M-ik}\right)_{11} = \frac{M_{22} - ik_{22}}{(M_{11}-ik_{11})(M_{22}-ik_{22})-(M_{12})^2} \qquad (6.41)$$

therefore

$$\left(\frac{1}{M-ik}\right)^{-1} = M_{11} - ik_{11} - \frac{(M_{12})^2}{M_{22} - ik_{22}} \qquad (6.42)$$

and finally

$$k_{11} \cot \eta = M_{11} - \frac{|M_{12}|^2}{M_{22}+\lambda} \qquad (6.43)$$

where $k = i \cdot \lambda = K$ and where $k_{11} = k$. The value of the phase shift thus obtained can be compared with existing elastic scattering results.

The extrapolation above does not hold when long range potentials are present. It needs modification for that case.

6.5 Computation

For each energy of the incident particle a different set of linear algebraic equations was solved. As required for the accuracy of the reactance matrix obtained and its symmetry the number of points for the radial integration should not be less than forty-eight. They are distributed between zero and twenty five. This corresponds to a set of 96 linear equations (as will be seen later), and a matrix of coefficients consisting of 9216 elements.

Either we enter the subroutine of solving the equations with the coefficients in hand, in which case we need 9216 stores, or we solve them by taking two equations at a time. The latter case requires unnecessary repetition of evaluating the kernels (see following details).

There are 2304 different (bij)'s in the coefficient matrix. Each of them includes the summation of 48 terms with 48 kernels.

Unless repetition and symmetry are exploited there will be needed 2304 x 48 evaluations. From this we see what a large amount of computing time is consumed.

The capacity of the K. D. F.9 of the University of Newcastle-upon-Tyne is 14,000 stores. If 9216 of them are reserved for the coefficients less than 5,000 stores are to be used for different parts of the program and the program itself. That would not have been possible had we obtained bad accuracy in the results which would require more points and a larger matrix. If this had been the case we would have been forced to perform the longer procedure of taking two equations at a time. We have tested two rows of the matrix and found that in such a case the evaluation of the whole matrix would require about three hours. But if various steps of economizing are taken the time is squeezed to 10 minutes.

Another difficulty causing time consumption was the behavior of the kernels at some points. They have singularities at r = R and at r = 2R. One way of going about this was to have two different mesh points for r and R. But this is not very effective as when the intervals between these points are divided according to a Gaussian integration method some of the dividing points might coincide with the mesh of the other r. Another way is explained in the following.

Because we use the Gaussian method for the interval -1 to +1 we need to change the variables so as to transform the region -1 to +1. Two of the points dividing each interval are very close to, but not on the ends. Therefore if we divide the r first, then for each point we have a different mesh for the R by inserting this point in the mesh of R.

When Gauss division comes this point will be automatically avoided. This method had its success. But when the accuracy required many points the points crowded enough to give rise to a singularity again.

Finally we turned to the kernel itself. With some simple change of variables the singularity was removed. Then we were free to increase the points without fear of the kernel blowing up. In fact although the kernel goes through a singularity its integration is meaningful. The error comes from the discreteness of numerical techniques (representing curves by steps).

The program briefly goes as follows. Let us consider the elements $b_{ij} = h(r_i, R_j)$ of equation (6.21). Because of the integration it is a summation of terms dependent on r^1. To see the construction move precisely we introduce the elements of a three dimensional matrix (see diagram in figure (6). As in the diagram, these elements occupy stores which are numbered in three directions. The horizontal one is i, the vertical one is j and the third one is k. From equation (6.10) it is seen that $\bar{b}_{ijk}$ can be factored into $\bar{b}_{ik}{}^{1}$ x $\bar{b}_{jk}$ where

$$\bar{b}^{1}_{ik} = L_n(r, r^1) \text{ and, } \bar{b}_{jk} = k(r^1_k\ , R_j) r^1_k, R_j \qquad (6.44)$$

This enables us to evaluate $\bar{b}_{jk}$ once and for all for each column i, store copies of it in the appropriate stores, and multiply each with $\bar{b}_{ik}$. By doing that the time of calculating the kernels is saved. If this is repeated for all the other elements k (the third dimension) from 1 to 48, each time adding a new $\bar{b}_{ijk}$ to what has been accumulated in the corresponding store, we end up by having all the integrations in one column done. The procedure is repeated for all columns. The symmetry of the kernels is exploited by storing copies of them when forming the b sub-matrix, and then using them later for forming the c sub-matrix. In order to be able to reverse the k matrix it must be square. Unfortunately when we used 48 points for the intermediate integration it was not accurate enough. By increasing the number the matrix became rectangular. The other dimension of it is already in its maximum. Therefore this symmetry was not used.

