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CALCULATION OF THE BINDING ENERGY

AND

SCATTERING CROSS-SECTIONS OF THE THREE-NUCLEON SYSTEM

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الى الراحلين .. والدتي ووالدي

والى الأعزاء الذين جاهدوا وصمدوا

من اجل ان يتم هذا البحـــث

زوجتي واطفالنـــا

اليهم جميعا اهدي هذا الجهد المتواضع

PREFACE

The work presented in this thesis was carried out in the Department of Mathematics, Imperial College of Science and Technology, London, S.W.7., under the supervision of Dr. S. Hochberg, B.SC., PH.D., A.R.C.S.

In part (1) a brief account is given to the problem of nuclear interaction potential and of the deuteron wave functions. This includes another derivation of the integro-differential equations using the properties of the spherical harmonics and Clebsch-Gordon coefficients. Part (2) deals with the problem of scattering of protons by deuterons.

The numerical analysis and computations of the problem are given in part (3). This includes the results obtained for the phase-shifts, differential and total cross-sections, as well as the binding energy of ^{3}He.

It is my pleasure to take this apportunity to express my gratitude to Dr. S. Hochberg, for suggesting the problem and for his encouragement throughout this work. I would also like to thank Mr. R. Shephered, the director of the computer centre, Chelsea College, for the generous use of the computers and computing facilities provided during the course of computations. Also, I wish to thank Dr. R. Sibbel, Miss. H. Legge, Mr. M.R. Langton, Mr. P.E. Johnston, Mr. R.E. Chapman, and the staff at the computer centre of Chelsea College of Science and Technology for the valuable discussion I have had with them in dealing with some of the programs.

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ABSTRACT

The following points are discussed:

(a) The problem of scattering of protons by deuterons was using the resonating group method of J.A. Wheeler (1937). Starting from three-nucleon wave functions, simultaneous integrodifferential equations were derived from Schroedinger wave equation. The s- and the D- redial wave functions are taken in double Gaussian form in order that we can further the analysis.

(b) The Hamada and Johnston potential (1962) which satisfies the N-N data up to 310 MeV is used, and the potential function was also expressed in double Gaussian form.

(c) A spline interpolation procedure written by Christian H. Reinsch (Numerisch Mathematik 10 , (1967), 177), was used to interpolate the data given by Hamada and Johnston, for the potential-and wave-functions, and a least square method was then applied to determine the constants A, α, U and μ respectively. A reasonable accuracy for these constants were obtained and they are given in tables (VIII) and (IX).

(d) The (s-D) interaction terms due to the quadratic spin-orbit force were omitted, because of their small contributions.

(e) The resulting integrodifferential equations describing the problem are expressed in terms of finite differnces (Robertson, 1955; and Buckingham, numerical methods, 1957),

and finally put into matrix form. Programs for computing the direct and exchange terms, as well as the solution of the matrix equations are all written in Algol language. These matrix equations ($\underline{A}\ \underline{F}=\underline{B}+\mathcal{E}$) are then solved for incident proton energies (E_p(c.m) = 1.85 to 11.50 MeV) and values of ℓ=0,1,2 and 3.

(f) Phase-shifts, differential and total cross-sections were obtained from the direct solution of the integro-differential equations and compared with previous work.

(g) The binding energy of ^{3}He has also been calculated.

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INTRODUCTION

The three-body scattering problem in nuclear physics has been the subject of considerable theoretical and experimental studies. Initial theoretical work was done by Buckingham and Massey (1941)employing the resonating group method of Wheeler (1937). The work of Christian and Gammel (1953), De Borde and Massey (1955), Burke and Robertson (1957), who used the central force approximation, showed that simple central nuclear potentials cannot simultaneously account for the binding energies of the deuteron, triton, and alpha particles. This result was subsequently attributed to the presence of the non-central forces.

Gerjuoy and Schwinger (1942), gave the first quantitative calculations of the triton binding energy with the inclusion of the tensor force. Later calculations, however, established that a central plus tensor force was sufficiently flexible, to fit both the existing two-nucleon data and the triton binding energy (Clapp 1949, Hu and Hsu 1951, Pease and Feshbach 1952). Bransden, Smith and Tate (1958), gave a detailed study of the problem of scattering of nucleons by deuterons employing a tensor force and taking into account the distortion of the deuteron wave function occasioned by the interaction, together with the admixture of the deuteron D-state wave function.

Buckingham and Massey (1941); Buckingham, Hubbard and Massey (1952); Hochberg, Massey and Underhill (1954); Bransden, Smith and Tate (1958); and others, applied the resonating group method to the problem of three, four, and five nucleons using different kinds of potentials and wave functions.

The Hamada and Johnston potential (1962), which not only includes one-pion exchange and a repulsive hard-core, but also tensor, spin-orbit and quadratic spin-orbit forces, was used in three-, four- and five-nucleon problems (Sribhibhadh 1966, Omojola 1968, Pramanik 1971).

This thesis extends previous work (Sribhibhadh 1966) to the problem of scattering of protons by deuterons and the binding energy of Helium-three (^{3}He). It is hoped that solving the three-nucleon problem with a potential which contains both central and non-central forces and a repulsive core will allow us not only to gain further insight into the nuclear forces, but will also provide a test for the resonating group method with Gaussian 2-body amplitudes and potential shapes.

