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THE SCATTERING OF POSITRONS BY ATOMIC  
HYDROGEN: FORMULATION

by

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# THE SCATTERING OF POSITRONS BY ATOMIC HYRDOGEN: FORMULATION

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## ABSTRACT

This report contains the derivation of the coupled systems of second-order integrodifferential equations which must be solved numerically in order to obtain the cross sections for the elastic and inelastic scattering of positrons by atomic hydrogen and the cross sections for the formation of positronium into the 1s and 2s states.

The numerical method to be used to solve the equations at incident energies above excitation thresholds is also discussed.

## I. INTRODUCTION

As noted by Massey and Mohr (1954) and Massey and Moussa (1958), the recent advances in experimental techniques associated with the study of a stream of positrons in a gas now justifies theoretical investigations of the various processes involved.

Massey and Moussa (1958) calculated the elastic scattering cross sections for positrons with various atoms, including hydrogen, using the adiabatic one-body approximation, and concluded that distortion effects are negligible. This conclusion has received support from the work of Smith, Miller and Mumford (1960), who assumed distortive effects to exist only in the sense of real excitation to the 2s- and 3s-states of atomic hydrogen, rather than a distortion due to an added induced potential between the positron and the hydrogen atom [see Massey and Moussa (1958)].

However, both Moussa (1959) and Spruch and Rosenberg (1960) have shown that at very low energies (about 5 ev) the effect of virtual positronium formation on the elastic scattering cross section is important, in contradiction to those calculations which neglect positronium formation. Both sets of calculations were carried out by variational methods.

The present report formulates the problem from the usual eigenfunction-expansion approach and presents the coupled systems of radial equations which must be solved numerically for the phase shifts

and amplitudes in order to obtain the various cross sections. It is hoped that numerical calculations based on this formulation will settle the disagreement between the above two sets of calculations.

In Section II we present the derivation of the radial equations; the various kernels are analyzed in Section III. In Section IV we discuss the various cross sections we intend to calculate. The numerical details are given in Section V.

## II. DERIVATION OF THE RADIAL EQUATIONS\*

The Schrödinger equation for a positron-atomic hydrogen system can be written as

$$[T + V - E] \Psi(\underline{r}_1, \underline{r}_2) = 0 \quad , \quad (2.1)$$

where  $E$  is the total energy of the system, the potential energy is

$$V = - \frac{e^2}{|\underline{r}_1 - \underline{r}_2|} + \frac{e^2}{r_2} - \frac{e^2}{r_1} \quad , \quad (2.2)$$

and the kinetic energy can be written in the form:

$$T = - \frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 \quad , \quad (2.3)$$

or

$$T = - \frac{\hbar^2}{m} \nabla_\rho^2 - \frac{\hbar^2}{4m} \nabla_R^2 \quad , \quad (2.4)$$

and where

$$\underline{\rho} \equiv \underline{r}_1 - \underline{r}_2 \quad \text{and} \quad \underline{R} \equiv (\underline{r}_1 + \underline{r}_2)/2 \quad ;$$

also

$$\underline{r}_1 = 2\underline{R} - \underline{r}_2 \quad \text{and} \quad \underline{\rho} = 2(\underline{R} - \underline{r}_2) \quad .$$

Here  $\underline{r}_1$  and  $\underline{r}_2$  denote the vectors from the "infinitely" heavy proton to the electron and positron, respectively.

The exact overall wave function  $\Psi$  has the property that

$$I \equiv \int \Psi^* [T + V - E] \Psi d\underline{r} = 0 \quad . \quad (2.6)$$

---

\*We are indebted to Dr. P. G. Burke for a discussion on this section.

The approximate calculation of  $\Psi$  is based on the following considerations. We construct trial functions of the type

$$\Psi_t(\underline{r}_1, \underline{r}_2) = \sum_{\alpha} \psi_{\alpha}(\underline{r}_1) F_{\alpha}(\underline{r}_2) + \sum_i \phi_i(\underline{\rho}) G_i(\underline{R}) \quad , \quad (2.7)$$

where  $\psi_{\alpha}$  and  $\phi_i$  are the eigenfunctions of the hydrogen atom and positronium, respectively. In this report, the summations in Eq. (2.7) will be restricted to the first few discrete s-states of the bound systems.