CHAPTER 7

Results and Conclusion

7.1 One channel case:

The s- and p- wave phase shifts for various polarization potentials calculated in the one-channel treatment are shown in tables (1) and (2) respectively. In column (1) of these tables the phase shifts are listed when only the dipole part of the polarization is included. This is the most important contribution to polarization. The next most important part is the quadrupole. Column (2) of the table shows the phase shifts when the dipole and the quadrupole terms are included. The monopole contribution to the polarization is of short range. Drachman (1965) has shown that the monopole term provides a potential which is too large. The phase shifts when including dipole, quadrupole, and monopole terms are shown in column (3).

In column (4) we include the phase shifts using the complete polarization calculated by Dalgarno and Lynn (1957) and used by Deachman (1965). In column (6) we include Schwartz's wave phase shifts (1961). Schwartz results are expected to be accurate. But there is some doubt about that. Cody et. al(1964) found that by allowing for virtual positronium formation the results exceeded those of Schwartz' bounds. Stone (1966) suggested that the results should improve when more multipoles are added in the polarization. He considered Schwartz results as accurate and hence showed some doubt about the results of Drachman whose phase shifts, with the complete potential exceed those of Schwartz considerably. We have recalculated the phase shifts with the complete potential and obtained results which agree to within 1% with those of Drachman.

Temkin and Lamkin (1961) introduced a polarization potential based on a wave function containing a step function that forces the perturbed wave function to be zero when the incident particle lies within the target atom. In table (1) column (5) we include the phase shifts calculated by Cody et. al (1964) based on this approximation. Their approximation is in principle equivalent to the dipole approximation.

The results of Stone (1966) using a dipole wave function obtained by variational methods are in good agreement with the corresponding approximation (column 1). They are not included in the tables.

7.2 The two-channel case

The elastic scattering cross-sections Q_{11} have been calculated for incident wave numbers up to 1 atomic unit. The results for the s-wave are shown in figure (2). Those of the p-wave are shown in figure (3). The different graphs correspond to different approximations which have been used in the calculations. A is the approximation of including vertual positronium formation, and no polarization is included. B(1) is the same as A but with the dipole potential included in channel 1 and channel 2. B(2) is the same as A but with the dipole and quadrupole potentials included in the first channel and only the dipole in the second channel. B(3) is the same as A but with the dipole, quadrupole and the monopole potentials included in the first channel and only the dipole in the second channel.

The reason for including only the dipole in the second channel in approximations B(2) and B(3) is that they are identically zero in that channel.

The cross section for positronium formation Q_{12} is shown in figure (4) for the s-wave and in figure (5) for the p-wave. Approximations A and B(1) have been used to calculate the cross sections for $l = 2$ Table (4). They show that the $l = 2$ wave has little contribution to make for the cross sections compared with the $l = 0$ and $l = 1$

cases. Polarization emphasises the effect of this wave in the elastic scattering.

If the reactance matrix is diagonalized we obtain results that can be compared with the phase shifts of the existing one-channel approximation results, for the multichannel scattering process is determined by the specification of the eigenphase shifts and of the mixing parameters. Diagonalizing the reactance matrix was done by help of the real orthogonal U matrix defined in equation (6.31). In Table (6) the mixing parameters are included together with the eigenphase shifts. It must be noted that physical effects are not affected by the addition of multiples of 2Π in eigen phase shifts.

In figures (4) and (5) cross sections are included for the Positronium formation Q_{12} in two cases 1 = 0 and 1 = 1 respectively. It is noticed that in the no-polarization case the cross section for positronium formation is very small. We can interpret that as the result of decoupling of the two channels when ε is too small. Although the feature has often been noticed (Bransden 1965) in methods based on variational principles, it seems that this case is an extreme. The behaviour of the total positronium formation cross sections

$$Q_{12} = \sum_{\ell} Q_{12}(\ell) \qquad (7.1)$$

which rise to a miximum in magnitude of order a_0^2 at momentum k = 1.0 (a.u.) is, in contrast, entirely what would be expected.

It was interesting to check numerical work by comparing the extrapolation of our results to the region below the threshold of positronium formation with those of Cody et. al. (1964). The M matrix (Ross and Shaw 1961) was extrapulated for $l = 0$. The agreement was very good considering the extrapolation involved.