PART (1)

THE INTEGRODIFFERENTIAL EQUATIONS FOR THE PROBLEM OF SCATTERING OF PROTONS BY DEUTERONS

CHAPTER I

(I.1.) THE NUCLEAR INTERACTION POTENTIAL

Many studies have been caried out aimed at improving the nuclear interaction potential which is considered to include both central and non central forces. The work of Signell-Marshak (1957), has confirmed the existence of the tensor and the linear spin-orbit forces. The quadratic spin-orbit term of the potential has been introduced by Hamada-Johnston (1962), in order to produce all the available data below 310 MeV of pp as well as np phenomena. According to Hamada and Johnston, the potential between the i^{th} and j^{th} nucleon must have the following form:

$$V_{ij} = \sum_{\lambda,\nu=1} \frac{1}{4} \left(\overset{\pm}{W} + \overset{\pm}{b}\, B_{ij} + \overset{\pm}{m}\, M_{ij} + \overset{\pm}{h}\, H_{ij} \right)_{\nu} \overset{\nu}{V}_{\lambda}(\underline{r}_{ij}\ ;\ \underline{\sigma}_1, \underline{\sigma}_j)$$

$$+ \mathcal{E}_{ij} \frac{e^2}{r_{ij}} \qquad \ldots \quad (I.1.1)$$

Where $\mathcal{E} = 1$ if i and j are protons; $\mathcal{E} = 0$, otherwise.

B_{ij}, M_{ij} and H_{ij} are the usual Bartlett, Majorana, and Heisenberg projection operators. These operators are introduced in order to take care of the exchange nature of the nuclear forces between nucleons i and j. we have $B^{\sigma}_{ij} = \frac{1}{2}(1 + \underline{\sigma}_i \cdot \underline{\sigma}_j)$, $H^{\tau}_{ij} = -\frac{1}{2}(1 + \tau_i \cdot \tau_j)$ and $M_{ij} = B_{ij} H_{ij}$.

The summation over λ in (I.1.1) includes most known types of nuclear forces (i.e. central, tensor, linear spin-orbit and quadratic spin-orbit forces). The other summation over ν represents the various states (i.e. triplet even, triplet odd, singlet even and singlet odd).

The function ${}^{\nu}V_{\lambda}(\underline{r}_{ij} \; ; \underline{\sigma}_i \; , \underline{\sigma}_j)$ is defined as:

$$
\begin{aligned}
{}^{\nu}V_{\lambda}(\underline{r}_{ij} \; ; \underline{\sigma}_i \; , \underline{\sigma}_j) = {}^{\nu}V_{\lambda}(\underline{r}_{ij}) \Big\{ & \delta(\lambda,1) + \delta(\lambda,2) \Big[\frac{3(\underline{\sigma}_i \cdot \underline{r}_{ij})(\underline{\sigma}_j \cdot \underline{r}_{ij})}{r_{ij}^2} \\
& - \underline{\sigma}_i \cdot \underline{\sigma}_j \Big] + \delta(\lambda,3) \Big[\frac{1}{2} (\underline{\sigma}_i + \underline{\sigma}_j) \cdot \underline{L}_{ij} \Big] + \delta(\lambda,4) \\
& \times \Big[(\underline{\sigma}_i \cdot \underline{\sigma}_j) \underline{L}_{ij}^2 - \frac{1}{2} (\underline{\sigma}_i \cdot \underline{L}_{ij})(\underline{\sigma}_j \cdot \underline{L}_{ij}) - \frac{1}{2} (\underline{\sigma}_j \cdot \underline{L}_{ij})(\underline{\sigma}_i \cdot \underline{L}_{ij}) \Big] \Big\}
\end{aligned}
\qquad \ldots \; (I.1.2)
$$

${}^{\nu}V_{\lambda}(r_{ij})$ is the potential radial function and $\underline{L}_{ij}$ is the angular momentum vector given by

$$
\underline{L}_{ij} = (\underline{r}_i - \underline{r}_j) \wedge (\underline{p}_i - \underline{p}_j) \qquad \ldots \; (I.1.3)
$$

Where $\underline{\sigma}_i$ and $\underline{p}_i$ are the spin and the momentum vectors of the nucleon i, respectively. $\delta(\lambda, \lambda')$ is the Kronecker delta.

The parameters U_k and μ_k are determined by a least square fit to Hamada and Johnston potential and are given in table (IX).

(I.2.) THE DEUTERON WAVE FUNCTION

The following description is well known and can be found in previous publication such as (Buckingham & Massey 1941; Buckingham, Hubbard and Massey, 1952; and Sribhibhadh, 1966) we are quoting it here for completeness sake and also to define the notation so as to avoid confusion in later chapters.

The deuteron ground state wave function is a mixture of the s- and the D- states and is given by:

$$\Phi(\underline{r}_{23}) = \Phi(\underline{r}_{23} \; ; \underline{\sigma}_2 \; , \underline{\sigma}_3) \; X^1_m(23) \qquad \ldots \quad (I.2.1)$$

where

$$\Phi(\underline{r}_{23} \; ; \underline{\sigma}_2 \; , \underline{\sigma}_3) = \phi_S(r_{23}) + S_{23}(\underline{r}^2_{23}) \; \phi_D(r_{23}) \qquad \ldots \quad (I.2.2)$$

and

$X^1_m(23)$ is the deuteron spin function in the triplet state. The wave function $\Phi(r_{23}; \underline{\sigma}_2 \; , \underline{\sigma}_3)$ is normalized so that

$$\sum_{spin} \int d\underline{r}_{23} \left| \Phi(\underline{r}_{23} \; ; \underline{\sigma}_2 \; , \underline{\sigma}_3) \right|^2 = 1$$

ϕ_S and ϕ_D are the radial parts of the s- and the D- state of the deuteron wave function; and these are given in double Gaussian form:

$$\phi_S(\underline{r}_{23}) = \sum_{i=1}^{2} A_i \; \mathrm{Exp}(- \alpha_i \; r^2_{23}) \qquad \ldots \quad (I.2.3)$$

$$\phi_D(\underline{r}_{23}) = \sum_{i=1}^{2} r^2_{23} \; A'_i \; \mathrm{Exp}(- \alpha'_i \; r^2_{23}) \qquad \ldots \quad (I.2.4)$$

The constants $A_i, A_i^{'}, \alpha_i$ and $\alpha_i^{'}$ are determined by the least square method from the data given by Hamada and Johnston(1962), the values of these constants are all given in table (VIII).