Following Bransden, Dalgarno, John and Seaton (1958), we define the integral

$$I_t \equiv \int d\underline{r} \Psi_t^* [T + V - E] \Psi_t \quad . \quad (2.8)$$

For small variations  $\delta\Psi_t$  of  $\Psi_t$ , it is required that the expressions

$$\int \delta\Psi_t^* [T + V - E] \cdot \Psi_t d\underline{r}$$

be stationary. This yields the equations

$$\int \psi_{\beta}^*(\underline{r}_1) [T + V - E] \Psi_t d\underline{r}_1 = 0 \quad (2.9)$$

and

$$\int \phi_j^*(\underline{\rho}) [T + V - E] \Psi_t d\underline{\rho} = 0 \quad . \quad (2.10)$$

Kohn (1948) has shown that the errors in the values obtained for the elements of the S-matrix from Eqs. (2.9) and (2.10) will be proportional to expressions which are quadratic in the errors in the wave functions.

Upon expanding the functions F and G in terms of Legendre polynomials and surface harmonics, respectively, Eq. (2.9) reduces to the radial equation

$$\left[ \frac{d^2}{dx^2} + (k_{\beta} a_0)^2 - \frac{\ell(\ell+1)}{x^2} \right] f_{\beta\ell}(x) + \sum_{\alpha} V_{\beta\alpha}(x) f_{\alpha\ell}(x) + \sum_i \int_0^{\infty} K_{\beta i \ell}^{(1)}(x, x') g_{i\ell}(x') dx' = 0 \quad , \quad (2.11)$$

where  $x$  and  $x'$  are dimensionless variables defined by

$$x = r_2/a_0; \quad x' = R/a_0; \quad a_0 = \hbar^2/me^2 \quad , \quad (2.12)$$

and

$$V_{\beta\alpha}(\mathbf{x}) \equiv -2a_0 \int d\underline{r}_1 \psi_{\beta}^*(\underline{r}_1) \left[ -\frac{1}{\rho} + \frac{1}{r_2} \right] \psi_{\alpha}(\underline{r}_1) \quad . \quad (2.13)$$

For the s-states of the hydrogen atom,

$$-V_{11}(\mathbf{x}) = 2 \left[ \frac{1}{x} + 1 \right] e^{-2x} \quad (2.14a)$$

$$-V_{22}(\mathbf{x}) = 2 \left[ \frac{1}{x} + \frac{3}{4} + \frac{x}{4} + \frac{x^2}{8} \right] e^{-x} \quad (2.14b)$$

$$-V_{33}(\mathbf{x}) = 2 \left[ \frac{1}{x} + \frac{5}{9} + \frac{4x}{27} + \frac{4x^2}{81} - \frac{4x^3}{729} + \frac{4x^4}{2187} \right] e^{-2x/3} \quad (2.14c)$$

The nondiagonal potential terms are given by

$$V_{ij}(\mathbf{x}) = V_{ji}(\mathbf{x}) \quad , \quad (2.15)$$

and

$$V_{12}(\mathbf{x}) = \frac{4\sqrt{2}}{9} \left( \frac{2}{3} + x \right) e^{-3x/2} \quad (2.16a)$$

$$V_{13}(\mathbf{x}) = \frac{1}{\sqrt{3}} \left( \frac{3}{8} + \frac{x}{2} - \frac{x^2}{9} \right) e^{-4x/3} \quad (2.16b)$$

$$V_{23}(\mathbf{x}) = 8\sqrt{6} \left( \frac{23}{3125} + \frac{23x}{3750} - \frac{7x^2}{3375} + \frac{x^3}{675} \right) e^{-5x/6} \quad (2.16c)$$

Similarly, Eq. (2.10) reduces to the radial equation

$$\left[ \frac{d^2}{dx'^2} + (k_j a_0)^2 - \frac{\ell(\ell+1)}{x'^2} \right] g_{j\ell}(x') + \sum_{\alpha} \int_0^{\infty} K_{j\alpha\ell}^{(2)}(x',x) f_{\alpha\ell}(x) dx = 0 \quad . \quad (2.17)$$

The wave numbers of Eqs. (2.11) and (2.17) are related by the expression

$$(k_j a_0)^2 = 2 \left[ (k_{\alpha} a_0)^2 - \frac{1}{\alpha^2} + \frac{1}{2j^2} \right] \quad . \quad (2.18)$$