When polarization is present, the picture gets more complicated. In the case when $l = 0$ the mixing parameter is large now. The coupling is consequently important. The scattering is affected by producing a bigger probability of positronium formation. Q_{12} is then increased considerably, while Q_{11} is reduced. This is not the case when $l = 1$. For then an opposite effect is produced. Q_{12} which was large for no-polarization is reduced and Q_{11} increased. In this case Q_{12} rises slowly above threshold but for $l = 0$ Q_{12} has a peak just above threshold, then drops very steeply when the energy increases. The position of the peak is (k = 0.7071). But since it is not possible to get very good calculations in the neighburhood of the threshold we say that the peak is near (k = 0.71).

The general feature of the s-wave scattering cross section suggests that the reactance matrix has a pole just below threshold, probably representing a bound state in the positron-proton channel. The behaviour of δ_2 is inconsistent with this. Our first attempt to confirm this picture was to extrapolate below threshold using the M matrix method. The second attempt was to calculate directly from the scattering equations. The M matrix elements were too sensitive for accurate results to be obtained. Direct calculations break down just below threshold. However, the results strongly suggest that a bound state exists in channel 2, giving rise to a resonance in the e^+ - H channel near $k = 0.706$. For $l = 1$ and $l = 2$ no trace of a pole is seen.

7.3 Conclusion

The conclusion that can be drawn from the results of our one-channel calculations is that polarization effects arise mainly from the contribution of the dipole and quadrupole terms of the polarization series. All higher terms are unimportant. We also conclude that the monopole should not be included for s-wave scattering. Perhaps instead of the monopole one should use long-range correlation terms to be determined variationally, as has been done by Burme and Taylor (1966) for electron-hydrogen scattering.

As in the one-channel treatment the cross sections in the two-channel treatment are seen to be rather sensitive to the details of the polarization potential used. It is noticed, though, that the difference between approximation A and any of the approximations (B) is large compared with the differences between the different approximations (B). This leads us to derive the conclusion that proper account must be taken of polarization effects in this reaction. We feel that this is most probably the case for rearrangement collisions in general.

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FIGURE LEGENDS

FIGURE 1

The cross-section for positronium formation calculated by Massy and More (1954).

Curve 1: First Born Approximation

Curve 2: Distorted wave Approximation

FIGURE 2

The elastic partial cross-section for e^+-H scattering for the partial wave $\ell = 0$

Curve (A): No polarization included

Curve (B1): Dipole potential included

Curve (B2): Dipole and Quadrupole potentials included

Curve (B3): Dipole Quadrupole and Monopole potentials included

FIGURE 3

The elastic partial cross-section for e^+-H scattering for the partial wave $\ell = 1$ (A), (B1), (B2), and (B3) represent the same approximations mentioned above.

FIGURE 4

The positronium formation cross-section for e^+-H scattering for the partial wave $\ell = 0$

FIGURE 5

The positronium formation cross-section for e^+-H scattering for the partial wave $\ell = 1$

FIGURE 6

Illustration of storage for kernels $K_{01}(r,R)$ and $K_{10}(R,r)$ in a three dimensional matrix.

FIG. 1.