$S_{23}(\underline{r}_{23}^2)$ is the tensor operator defined by

$$S_{23}(r_{23}^2) = 3(\underline{\sigma}_2 \cdot \underline{r}_{23})(\underline{\sigma}_3 \cdot \underline{r}_{23}) / r_{23}^2 - \underline{\sigma}_2 \cdot \underline{\sigma}_3 \ldots \quad (I.2.5)$$

(I.3.) THE THREE-BODY WAVE FUNCTION

If particles 1 and 2 are protons, and particle 3 is the neutron. Particles 2 and 3 form a deuteron.

Then the complete wave function antisymmetric in proton in the resonating group method (Buckingham and Massey, 1941), which describes the system is given by:

$$\Psi(12,3) = \Psi(1,\overline{23}) - \Psi(2,\overline{13}) \quad \ldots \quad (I.3.1)$$

In this system in which there exist non-central forces, the potential couples the space and the spin co-ordinates of each pair of particles and hence couples their orbital and spin angular momenta. As a result, the orbital-and the spin-angular momenta are no longer constants of motion, but the total angular momentum $\underline{J}$ and its z- components J_z are, together with their respective eigenvalues J and M.

The wave function $\Psi(1,\overline{23})$ is then expanded into eigen-functions of total angular momenta $\underline{J}$ and its z- components J_z, with eigenvalues J and M respectively.

Thus

$$\Psi(1,\overline{23}) = \sum_{JM} \Psi_{JM}(1,\overline{23}) \qquad \ldots \quad (I.3.2)$$

where

$$\Psi_{JM}(1,\overline{23}) = \sum_{S} \Phi(\underline{r}_{23};\ \underline{\sigma}_2\ ,\ \underline{\sigma}_3)\ F^{S}_{JM}(1-\overline{23}) \qquad \ldots \quad (I.3.3)$$

and

$$F^{S}_{JM}(1-\overline{23}) = \sum_{\ell=|J-S|}^{J+S} \mathcal{Y}^{S}_{J\ell M}(1,\overline{23}\ ;\ \theta,\varphi)\frac{1}{r}\, f^{S}_{J\ell M}(r) \qquad \ldots \quad (I.3.4)$$

The function $\Phi(\underline{r}_{23}\ ;\ \underline{\sigma}_2\ ,\ \underline{\sigma}_3)$ is given in (I.2.2), and $f^{S}_{J\ell M}(r)$ is the radial wave function for the incident proton, while $\mathcal{Y}^{S}_{J\ell M}(1,\overline{23};\theta,\varphi)$ is defined by (Blatt and weiskopf, 1952) and given by

$$\mathcal{Y}^{S}_{J\ell M}(1,\overline{23}\ ;\ \theta\ ,\varphi) = \sum_{m=|M-S|}^{M+S} C_{\ell S}(J\ M;m\ M-m)\ \mathcal{Y}^{\ell}_{m}(\theta,\varphi)\ |X^{S}_{M-m}(1,\overline{23})\rangle \qquad \ldots \quad (I.3.5)$$

Where $C_{\ell S}(J\ M;m\ M-m)$ are the Clebsch-Gordan coefficients, $\mathcal{Y}^{\ell}_{m}(\theta,\varphi)$ are the spherical harmonics of the solid angle (θ,φ), and $|X^{S}_{M-m}(1,\overline{23})\rangle$ are the spin functions for the three-nucleon system. The wave function $\Psi_{JM}(1,\overline{23})$ satisfies the following orthonormality property

$$\sum_{spins} \iint \left[\Phi(\underline{r}_{23}\ ;\ \underline{\sigma}_2\ ,\ \underline{\sigma}_3)\, \mathcal{Y}^{S}_{J\ell M}(1,\overline{23}\ ;\ \theta,\varphi) \right]^{*} \left[\Phi(\underline{r}_{23}\ ;\ \underline{\sigma}_2\ ,\underline{\sigma}_3) \right.$$

$$\times \overset{S}{\mathcal{Y}}_{J'\ell'M'}(1,\overline{23}\ ;\ \theta,\varphi)\Big] d\underline{r}_{23}\ d\Omega(\theta,\varphi) = \delta(\ell',\ell)\ \delta(J,J')$$

$$\times\ \delta(M,M') \qquad \ldots \quad (I.3.6)$$

CHAPTER II

(II.1.) DERIVATION OF THE INTEGRO-DIFFERENTIAL EQUATIONS

We start from the Schroedinger wave equation of the system

$$\left(T_{123} + \sum_{i>j=1}^{3} V_{ij} \right) \Psi(12,3) = E\, \Psi(12,3) \qquad \ldots \quad (II.1.1)$$

T_{123}, V_{ij} and E are the kinetic-, potential- and total energy operators respectively for the three nucleon system. Thus

$$T_{123} = T_{1-23} + T_{23} = T_{2-13} + T_{13} = -\frac{\hbar^2}{2M}\left(\frac{3}{2}\nabla^2_{1-23} + \frac{2}{1}\nabla^2_{23}\right)$$

$$= -\frac{\hbar^2}{2M}\left(\frac{3}{2}\nabla^2_{2-13} + \frac{2}{1}\nabla^2_{13}\right) \qquad \ldots \quad (II.1.2)$$

and

$$E = E_p + E_d \qquad \ldots \quad (II.1.3)$$

E_p and E_d are the energy of the incident proton and the binding energy of the deuteron respectively. Omitting details of the mathematical analysis, the following sets of coupled integro-differential equations are, finally obtained for the radial functions $f^{S}_{J\ell M}(r)$.