The kernels of the radial integrodifferential equations are defined by

$$\begin{aligned} K_{\beta i \ell}^{(1)}(\mathbf{x}, \mathbf{x}') &= 8x x' \iint d\omega_{\mathbf{x}} d\omega_{\mathbf{x}'} Y_{\ell 0}^*(\mathbf{x}) Y_{\ell' m'}(\mathbf{x}') \\ &\times \left[ \frac{1}{2} \left( \nabla_{\mathbf{x}'}^2 + k_1^2 a_0^2 \right) - 2 \left( -\frac{1}{|2\underline{x}' - \underline{x}|} + \frac{1}{x} \right) \right] \psi_{\beta}^*(2\underline{x}' - \underline{x}) \phi_i(2\underline{x}' - 2\underline{x}) \end{aligned} \quad (2.19)$$



and

$$K_{j\alpha\ell}^{(2)}(\mathbf{x}',\mathbf{x}) = -8\mathbf{x}\mathbf{x}' \iint d\omega_{\mathbf{x}} d\omega_{\mathbf{x}'} Y_{\ell'm'}^*(\mathbf{x}') Y_{\ell 0}(\mathbf{x}) \\ \times \left[ 2(\nabla_{\mathbf{x}}^2 + k_{\alpha}^2 a_0^2) - 4 \left( -\frac{1}{|2\mathbf{x}' - 2\mathbf{x}|} + \frac{1}{\mathbf{x}} \right) \right] \phi_j^*(2\mathbf{x}' - 2\mathbf{x}) \psi_{\alpha}(2\mathbf{x}' - \mathbf{x}) \quad , \quad (2.20)$$

where  $d\omega$  denotes solid angle integrations. We note here that in writing the kernels and the  $g$ 's as functions of  $\ell$  only, we have included the result of performing the angular integrations, since all kernels have the same angular factor, namely,

$$\iint d\omega_{\mathbf{x}} d\omega_{\mathbf{x}'} Y_{\ell_0}^*(\hat{\mathbf{x}}) P_{n_1}(\hat{\mathbf{x}} \cdot \hat{\mathbf{x}}') P_{n_2}(\hat{\mathbf{x}} \cdot \hat{\mathbf{x}}') Y_{\ell'm'}(\hat{\mathbf{x}}') \\ = \frac{4\pi}{2\ell+1} (n_1 n_2 / \ell)^2 \delta_{\ell\ell'} \delta_{m'm'} \quad , \quad (2.21)$$

where  $(ab/c)$  is the vector addition coefficient with vanishing magnetic quantum numbers [see Blatt, Biedenharn and Rose (1952)],  $Y_{\ell 0}$  is the Legendre polynomial associated with  $F$ , and  $Y_{\ell'm'}$  is the surface harmonic associated with  $G$ .

At this point we note the connection between the formalism developed above and the approximations of previous calculations. The results of Smith, Miller and Mumford (1960) were obtained using Eq. (2.11) but neglecting the integral terms. The Born approximation of Massey and Mohr (1954) can be obtained from Eq. (2.10) by writing this equation as

$$\int d\underline{\rho} \phi_j^*(\underline{\rho}) \left[ T - \frac{e^2}{\rho} - E \right] \Psi_t = - \int d\underline{\rho} \phi_j^*(\underline{\rho}) \left[ \frac{e^2}{r_2} - \frac{e^2}{r_1} \right] \Psi_t \quad , \quad (2.22)$$

substituting the second term of Eq. (2.7) on the left-hand side of Eq. (2.22), and assuming

$$\Psi_t = \psi_{\alpha}(\underline{r}_1) e^{i\mathbf{k}_i \cdot \underline{R}} \quad (2.23)$$

on the right-hand side.

### III. ANALYSIS OF THE KERNELS

In this report, we shall confine our attention to a maximum of two terms in the eigenfunction expansions of Eq. (2.7). This means that we shall have to evaluate only  $K_{ab}^{(x)}$ , where  $x, a, b = 1, 2$ .

The relevant bound-state wave functions are

$$\psi_1(r) = e^{-r/\pi^{1/2}} ; \quad \phi_1(\rho) = e^{-\rho/2}/(8\pi)^{1/2} \quad (3.1)$$

$$\psi_2(r) = (2-r) e^{-r/2}/4(2\pi)^{1/2} ; \quad \phi_2(\rho) = (2-\rho/2) e^{-\rho/4}/16\pi^{1/2} \quad (3.2)$$

$$\frac{d\psi_1(r)}{dr} = -\psi_1(r) ; \quad \frac{d\phi_1(\rho)}{d\rho} = -\frac{1}{2}\phi_1(\rho) \quad (3.1a)$$

$$\frac{d\psi_2(r)}{dr} = r e^{-r/2}/8(2\pi)^{1/2} - e^{-r/2}/2(2\pi)^{1/2} ; \quad (3.2a)$$

$$\frac{d\phi_2(\rho)}{d\rho} = \rho e^{-\rho/4}/128\pi^{1/2} - e^{-\rho/4}/16\pi^{1/2}$$