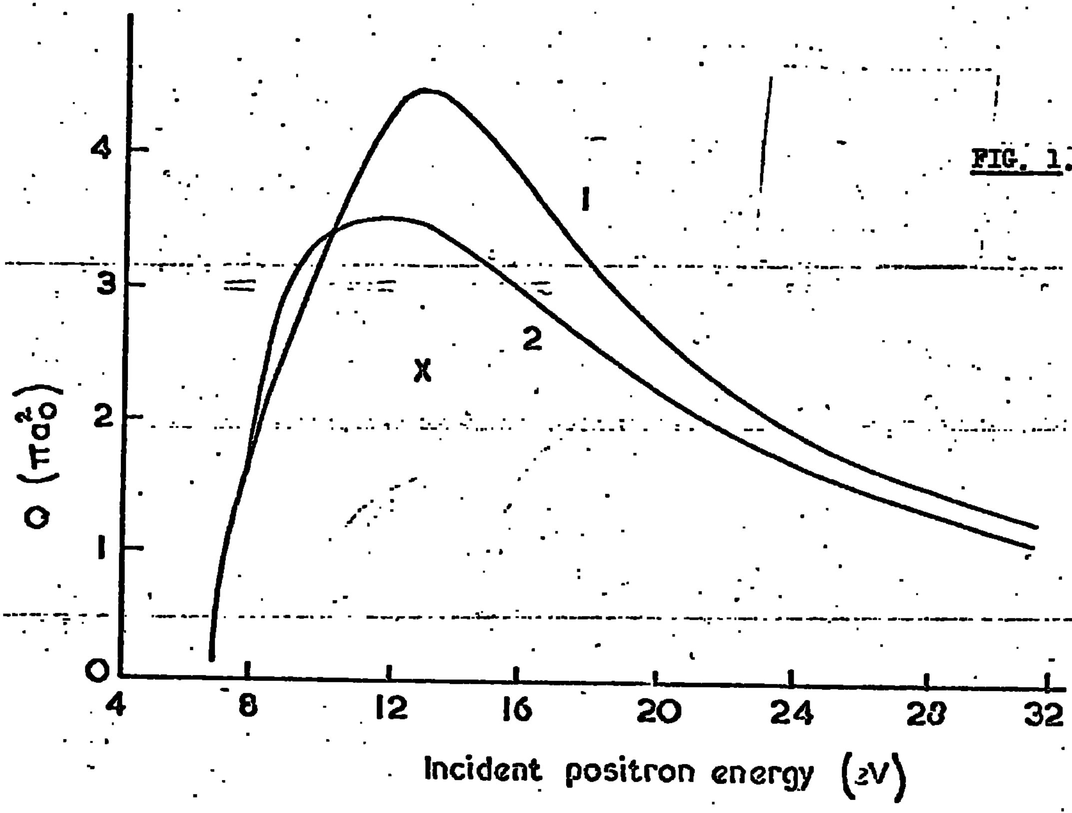

Q (πa_0^2)
0
1
2
3
4
4
8
12
16
20
24
28
32
Incident positron energy (eV)
1
2
X

FIG. 2.