$$D^2_{\ell'}\, f^{S'}_{J\ell' M}(r) = \sum_{\ell, S, m', m} C_{\ell' S'}(J\ M; m'\ M-m')\ C_{\ell S}(J\ M; m\ M-m)$$

$$\times \left\{ \frac{4Mr}{3\hbar^2} \int d\underline{R}\ d\Omega(\theta,\varphi) \left[\Phi(\underline{r}_{23}\ ;\ \underline{\sigma}_2\ ,\ \underline{\sigma}_3)\ Y^{\ell'}_{m'}(\theta,\varphi)\ \left|\chi^{S'}_{M-m'}(1,\overline{23})\right\rangle \right]^{*} \right.$$

$$\times \sum_{\lambda,\nu=1}^{4} \Big[\tfrac{1}{4}(2w - h)_{\nu} \; {}^{\nu}_{\lambda}V(\underline{r}_{12} ; \underline{\sigma}_1 , \underline{\sigma}_2) \; \Phi(\underline{r}_{23} ; \underline{\sigma}_2 , \underline{\sigma}_3)$$

$$\times \; |X^{S}_{M-m} (1,\overline{23})\rangle + \tfrac{1}{4}(2b - m)_{\nu} \; {}^{\nu}_{\lambda}V(\underline{r}_{12} ; \underline{\sigma}_1 , \underline{\sigma}_2) \; \Phi(\underline{r}_{23} ; \underline{\sigma}_1 , \underline{\sigma}_3)$$

$$\times \; |X^{S}_{M-m} (2,\overline{13})\rangle \Big] \; Y^{\ell}_{m}(\theta,\varphi) \; \frac{1}{r} \; f^{S}_{J\ell M}(r) + \frac{4Mr}{3\hbar^2} \int d\underline{R} \; d\Omega(\theta,\varphi)$$

$$\times \Big[\phi(\underline{r}_{23} ; \underline{\sigma}_2 , \underline{\sigma}_3) \; Y^{\ell'}_{m'}(\theta', \varphi') \;\; |X^{S'}_{M-m'} (1,\overline{23})\rangle \Big]^{*} \frac{e^2}{r_{12}} \; \Phi(\underline{r}_{23};\underline{\sigma}_2,\underline{\sigma}_3)$$

$$\times \; |X^{S}_{M-m} (1,\overline{23})\rangle \, Y^{\ell}_{m}(\theta,\varphi) \; \frac{1}{r} \; f^{S}_{J\ell M}(r) - \int d\underline{r}' \; d\Omega(\theta,\varphi) \; (4/3)^4 \; \frac{Mr}{\hbar^2}$$

$$\times \Big[\Phi(\underline{r}_{23} ; \underline{\sigma}_2 , \underline{\sigma}_3) \; Y^{\ell'}_{m'}(\theta,\varphi) \;\; |X^{S}_{m-m'} (1,\overline{23})\rangle \Big]^{*} \sum_{\lambda,\nu=1}^{4} \Big[\tfrac{1}{4}(W-2h)_{\nu}$$

$$\times \; {}^{\nu}_{\lambda}V(\underline{r}_{12} ; \underline{\sigma}_1 , \underline{\sigma}_2) \; \Phi(\underline{r}_{13} ; \underline{\sigma}_1 , \underline{\sigma}_3) \;\; |X^{S}_{M-m} (1,\overline{23})\rangle + \tfrac{1}{4}(b-2m)_{\nu}$$

$$\times \; {}^{\nu}_{\lambda}V(\underline{r}_{12} ; \underline{\sigma}_1 , \underline{\sigma}_2) \; \Phi(\underline{r}_{13} ; \underline{\sigma}_2 , \underline{\sigma}_3) \; |X^{S}_{M-m} (1,\overline{23})\rangle \Big] \; Y^{\ell}_{m}(\theta', \varphi')$$

$$\times \; \frac{1}{r'} \; f^{S}_{J\ell M}(r') - \int d\underline{r}' \; d\Omega(\theta,\varphi) \Big[\Phi(\underline{r}_{23} ; \underline{\sigma}_2 , \underline{\sigma}_3) \;\; Y^{\ell'}_{m'}(\theta,\varphi)$$

$$\times \; |X^{S'}_{M-m'} (1,\overline{23})\rangle \Big]^{*} (4/3)^4 \; \frac{e^2}{r_{12}} \;\; \frac{Mr}{\hbar^2} \;\; \Phi(\underline{r}_{13} ; \underline{\sigma}_1 , \underline{\sigma}_3) \; |X^{S}_{M-m} (2,\overline{13})\rangle$$

$$\times \; Y^{\ell}_{m}(\theta', \varphi') \; \frac{1}{r'} \; f^{S}_{J\ell M}(r') + (E_p - E_d) \int d\underline{r}' \; d\Omega(\theta,\varphi) \; (4/3)^4 \; \frac{Mr}{\hbar^2}$$

$$\times \Big[\Phi(\underline{r}_{23} ; \underline{\sigma}_2 , \underline{\sigma}_3) \; Y^{\ell'}_{m'}(\theta,\varphi) \;\; |X^{S'}_{M-m'} (1,\overline{23})\rangle \Big]^{*} \Phi(\underline{r}_{13} ; \underline{\sigma}_1 , \underline{\sigma}_3)$$

$$\times \; |X^{S}_{M-m} (2,\overline{13})\rangle \, Y^{\ell}_{m}(\theta', \varphi') \; \frac{1}{r'} \; f^{S}_{J\ell M}(r') + \int d\underline{r}' \; d\Omega(\theta,\varphi) \; (4/3)^3 \; r$$