Inspection of the kernels reveals that three expansions will be needed repeatedly in order to perform the angular integrations analytically; these are [see Mott and Sneddon (1948)]

$$(1) \frac{e^{-k|\underline{r}_1 - \underline{r}_2|}}{|\underline{r}_1 - \underline{r}_2|} = \sum_{n=0}^{\infty} \frac{2n+1}{(r_1 r_2)^{1/2}} w_n(k; r_b; r_a) P_n(\underline{r}_1 \cdot \underline{r}_2) \quad , \quad (3.3)$$

where

$$w_n(k; r_b; r_a) = I_{n+1/2}(kr_a) K_{n+1/2}(kr_b) \quad . \quad (3.4)$$

Here  $r_a$  is the smaller of  $r_1$  and  $r_2$ , and  $I_n$  and  $K_n$  are the usual Bessel functions as adopted by Watson (1944).

$$(2) e^{-k|\underline{r}_1 - \underline{r}_2|} = \sum_{n=0}^{\infty} \frac{2n+1}{(r_1 r_2)^{1/2}} p_n(k; r_b; r_a) P_n(\underline{r}_1 \cdot \underline{r}_2) \quad , \quad (3.5)$$

where

$$p_n(k; r_b; r_a) = r_b I_{n+1/2}(kr_a) K_{n+3/2}(kr_b) - r_a I_{n-1/2}(kr_a) K_{n+1/2}(kr_b) ; \quad (3.6)$$

also,

$$(3) |\underline{r}_1 - \underline{r}_2| e^{-k|\underline{r}_1 - \underline{r}_2|} = \sum_{n=0}^{\infty} \frac{2n+1}{(r_1 r_2)^{1/2}} q_n(k; r_b; r_a) P_n(\underline{r}_1 \cdot \underline{r}_2) \quad , \quad (3.7)$$

where

$$\begin{aligned}
q_n(k; r_b; r_a) &= (r_a^2 + r_b^2) I_{n+1/2}(kr_a) K_{n+1/2}(kr_b) \\
&\quad - \frac{2n}{2n+1} r_a r_b I_{n-1/2}(kr_a) K_{n-1/2}(kr_b) \\
&\quad - \frac{2(n+1)}{2n+1} r_a r_b I_{n+3/2}(kr_a) K_{n+3/2}(kr_b) \quad . \quad (3.8)
\end{aligned}$$

In the kernel definitions, Eqs. (2.19) and (2.20), we note that the terms involving the Laplacian can be rewritten as follows:

$$\begin{aligned}
&\nabla_{\underline{x}'}^2 [\psi(|2\underline{x}' - \underline{x}|) \phi(|2\underline{x}' - 2\underline{x}|)] \\
&= 4 [\psi(r_1) \nabla_{\rho}^2 \phi(\rho) + \phi(\rho) \nabla_1^2 \psi(r_1) + 2\nabla_1 \psi \cdot \nabla_{\rho} \phi] \quad , \quad (3.9)
\end{aligned}$$

and

$$\begin{aligned}
&\nabla_{\underline{x}}^2 [\psi(|2\underline{x}' - \underline{x}|) \phi(|2\underline{x}' - 2\underline{x}|)] \\
&= \phi(\rho) \nabla_1^2 \psi(r_1) + 4\psi(r_1) \nabla_{\rho}^2 \phi(\rho) + 4\nabla_{\rho} \phi \cdot \nabla_1 \psi \quad , \quad (3.10)
\end{aligned}$$

where  $r_1$  and  $\rho$  on the right hand sides are dimensionless, i.e., divided by  $a_0$ .

Substituting Eqs. (3.9) and (3.10) into the kernel definitions and using the Schrödinger equation for the bound systems, we derive the following simplified forms for the kernels:

$$\begin{aligned}
K_{\beta i \ell}^1(\underline{x}, \underline{x}') &= 8\underline{x}\underline{x}' \iint d\underline{w}_x d\underline{w}_{x'} Y_{\ell_0}^*(\underline{x}) Y_{\ell' m'}(\underline{x}') \\
&\quad \times \left[ \left\{ \frac{(k_i a_0)^2}{2} - \frac{2}{|2\underline{x}' - \underline{x}|} - \frac{2}{x} + \frac{1}{2i^2} - \frac{2}{|2\underline{x}' - 2\underline{x}|} + \frac{2}{\beta^2} \right\} \psi_{\beta} \phi_i + 4 \frac{d\psi_{\beta}}{dr_1} \frac{d\phi_i}{d\rho} \hat{\underline{r}}_1 \cdot \hat{\underline{\rho}} \right] \quad (3.11)
\end{aligned}$$