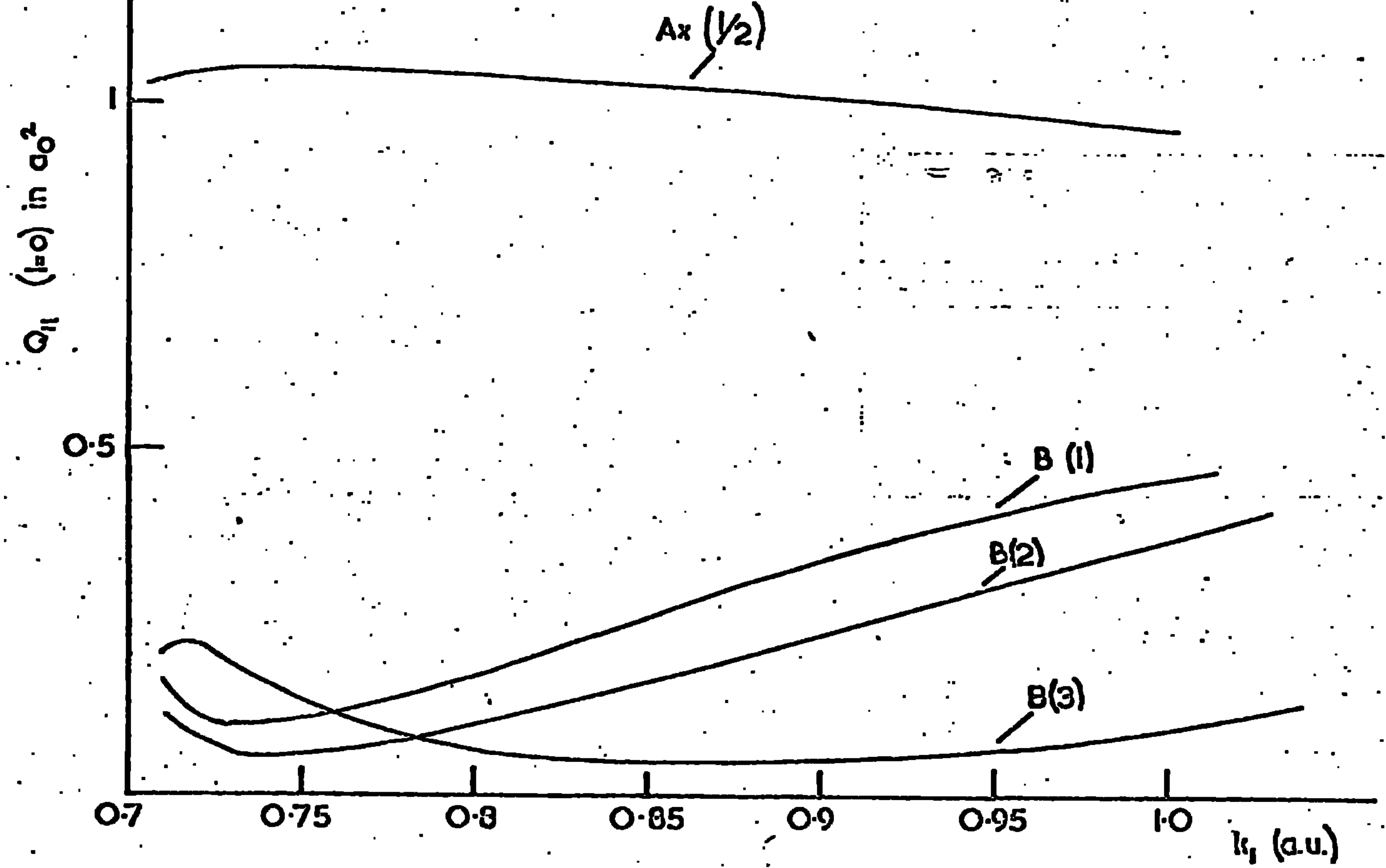


FIG. 3.