$$\times \overset{\ell'*}{\underset{m'}{Y}}(\theta,\varphi) \left|X^{S'}_{M-m'}(1,\overline{23})\right\rangle^{*} \left[\nabla^2_{r'} \Phi(\underline{r}_{23} ; \underline{\sigma}_2 , \underline{\sigma}_3) \Phi(\underline{r}_{13} ; \underline{\sigma}_1, \underline{\sigma}_3) \right]$$

$$\times \left|X^{S}_{M-m}(2,\overline{13})\right\rangle \overset{\ell}{\underset{m}{Y}}(\theta',\varphi') \frac{1}{r'} \overset{S}{\underset{J\ell M}{f}}(r') - \int d\underline{r}' \, d\Omega(\theta,\varphi) \, (4/3)^4 \, r$$

$$\times \left[\nabla^2_R \Phi(\underline{r}_{23} ; \underline{\sigma}_2 , \underline{\sigma}_3) \overset{\ell'}{\underset{m'}{Y}}(\theta,\varphi) \right]^{*} \left|X^{S'}_{M-m'}(1,\overline{23})\right\rangle^{*} \Phi(\underline{r}_{13};\underline{\sigma}_1,\underline{\sigma}_3)$$

$$\times \left| X^{S}_{M-m}(2,\overline{13})\right\rangle \overset{\ell}{\underset{m}{Y}}(\theta',\varphi') \frac{1}{r'} \overset{S}{\underset{J\ell M}{f}}(r') \Big\} \qquad \ldots \quad (II.1.4)$$

where

$$D^2_{\ell'} = \frac{d^2}{dr^2} - \frac{\ell'(\ell'+1)}{r^2} + K^2 \qquad \ldots \quad (II.1.5)$$

and K^2 is a wave number defined by

$$K^2 = \frac{4}{3} \frac{M}{\hbar^2} E_p(C.M) \qquad \ldots \quad (II.1.6)$$

METHOD OF REPRESENTATION

The resulting integrals are of two types and are classified as direct (D), and exchange (E). All direct terms are completely evaluated, but the exchange terms are left in the form of integrands.

The final step in the calculation consists in solving numerically the resulting integro-differential equations for the radial functions $f^{S}_{J\ell M}(r)$. In the evaluation of the central, coulomb,....,etc. terms; the following cases have been considered:

(a) The (s-s) terms; in which both the Bra and Ket functions are in the s-state.,

(b) The (s-D) and the (D-s) terms in which one of the deuteron wave function is in the s-state, while the other is in the D-state.,

(c) The (D-D) terms are neglected due to the small percentage of the D-state admixture (4%).

PART (2)

PROTON-DEUTERON SCATTERING

CHAPTER III

DIRECT (s-s) INTERACTION TERMS

The direct interaction terms in the resulting integro-differential equations (II.1.4) are given below:

(III.1.) THE CENTRAL TERM

The term for the direct interaction of the central force $\overset{c}{D}{}^{S'}_{J\ell' M(s-s)}(r)$ is given by:

$$\overset{c}{D}{}^{S'}_{J\ell' M(s-s)}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m)$$

$$\times \int d\underline{R}\ d\Omega(\theta,\phi) \left[\phi_S(\underline{R})\ Y^{\ell'}_{m'}(\theta,\phi)\ \left|X^S_{M-m}(1,\overline{23})\right\rangle\right]^* \sum_{\nu=1}^{4} \left[\frac{1}{4}(2W-h)_\nu\right.$$

$$\times {}^{\nu}V_c(|\underline{r} - \tfrac{1}{2}\underline{R}|)\ \left|X^S_{M-m}(1,\overline{23})\right\rangle + \frac{1}{4}(2b-m)_\nu\ {}^{\nu}V_c(|\underline{r} - \tfrac{1}{2}\underline{R}|)$$

$$\times \left.\left|X^S_{M-m}(2,\overline{13})\right\rangle\right] \phi_S(\underline{R})\ Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) = \frac{3M}{3\hbar^2} \sum_{\ell,S} \sum_{m',m}$$

$$\times C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m)\ \delta(S',S)\ \delta(m',m) \int d\underline{R}\ d\Omega(\theta,\phi)$$

$$\times \phi_S(\underline{R})\ Y^{\ell' *}_{m'}(\theta,\phi) \sum_{\nu=1}^{4} \frac{1}{4} \left[(2W-h)_\nu + g(S)\ (2b-m)_\nu\right]$$

$$\times {}^{\nu}V_c(|\underline{r} - \tfrac{1}{2}\underline{R}|)\ \phi_S(\underline{R})\ Y^{\ell}_{m}(\theta,\phi)\ f^S_{J\ell M}(r) \qquad \ldots \quad \text{(III.1.1)}$$

Where $g(S) = -\frac{1}{2}$ for $S=\frac{1}{2}$; and $g(S) = 1$ for $S=3/2$.