$$\begin{aligned}
K_{j \alpha \ell}^2(\underline{x}', \underline{x}) &= -8\underline{x}'\underline{x} \iint d\underline{w}_x d\underline{w}_{x'} Y_{\ell' m'}^*(\underline{x}') Y_{\ell_0}(\underline{x}) \\
&\quad \times \left[ \left\{ 2(k_{\alpha} a_0)^2 - \frac{4}{|2\underline{x}' - 2\underline{x}|} - \frac{4}{x} + \frac{2}{\alpha^2} + \frac{2}{j^2} - \frac{4}{|2\underline{x}' - \underline{x}|} \right\} \psi_{\alpha} \phi_j + 8 \frac{d\psi_{\alpha}}{dr_1} \frac{d\phi_j}{d\rho} \hat{\underline{r}}_1 \cdot \hat{\underline{\rho}} \right] \quad (3.12)
\end{aligned}$$

Expanding  $\psi_\beta$  and  $\phi_i$  using Eqs. (3.1) - (3.8), we obtain the following explicit forms for the kernels:

$$\begin{aligned}
K_{\beta i \ell}^{(1)}(\mathbf{x}\mathbf{x}') &= \frac{\sqrt{2}}{2\ell+1} \sum_{n_1, n_2} (2n_1+1)(2n_2+1)(n_1 n_2 / \ell)^2 \\
&\times \left[ 16 \left\{ \frac{(k_{i\alpha_0})^2}{2} - \frac{2}{x} + \frac{1}{2i^2} + \frac{2}{\beta^2} \right\} k_{\beta i}^A(\mathbf{x}\mathbf{x}') \right. \\
&- 32 k_{\beta i}^B(\mathbf{x}\mathbf{x}') - 16 k_{\beta i}^C(\mathbf{x}\mathbf{x}') + 32 (2x'^2 + x^2) k_{\beta i}^D(\mathbf{x}\mathbf{x}') \left. \right] \\
&- \frac{96\sqrt{2}}{2\ell+1} \frac{\mathbf{x}\mathbf{x}'}{L} \sum_{n_1, n_2, L} (2n_1+1)(2n_2+1)(n_1 n_2 / L)^2 (L\ell / \ell)^2 k_{\beta i}^D(\mathbf{x}\mathbf{x}')
\end{aligned} \tag{3.13}$$

$$\begin{aligned}
-K_{j\alpha\ell}^{(2)}(\mathbf{x}'\mathbf{x}) &= \frac{\sqrt{2}}{2\ell+1} \sum_{n_1, n_2} (2n_1+1)(2n_2+1)(n_1 n_2 / \ell)^2 \\
&\times \left[ 16 \left\{ 2(k_{\alpha a_0})^2 + \frac{2}{j^2} + \frac{2}{\alpha^2} - \frac{4}{x} \right\} k_{\alpha j}^A(\mathbf{x}\mathbf{x}') - 64 k_{\alpha j}^B(\mathbf{x}\mathbf{x}') \right. \\
&- 32 k_{\alpha j}^C(\mathbf{x}\mathbf{x}') + 64 (2x'^2 + x^2) k_{\alpha j}^D(\mathbf{x}\mathbf{x}') \left. \right] \\
&- \frac{192\sqrt{2}}{2\ell+1} \frac{x'\mathbf{x}}{L} \sum_{n_1, n_2, L} (2n_1+1)(2n_2+1)(n_1 n_2 / L)^2 (L\ell / \ell)^2 k_{\alpha j}^D(\mathbf{x}\mathbf{x}')
\end{aligned} \tag{3.14}$$

where

$$k_{11}^A = \frac{1}{\sqrt{8}} p_{n_1} (1 \ x_b \ x_a) p_{n_2} (1 \ x_d \ x_c) \tag{3.15}$$

$$k_{12}^A = \frac{1}{16} p_{n_1} (1 \ x_b \ x_a) \left\{ 2 p_{n_2} \left( \frac{1}{2} x_d \ x_c \right) - q_{n_2} \left( \frac{1}{2} x_d \ x_c \right) \right\} \tag{3.16}$$

$$k_{21}^A = \frac{1}{16} \left\{ 2 p_{n_1} \left( \frac{1}{2} x_b \ x_a \right) - q_{n_1} \left( \frac{1}{2} x_b \ x_a \right) \right\} p_{n_2} (1 \ x_d \ x_c) \tag{3.17}$$

$$k_{22}^A = \frac{1}{64\sqrt{2}} \left\{ 2 p_{n_1} \left( \frac{1}{2} x_b \ x_a \right) - q_{n_1} \left( \frac{1}{2} x_b \ x_a \right) \right\} \left\{ 2 p_{n_2} \left( \frac{1}{2} x_d \ x_c \right) - q_{n_2} \left( \frac{1}{2} x_d \ x_c \right) \right\} \tag{3.18}$$