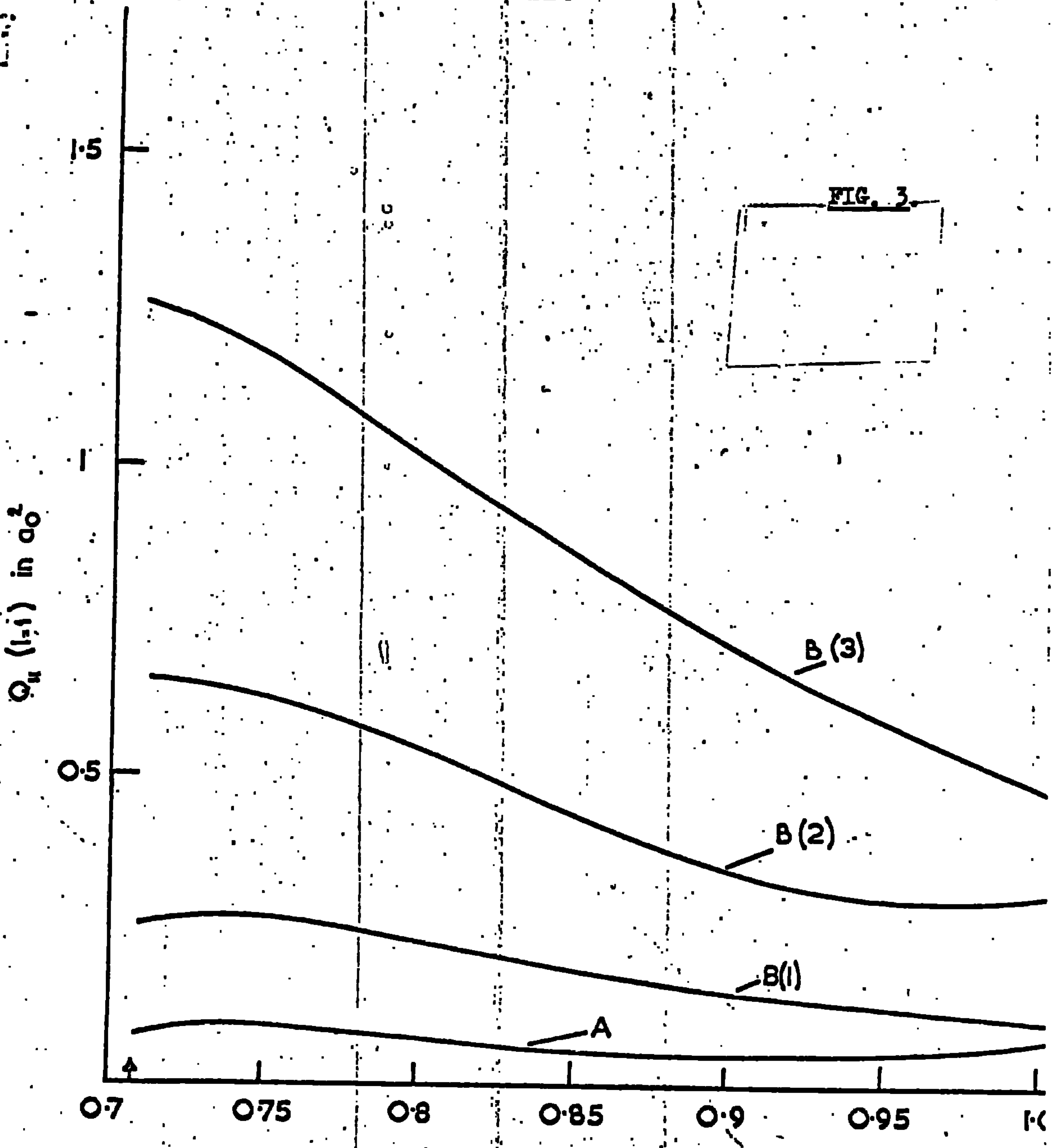
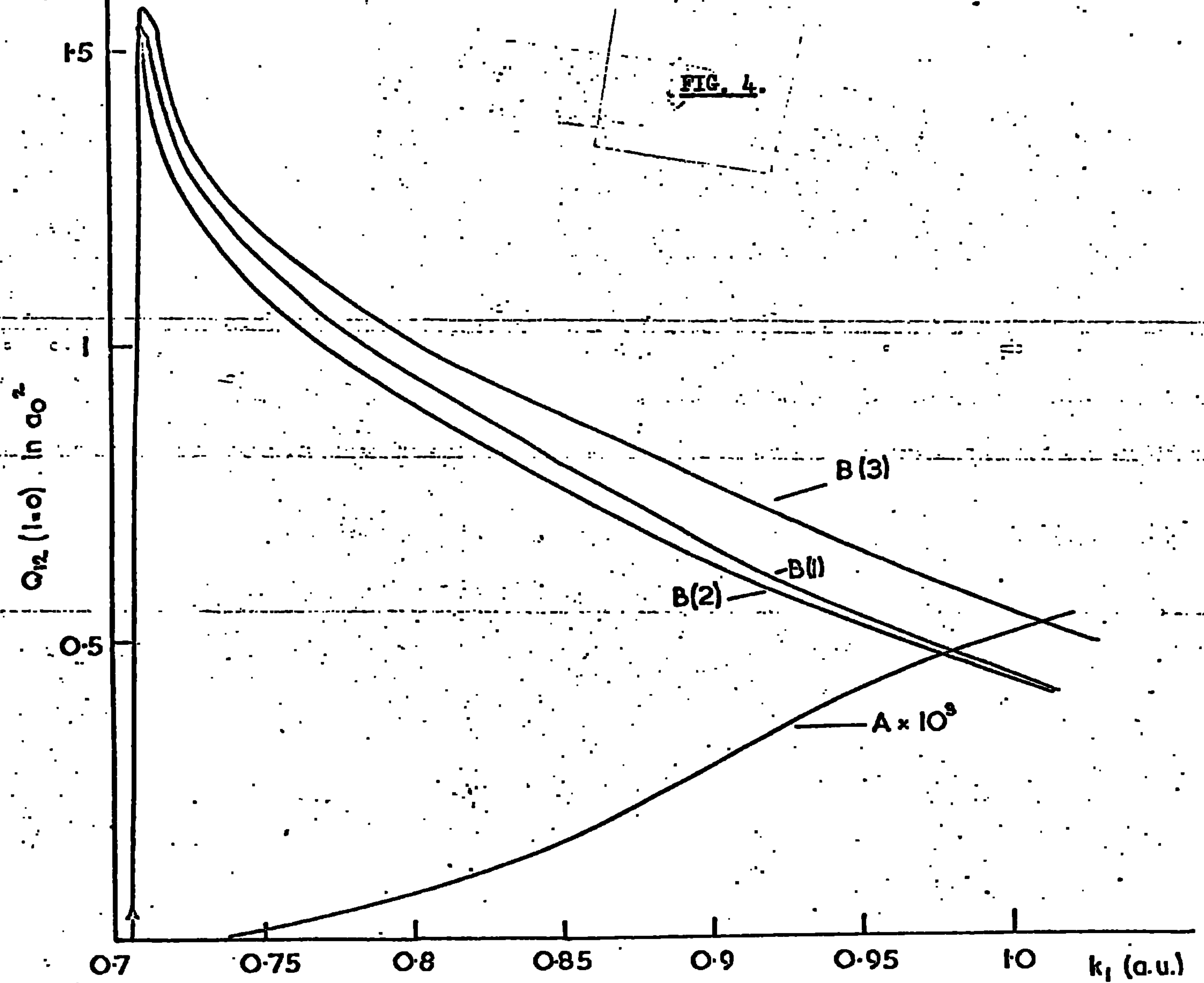


FIG. 4.