The potential in the direct central force is now given in double Gaussian form for two distinct cases:

(a) THE DOUBLET STATE($s=\frac{1}{2}$)

$$ {}^{c}V^{(1)}(|\underline{r} - \tfrac{1}{2}\underline{R}|) = \sum_{\nu=1}^{4} \frac{1}{4}\left[(2W - h)_\nu - \frac{1}{2}(b - 2m)_\nu \right] $$

$$ x\,{}^{\nu}V_c(|\underline{r} - \tfrac{1}{2}\underline{R}|) = \sum_{k=1}^{2} {}^{c}U_k^{(1)} \, Exp(- {}^{c}\mu_k^{(1)} (|\underline{r} - \tfrac{1}{2}\underline{R}|)^2) $$

... (III.a.1)

(b) THE QUARTET STATE ($S=3/2$)

$$ {}^{c}V^{(2)}(|\underline{r} - \tfrac{1}{2}\underline{R}|) = \sum_{\nu=1}^{\nu} \frac{1}{4}\left[(2W - h)_\nu + (b - 2m)_\nu \right] {}^{\nu}V_c(|\underline{r} - \tfrac{1}{2}\underline{R}|) $$

$$ = \sum_{k=1}^{2} {}^{c}U_k^{(2)} \, Exp(- {}^{c}\mu_k^{(2)} (|\underline{r} - \tfrac{1}{2}\underline{R}|)^2) \qquad \text{... (III.b.1)} $$

The values of the parameters ${}^{c}\mu_k^{(II)}$ and ${}^{c}U_k^{(II)}$ (II=1,2) were calculated and are given in table (IX).

Now, using (III.a.1) and (III.b.1), and integrating over all coordinates with exception of r, expression (III.1.1) finally becomes:

$$ {}^{c}D^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell, S} {}^{c}B_1(r) \; \delta(\ell', \ell) \; \delta(S', S) \; f^{S}_{J\ell M}(r) $$

... (III.1.2)

where

$$ {}^{c}B_1(r) = \frac{4\,M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \, {}^{c}U_k^{(\pi)} \left(\pi / \lambda_{ijk} \right)^{3/2} Exp(- {}^{c}\mu_k^{(\pi)} (1 - \gamma_{ijk}) r^2) $$

... (III.1.3)

and

$$\lambda_{ijk} = \alpha_i + \alpha_j + \frac{1}{4}\, \overset{c(\pi)}{u_k} \; ; \quad \gamma_{ijk} = \overset{c(\alpha)}{u_k} \Big/ 4\, \lambda_{ijk}$$

(III.2.) THE COULOMB TERM

The interaction between two protons, is given below by:

$$\overset{coul\ S'}{D}_{J\ell' M(s-s)}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell, S, m', m} C_{\ell' S'}(J\ M; m'\ M-m')\ C_{\ell S}(J\ M; m\ M-m)$$

$$\times \int d\underline{R}\ d\Omega(\theta,\phi)\ \overset{\ell' *}{Y}_{m'}(\theta,\phi)\ \phi_s(\underline{R})\ g(S)\ \left|X^{S'}_{M-m'}(1,\overline{23})\right\rangle^{*}\ \overset{coul}{V}(\underline{r}_{12})$$

$$\times \left|X^{S}_{M-m}(1,\overline{23})\right\rangle \phi_s(\underline{R})\ \overset{\ell}{Y}_m(\theta,\phi)\ \frac{1}{r}\ f^{S}_{J\ell M}(r) \qquad \ldots \quad (III.2.1)$$

where

$$\overset{coul}{V}(\underline{r}_{12}) = \frac{e^2}{r_{12}} \qquad \ldots \quad (III.2.2)$$

The potential function $\overset{coul}{V}(\underline{r}_{12})$ can be expanded in the following way:

$$\overset{coul}{V}(\underline{r}_{12}) = \sum_{p,\eta} \overset{coul}{U}_p(r,R)\ \overset{p *}{Y}_{\eta}(\theta_R,\phi_R)\ \overset{p}{Y}_{\eta}(\theta,\phi) \ldots \quad (III.2.3)$$

so that

$$\overset{coul}{U}_p(r,R) = 2 \int_{-1}^{+1} d\mu\ p_p(\mu)\ \overset{coul}{V}(\underline{r}_{12}) \qquad \ldots \quad (III.2.4)$$

Using (III.2.3) in (III.2.1) and performing the spin summation we get:

$$\overset{coul}{D}{}^{S'}_{J\ell' M(s-s)}(r) = \frac{4Me^2}{3\hbar^2} \sum_{i,j=1}^{2} A_i A_j \sum_{\ell, S} g(S) \int_0 dR\, R^2$$

$$\times \mathrm{Exp}(-(\alpha_i + \alpha_j)R^2) \overset{coul}{U_p}(r,R)\, f^S_{J\ell M}(r) \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')$$

$$\times C_{\ell S}(J\ M;m\ M-m)\, \delta(S',S)\, \delta(m',m) \int d\Omega_R(\theta_R,\phi_R)\, Y^{p*}(\theta_R,\phi_R) \int d\Omega(\theta,\phi)$$

$$\times \overset{p}{Y}(\theta,\phi)\ Y^{\ell}_{m}(\theta,\phi) \qquad \ldots \quad (III.2.5)$$

Integrating the angular part in (III.2.5) and then summing over the magnetic quantum numbers, m' and m, we get:

$$\overset{coul}{D}{}^{S'}_{J\ell' M(s-s)}(r) = \frac{16\pi Me^2}{3\hbar^2 r} \sum_{i,j=1}^{2} A_i A_j \sum_{\ell, S} g(S)\, f^S_{J\ell M}(r)\, \delta(S',S)$$

$$\times \delta(\ell',\ell) \int_0 R^2\, dR\, \mathrm{Exp}(-(\alpha_i+\alpha_j)R^2) \qquad \ldots \quad (III.2.6)$$

Expression (III.2.6) is further simplifiedm and finaly reduced to the following form

$$\overset{coul}{D}{}^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell, S} \overset{coul}{B_1}(r)\, g(S)\, \delta(S',S)\, \delta(\ell',\ell)\, f^S_{J\ell M}(r)$$

$$\ldots \quad (III.2.7)$$

where

$$\overset{coul}{B_1}(r) = \sum_{i,j=1}^{2} \frac{8Me^2\pi}{3\hbar^2 r} A_i A_j\, (\pi/(\alpha_i + \alpha_j))^{1/2} \ldots \quad (III.2.8)$$

for $S' = S = \frac{1}{2}$ and $S' = S = 3/2$ respectively.