$k^B$  is the same as  $k^A$  with  $w_{n_1}$  replacing  $p_{n_1}$  and  $p_{n_1}$  replacing  $q_{n_1}$ .  
 $k^C$  is the same as  $k^A$  with  $p_{n_2}$  replaced by  $w_{n_2}$  and  $q_{n_2}$  replaced by  $p_{n_2}$ .  
 $k^D$  is also the same as  $k^A$  with  $p_{n_i}$  replaced by  $w_{n_i}$  and  $q_{n_i}$  replaced by  $\frac{1}{2} p_{n_i}$ .

$$\begin{aligned} x_a &= \min(2x', x); & x_b &= \max(2x', x) \\ x_c &= \min(x', x); & x_d &= \max(x', x) \end{aligned} \quad (3.19)$$

#### IV. CROSS SECTIONS

Taking two terms in the eigenfunction expansion allows us to determine:

- (a) the effect of real positronium formation (in either the 1s state or 2s state) on the elastic and inelastic scattering cross sections of positrons on hydrogen atoms,
- (b) the cross sections for the formation of positronium into either the 1s or 2s states, and
- (c) the de-excitation cross sections for the scattering of positronium in protons.

For a pair of coupled equations, i. e., a single term taken in the eigenfunction expansions, the explicit expression for inelastic cross section is given in Marriott (1958). For three, or more, coupled equations the relevant matrix expressions for the cross sections have been derived by Smith (1960).

The various cross sections are related to the asymptotic forms of the functions  $F_\alpha(\underline{r}_2)$  and  $G_j(\underline{R})$ . If all the hydrogen atoms are initially in the 1s state, then

$$F_\alpha(\underline{r}_2) \sim e^{i\mathbf{k}\alpha \cdot \underline{r}_2} \delta_{\alpha\beta} + \frac{e^{ik_\alpha r_2}}{r_2} f(\theta_{\alpha\beta}) \quad , \quad (4.1)$$

where  $f(\theta_{\alpha\beta})$  is the scattering amplitude for a positron "exciting" the hydrogen atom from the  $\beta$  to  $\alpha$  state, and

$$G_j(\underline{R}) \sim \frac{e^{ik_j R}}{R} f(\theta_{j\alpha}) \quad , \quad (4.2)$$

where  $f(\theta_{j\alpha})$  is the probability amplitude for the capture of an electron from the  $\alpha$  state of the hydrogen atom into the  $j$  state of positronium.

Alternatively, if we require those solutions of the radial equations (2.9) and (2.10) which satisfy the asymptotic boundary condition:

$$G_j(\underline{R}) \sim e^{i\mathbf{k}_j \cdot \underline{R}} \delta_{jk} + \frac{e^{ik_j R}}{R} f(\theta_{jk}) \quad , \quad (4.3)$$

then  $f(\theta_{jk})$  is interpreted as the scattering amplitude for positronium scattering from protons and being excited from the  $k$  to  $j$  state.

## V. NUMERICAL DETAILS

### An Iterative Method for Calculating Cross Sections in Atomic Collisions\*

In this section we shall describe a method which has been used to solve coupled ordinary second-order integrodifferential equations such as Eqs. (2.9) and (2.10). This type of equation is quite common in nuclear and atomic collision theory: see Bransden, Smith and Tate (1958) for the scattering of nucleons on deuterons, and Marriott (1958) for the scattering of electrons by hydrogen atoms. In general, we shall write the  $N$  coupled equations as

$$\frac{d^2 y_\alpha(\mathbf{x})}{dx^2} = \sum_{\beta=1}^N \left[ V_{\alpha\beta}(\mathbf{x}) y_\beta(\mathbf{x}) + \int_0^\infty K_{\alpha\beta}(\mathbf{x}, \mathbf{x}') y_\beta(\mathbf{x}') dx' \right] \quad , \quad (5.1)$$

with boundary conditions

$$y_\alpha(0) = 0 \quad . \quad (5.2)$$

$$y_{\alpha\ell}(\mathbf{x}) \sim A_{\alpha\ell} \sin(k_\alpha x - \ell\pi/2 + \delta_{\alpha\ell}) \quad , \quad (5.3)$$

$$\alpha = 1, 2, \dots, N \quad ,$$

where  $k_\alpha$  is the wave number of the emerging projectile, which can be calculated directly from the energy of the incident projectile using energy conservation [see, for example, Eq. (2.11)]. Here  $A_\alpha$  and  $\delta_\alpha$  are the asymptotic amplitude and phase shift, respectively. The relationship between these parameters and the cross sections has been shown elsewhere [see Smith (1960)]. Thus, it is the purpose of the numerical solution of Eq. (5.1) to determine  $A_\alpha$  and  $\delta_\alpha$ .