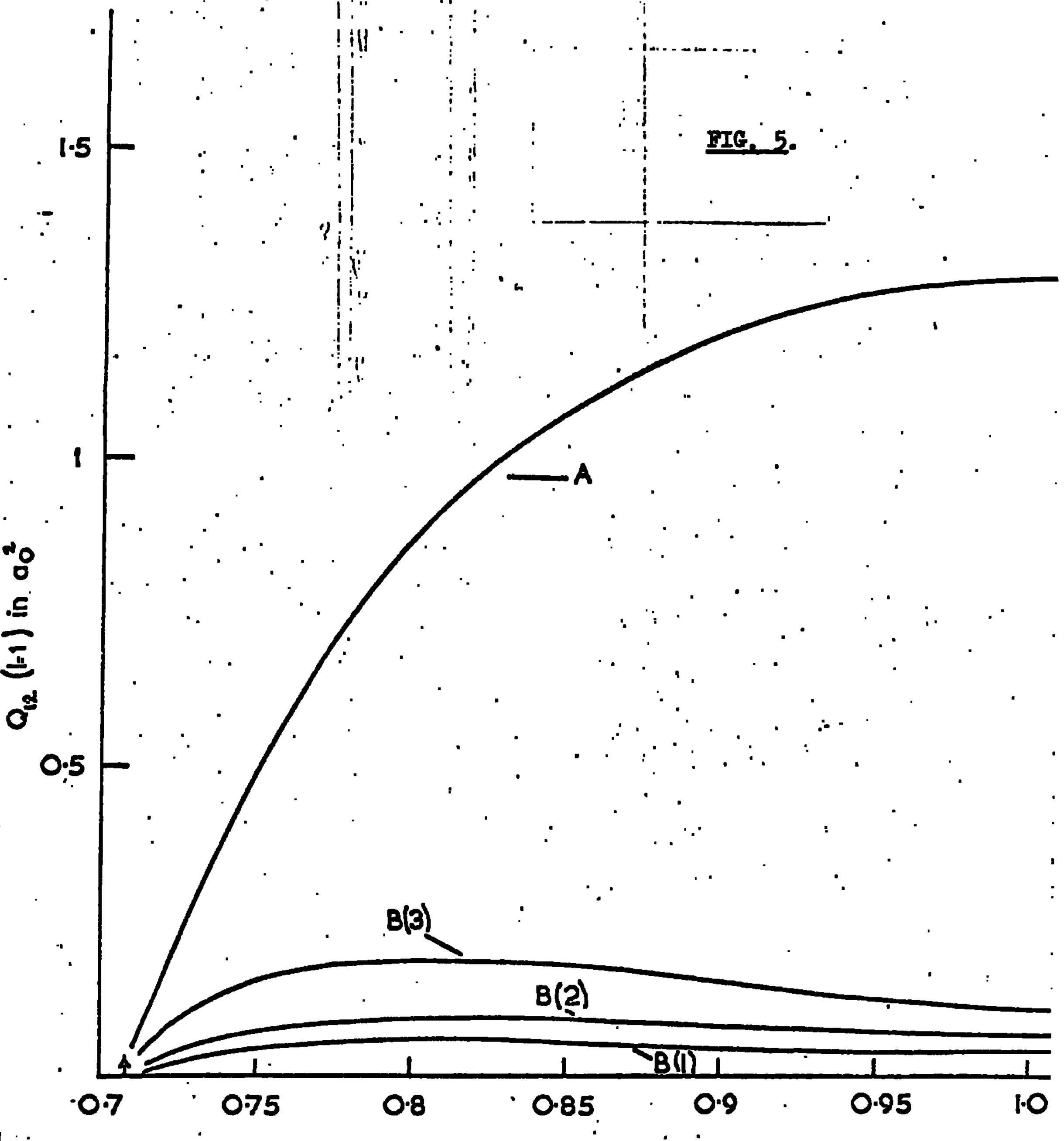


FIG. 5.