(III.3) THE TENSOR TERM

The direct term of the tensor force ${}^{t\,S'}D_{J\ell' M(s-s)}(r)$ is given in the quartet state by:

$$
\begin{aligned}
{}^{t\,S'}D_{J\ell' M(s-s)}(r) &= \frac{4Mr}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m) \\
&\times \int d\underline{R}\ d\Omega(\theta,\phi) \left[\phi_S(\underline{R})\ |X^S_{M-m}(1,\overline{23})\rangle^{*} Y^{\ell'}_{m'}(\theta,\phi) \right] \sum_{\nu=1}^{4} \frac{1}{4} \Big[(2w-h)_\nu \\
&\times {}^{\nu}V_t(\underline{r}_{12})\ S_{12}(\underline{r}^2_{12})\ |X^S_{M-m}(1,\overline{23})\rangle + (2b-m)_\nu\ {}^{\nu}V_t(\underline{r}_{12})\ S_{12}(\underline{r}^2_{12}) \\
&\times |X^S_{M-m}(1,\overline{23})\rangle \Big] \phi_S(\underline{R})\ Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) = \frac{4M}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} \\
&\times C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m) \int d\underline{R}\ d\Omega(\theta,\phi)\ Y^{\ell' *}_{m'}(\theta,\phi)\ \phi_S(\underline{R}) \\
&\times {}^{t}V(\underline{r}_{12}) \langle X^{S'}_{M-m'}(1,\overline{23})|\ S_{12}(\underline{r}^2_{12})\,|X^S_{M-m}(1,\overline{23})\rangle\ Y^{\ell}_{m}(\theta,\phi)\ \phi_S(\underline{R})\ f^S_{J\ell M}(r)
\end{aligned}
\qquad \ldots \text{(III.3.1)}
$$

where

$$
{}^{t(\nu)}V(\underline{r}_{12}) = \sum_{\nu=1}^{4} \frac{1}{4}(2w - h + 2b - m)_\nu\ {}^{\nu}V_t(\underline{r}_{12}) = r^2_{12} \sum_{k=1}^{2} {}^{t}U_k \times \mathrm{Exp}(-{}^{t(\nu)}\mu_k\ \underline{r}^2_{12}) \qquad \ldots \text{(III.3.2)}
$$

and $S_{12}(\underline{r}^2_{12})$ is a tensor operator defined in (I.2.5).

The spin matrix elements of the tensor operator $S_{12}(\underline{r}^2_{12})$ are expressed in terms of $Y^2_{m'-m}(\theta,\phi)_{r_{12}}$ harmonics.

The $Y^2(\theta,\phi)_{r_{12}}$ is then written in polar coordinates of $\underline{r}$ and $\underline{R}$ (Bransden, Smith and Tate, 1958)

$$\langle \chi^{S'}_{M-m'}(1,\overline{23})|\ S_{12}(\underline{r}^2_{12})\,|\chi^{S}_{M-m}(1,\overline{23})\rangle = g(S',S)\ (4\pi/5)^{\frac{1}{2}}$$

$$\times\ C_{S'S}(2\ ,\ m'-m\ ;\ m'-M,\ M-m)\ \overset{2}{\underset{m'-m}{Y}}(\theta,\phi)_{r_{12}} = g(S',S)\ (4\pi/5)^{\frac{1}{2}}$$

$$\times\ C_{S'S}(2,\ m'-m\ ;\ m'-M\ ,\ M-m)\ \frac{1}{r^2_{12}}\Big[r^2\ \overset{2}{\underset{m'-m}{Y}}(\theta,\phi) + \frac{1}{4}R^2\ \overset{2}{\underset{m'-m}{Y}}(\theta_R,\phi_R)$$

$$-\ \frac{1}{2}\,rR\ (40\pi/3)^{\frac{1}{2}} \sum_{\lambda,\eta} C_{11}(2,\ m'-m\ ;\eta\lambda)\ \overset{1}{\underset{\lambda}{Y}}(\theta,\phi)\ \overset{1}{\underset{\eta}{Y}}(\theta_R,\phi_R)\ \Big] \qquad \ldots\ (III.3.3)$$

where $g(S',S) = 4$ for $S' = S = 3/2$.

The potential function ${}^{t}V(\underline{r},\underline{R})$ is also expanded in spherical harmonics, thus

$${}^{t}V(\underline{r},\underline{R}) = \sum_{n,p} {}^{t}U_n(r,R)\ \overset{n_*}{\underset{p}{Y}}(\theta_R,\phi_R)\ \overset{n}{\underset{p}{Y}}(\theta,\phi) \qquad \ldots\ (III.3.4)$$

where

$${}^{t}U_n(r,R) = 2\pi \int_{-1}^{+1} d\mu\ p_n(\mu)\ {}^{t}V(\underline{r},\underline{R}) \qquad \ldots\ (III.3.5)$$

Therefore, in using (III.3.3) and (III.3.4), expression (III.3.1) reduces to its final form:

$${}^{t}D^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell} {}^{t}B_l(r)\ A(\ell' 3/2\ ;\ \ell 3/2)\ f^{3/2}_{J\ell M}(r) \qquad \ldots\ (III.3.6)$$

where

$${}^{t}B_l(r) = \frac{4Mr^2}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j\ {}^{t}U^{(l)}_k(\pi/\lambda_{ijk})^{3/2}\ (1-\tfrac{1}{2}\gamma_{ijk})^2$$

$$\times \, \mathrm{Exp}(-{}^{t}\mu_k^{(1)} (1 - {}^{t}\mu_k^{(1)} /4 \, \lambda_{ijk}) r^2) \qquad \ldots \quad (\mathrm{III.3.7})$$

and

$$A(\ell' 3/2 \, ; \, \ell 3/2) = 4(-1)^{J-3/2} \left[(2\ell + 1)(2\ell' + 1) \right]^{\frac{1}{2}} C_{\ell' \ell}(2)$$

$$\times \, W(\ell' 3/2 \, ; \, \ell 3/2 \, ; \, J2) \qquad \ldots \quad (\mathrm{III.3.8})$$

$C_{\ell' \ell}(2) = C_{\ell' \ell}(2,0;00)$ and $W(\ell' 3/2 \, ; \, \ell 3/2; J2)$ are the Clebsch-Gordan, and Racah coefficients respectively.