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The numerical problem is therefore a "two-point" boundary value problem which is more difficult to solve than an initial value problem. It is possible to treat the problems met in collision theory as initial value problems.\*

Let us re-write Eq. (5.1) as

$$\frac{d^2 y_\alpha(\mathbf{x})}{dx^2} = V_{\alpha\alpha}(\mathbf{x}) y_\alpha(\mathbf{x}) + \sum'_{\beta(\neq\alpha)} U_{\alpha\beta}(\mathbf{x}) y_\beta(\mathbf{x}) \quad , \quad (5.4)$$

where  $V_{\alpha\alpha}(\mathbf{x})$  and  $U_{\alpha\beta}(\mathbf{x})$  can be integral operators. Let us assume, for the moment, that the  $(N-1)$  functions  $y_\beta$  (where  $\beta \neq \alpha$ ) are known, which we label  $y_\beta^A$ . Then Eq. (5.4) becomes

$$\frac{d^2 y_\alpha}{dx^2} = V_{\alpha\alpha}(\mathbf{x}) y_\alpha(\mathbf{x}) + g_\alpha^A(\mathbf{x}) \quad , \quad (5.5)$$

where  $g_\alpha^A(\mathbf{x})$  is a known function. The solution of Eq. (5.5) is discussed in Mott and Massey (1949).

The general solution of Eq. (5.5), which also satisfies  $y_\alpha(0) = 0$ , is

$$y_\alpha(\mathbf{x}) = \bar{y}_\alpha(\mathbf{x}) + \bar{\bar{y}}_\alpha(\mathbf{x}) \quad , \quad (5.6)$$

where  $\bar{y}$  is any solution of the homogeneous equation

$$\frac{d^2 \bar{y}_\alpha}{dx^2} = V_{\alpha\alpha}(\mathbf{x}) \bar{y}_\alpha(\mathbf{x}) \quad , \quad (5.7)$$

$$\bar{y}_\alpha(0) = 0, \bar{y}_\alpha(\mathbf{x}) \sim \bar{A}_{\alpha\ell} \sin(k_\alpha x - \ell\pi/2 + \delta_{\alpha\ell}) \quad . \quad (5.8)$$

Since Eq. (5.7) is homogeneous in  $\bar{y}_\alpha$ , we can multiply the solution by any arbitrary factor, which implies that  $\bar{A}_{\alpha\ell}$  is arbitrary! This arbitrary constant can be fixed, for example, by the condition

$$y_{\alpha\ell}(\Delta x) = \text{constant}(\lambda_\alpha) \quad . \quad (5.9)$$

[We note that if  $\ell = 0$ , then this condition is equivalent to the condition

$$\left. \frac{dy_\alpha}{dx} \right|_{x=0} = \text{constant} \quad . \quad (5.10)$$

This equivalence is not true for  $\ell \neq 0$ , since  $\left. \frac{dy_\alpha}{dx} \right|_{x=0} = 0$  for  $\ell > 0$ . However, Eq. (5.9) is always true!]

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\*We are very grateful to Dr. B. H. Bransden for indicating the following procedure.

$\bar{y}_\alpha$  is a particular integral of the inhomogeneous Eq. (5.5) and does not contain any arbitrary constants. The method for constructing the relevant Green's function is given in Mott and Massey (1949).

Hence, if we are given  $y_\beta^A$ , then we only need to specify one arbitrary constant to obtain  $y_\alpha$ . The same considerations apply to all the  $N$  functions  $y_\alpha$ , with  $\alpha = 1, \dots, N$ . Thus, only  $N$  arbitrary constants are needed to specify a solution of the coupled system, and these may be taken to be the values  $y_\alpha(\Delta x)$ . We emphasize that the solutions could be chosen by specifying the values of  $y_\alpha$  at any point.