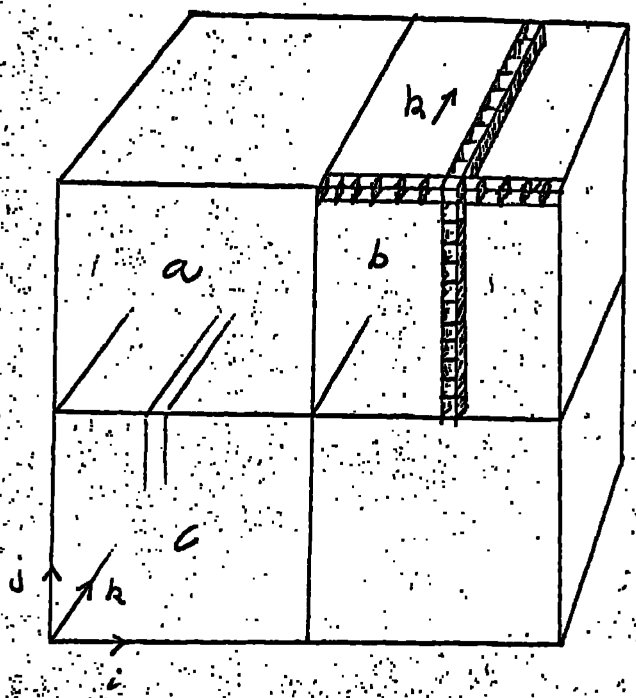


FIGURE 6

Table 1

s-wave phase shifts for positron scattering by hydrogen in the ground state

k	I	II	III	IV	V	VI
0.1	0.098	0.127	0.163	0.184	0.080	0.151
0.2	0.114	0.157	0.213	0.241	0.085	0.188
0.3	0.087	0.134	0.201	0.230	0.053	0.168
0.4	0.041	0.089	0.164	0.191	0.005	0.120
0.5	-0.010	0.034	0.115	0.141	-0.048	0.062
0.6	-0.062	-0.021	0.067	0.089	-0.099	0.007
0.7	-0.111	-0.074	0.020	0.040	-0.147	-0.054
0.8	-0.157	-0.123	-0.024	-0.006	-	-

I Computed from dipole part of the adiabatic potential.
II Computed from the dipole + quadrapole parts of the adiabatic potential.
III Computed from the monopole + diapole + quadrapole parts of the adiabatic potential.
IV Computed from the complete adiabatic potential (for k 0.7 from Drachman 1965).
V Dipole potential results of Cody et al. (1964).
VI The variational results of Schwartz (1961).

Table 2

p-wave phase shifts for positron scattering by hydrogen in the ground state

k	I	II	III	IV	V
0.1	0.007	0.007	0.007	0.009	0.008
0.2	0.027	0.029	0.030	0.031	0.031
0.3	0.049	0.056	0.058	0.061	0.062
0.4	0.067	0.079	0.084	0.090	0.099
0.5	0.079	0.096	0.103	0.113	0.128
0.6	0.084	0.103	0.115	0.125	0.150
0.7	0.081	0.103	0.119	0.131	0.166
0.8	0.074	0.097	0.117	0.129	-

I Computed from dipole part of the adiabatic potential

II Computed from quadrapole + dipole parts of the adiabatic potential

III Computed from monopole + dipole + quadrapole parts of the adiabatic potential

IV Computed from complete adiabatic potential (for k 0.7 from Drachman 1965).

V The variational results of Kleinman et al. (1965).

Table 3

Variational corrections to s-wave phase shifts including the dipole potential

k	Phase Shift	Correction
0.1	0.098	0.01025
0.2	0.114	0.00853
0.3	0.087	0.00688
0.4	0.041	0.00569
0.5	-0.010	0.00486
0.6	-0.062	0.00435
0.7	-0.111	0.00388
0.8	-0.157	0.00347

k_1(a.u)	A		B(1)	
	Q_{11}	Q_{12}	Q_{11}	Q_{12}
0.72	1.7×10^{-3}	1.6×10^{-3}	0.30	3.6×10^{-3}
0.74	2.0×10^{-3}	1.2×10^{-2}	0.31	3.2×10^{-2}
0.8	3.3×10^{-3}	6.3×10^{-2}	0.30	1.2×10^{-2}
0.9	7.6×10^{-3}	8.1×10^{-2}	0.30	8.3×10^{-2}

Table 4 The cross-sections for $l = 2$ using wave functions in approximations A and B(l)

Q_{11} = elastic cross-section for e^+-H scattering in units of a_0^2

Q_{12} = positronium formation cross-section in units of a_0^2

k(a.u)	δ	$\bar{\delta}$
0.7	-0.29	-0.286
0.6	-0.24	-0.238
0.5	-0.20	-0.186
0.4	-0.15	-0.134

Table 5 Phase shifts ($l = 0$) for elastic scattering of positrons by hydrogen.

δ is the $l = 0$ phase shift obtained by extrapolating the results of approximation (A) below the positronium formation threshold.

$\bar{\delta}$ is the $l = 0$ phase shift computed directly by Cody et al. in the same approximation.

Table 6

Eigenphase shifts and Mixing parameters for l = 0
near threshold

	No polarisation		Approximation A		Polarisation Approximation B(1)	
k:(a.u)	δ_1	δ_2	ε	δ_1	δ_2	ε
0.71	-0.294	-0.261	-0.006	-0.022	1.819	0.285
0.715	-0.296	-0.413	+0.004	-0.039	1.412	0.263
0.72	-0.299	-0.548	0.003	-0.052	1.198	0.292
0.73	-0.303	-0.721	0.003	-0.074	0.937	0.324
0.74	-0.307	-0.826	0.004	-0.096	0.768	0.440
0.77	-0.332	-1.168	0.005	-0.159	0.463	0.569

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