At the beginning of the iterative scheme, we neglect the integral terms in Eq. (5.1), which still leaves us with  $N$  coupled equations to solve:

$$\frac{d^2 y_\alpha}{dx^2} = \sum_{\beta=1}^N V_{\alpha\beta}(x) y_\beta(x) \quad (5.11)$$

We then assume that at some very small value of  $x$ , so small that we can set it equal to zero in the computing machine, the value of the first derivative is finite and is chosen to be  $y_\alpha(\Delta x)/\Delta x$ . Thus, we have specified the  $2N$  constants at the beginning of the integration and we can integrate out from the origin using Gill's (1951) version of the Runge-Kutta method.

We note that one of the major advantages of this method, over a method such as Hartree's method, is that we do not have to calculate a few starting values using a series expansion in sines.

Solution of the system (5.11) will give us  $y_\alpha^I$ , from which we must extract the parameters  $A_{\alpha\ell}^I$  and  $\delta_{\alpha\ell}^I$ .

The phase shift was calculated in the following way: Since the functions  $y_\alpha$  are oscillatory, a record was kept of the zeros,  $x_{\alpha i}^0$ , which were compared with the corresponding zero of the appropriate Bessel function,  $X_{\ell i}^0$ , and the phase shift is given by

$$\delta_{\alpha\ell i} = k_\alpha a_0 [X_{\ell i}^0 - x_{\alpha\ell i}^0] \quad (5.12)$$

where  $i$  is the number of the zero and  $a_0$  is a constant which makes  $k_\alpha a_0$  dimensionless. At large  $x$ ,

$$y_\alpha(x) \sim A_{\alpha\ell} x [\cos \delta_{\ell} (k_\alpha a_0 x) - \sin \delta_{\ell} (k_\alpha a_0 x)] \quad ; \quad (5.12)$$

hence, at a zero,  $y_{\alpha\ell}(x^0) = 0$ ,

$$\tan \delta_{\alpha\ell} = j_\ell / n_\ell \quad , \quad (5.13)$$



which gives  $\delta_{\alpha l}$  to within  $m\pi$ . Both the above methods were used and the value of  $\delta_{\alpha l}$  printed out at each zero. When the difference between  $\delta_i$  and  $\delta_{i+1}$  is less than some preassigned epsilon, the outward integration is stopped.

Since  $A_{\alpha l}$  is also needed in the cross-section formula, we use Eq. (5.12) in the form

$$\frac{1}{A_{\alpha l}} = \frac{x[\cos \delta_{j l} - \sin \delta_{n l}]}{y_{\alpha l}}, \quad (5.14)$$

and we calculate  $1/A_{\alpha l}$  at the maxima of  $y_{\alpha l}$ .

Thus, from  $y^I$  we obtain our first approximations to the required asymptotic parameters:  $\delta_{\alpha l}^I$  and  $A_{\alpha l}^I$ ; we also store the values of  $y^I$  at the mesh points.

The second step in the iteration scheme is to substitute  $y^I$  into the integral terms of Eq. (5.1), which gives

$$g_{\alpha\beta}^I(x) = \int_0^{\infty} K_{\alpha\beta}(x, x') y_{\beta}^I(x') dx' \quad (5.15)$$

Since  $y^I$  is an oscillatory function, one must be careful in the choice of the integration scheme. The method adopted here was to use the zeros of  $y^I$  as break-up points for the integral and integrate between the zeros, i.e.,

$$\int_0^{\infty} = \int_0^{x_1} + \int_{x_1}^{x_2} + \int_{x_2}^{x_3} + \dots \quad (5.16)$$

The values of the integrand are zero at the end points. One method for halting the integration is to compare the contribution of a loop to the entire sum and stop when the percentage contribution is less than some epsilon.

In the second iteration, instead of the homogeneous equation (5.11) we have the inhomogeneous equation

$$\frac{d^2 y_{\alpha}}{dx^2} = \sum_{\beta=1}^N [V_{\alpha\beta}(x) y_{\beta}(x) + g_{\alpha\beta}^I(x)] \quad (5.17)$$

which can again be solved as an initial value problem. This time we obtain  $\delta^{II}$  and  $A^{II}$  and  $y^{II}$  is in storage.

The iterative procedure is continued until  $\delta^i$  and  $\delta^{i+1}$  differ by a preassigned epsilon. It was found that four or so iterations were necessary in the electron-hydrogen atom problem.

If  $N > 1$ , the problem is not yet completed by only extracting one solution from the system (5.1). Since there are  $N$  arbitrary constants, there exist  $N$  linearly independent solutions to the system (5.1), and so  $N$  different choices of  $y'_\alpha$  must be made and the system solved  $N$  times.

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