(III.4.) THE SPIN-ORBIT TERM

This is given by

$$D^{s.o \, S'}_{J\ell' M(s-s)}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell, S} \sum_{m', m} C_{\ell' S'}(J \, M; m' \, M-m') \, C_{\ell S}(J \, M; m \, M-m)$$

$$\times \int d\underline{R} \, d\Omega(\theta,\phi) \left[\phi_S(\underline{R}) \, \middle| X^{S'}_{M-m'}(1,\overline{23}) \right\rangle Y^{\ell'}_{m'}(\theta,\phi) \Big]^* \sum_{=1}^{2} \frac{1}{4}$$

$$\times \Big[(2w - h)_\nu \, V^{\nu(I)}_{s.o}(\underline{r}_{12}) \, \frac{1}{2} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L}_{12} \left| X^S_{M-m}(1,\overline{23}) \right\rangle + (2b-m)_\nu$$

$$\times \, {}^{\nu}V^{(II)}_{s.o}(\underline{r}_{12}) \, \frac{1}{2} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L}_{12} \left| X^S_{M-m}(2,\overline{13}) \right\rangle \Big] \phi_S(\underline{R}) \, Y^{\ell}_{m}(\theta,\phi) \, \frac{1}{r}$$

$$\times \, f^S_{J\ell M}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell, S} \sum_{m', m} C_{\ell' S'}(J \, M; m' \, M-m') \, C_{\ell S}(J \, M; m \, M-m)$$

$$\times \sum_{i,j=1}^{2} A_i A_j \int d\underline{R} \, d\Omega(\theta,\phi) \; Y^{\ell'*}_{m'}(\theta,\phi) \, \mathrm{Exp}(-\alpha_i R^2) \left| X^{S'}_{M-m'}(1,\overline{23}) \right\rangle$$

$$\times \sum_{=1}^{4} \frac{1}{4} (2w - h + 2b + m)_\nu \, {}^{\nu}V_{s.o}(\underline{r}_{12}) \frac{1}{2} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L}_{12}$$

$$x \left|X^S_{M-m}(1,\overline{23})\right\rangle \mathrm{Exp}(-\alpha_i R^2)\ Y^{\ell}_m(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) \quad \ldots \quad (III.4.1)$$

The operator $\underline{L}_{12}$ has the following form

$$\underline{L}_{12} = \frac{1}{i}\left(\underline{r} - \tfrac{1}{2}\underline{R}\right)\wedge\left(\frac{3}{2}\frac{\partial}{\partial\underline{r}} - \frac{\partial}{\partial\underline{R}}\right) \quad \ldots \quad (III.4.2)$$

$$= -i\,\frac{3}{2}\,\underline{r}\wedge\frac{\partial}{\partial\underline{r}} \quad \ldots \quad (III.4.2a)$$

$$+\ i\,\underline{r}\wedge\frac{\partial}{\partial\underline{R}} \quad \ldots \quad (III.4.2b)$$

$$+\ \frac{3}{4}\,i\,\underline{R}\wedge\frac{\partial}{\partial\underline{r}} \quad \ldots \quad (III.4.2c)$$

$$-\ \frac{1}{2}\,i\,\underline{R}\wedge\frac{\partial}{\partial\underline{R}} \quad \ldots \quad (III.4.2d)$$

The potentials in the doublet and quartet states are given by:

$$\sum_{\nu=1}^{4} \frac{1}{4}\,(2w - h + 2b - m)_{\nu}\ {}^{\nu}V_{s.o}(\underline{r}_{12}) = \sum_{k=1}^{2} U_k^{s.o\,(II)}$$

$$x\ \mathrm{Exp}\left(-\mu_k^{s.o\,(II)}\ \underline{r}_{12}^2\right) = V^{s.o\,(II)}(\underline{r}_{12}) \qquad (II=1,2) \quad \ldots \quad (III.4.3)$$

The potential function $V^{s.o\,(II)}(\underline{r}_{12})$ is now expanded in spherical harmonics

$$V^{s.o\,(II)}(\underline{r},\underline{R}) = \sum_{L,M} U_L^{s.o\,(II)}(r,R)\ Y^L_M(\theta_R,\phi_R)\ Y^L_M(\theta,\phi)$$

$$\ldots \quad (III.4.4)$$

where

$$U_L^{s.o\,(II)}(r,R) = 2\pi\int_{-1}^{+1} d\mu\ p_L(\mu)\ V^{s.o\,(II)}(\underline{r},\underline{R}) \quad \ldots \quad (III.4.5)$$

Using (III.4.2) and (III.4.4), we finally write the spin-orbit interaction in the doublet and quartet states as:

$$D^{s.o\ S'}_{J\ell' M(s-s)}(r) = \sum_{\ell, S} B_1^{s.o\ (II)}(r)\ A(J\ell)\ f^S_{J\ell M}(r)\ \delta(S', S)\ \delta(\ell', \ell) \qquad \text{... (III.4.6)}$$

where

$$B_1^{s.o\ (II)}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j\ U_k^{s.o\ (II)}\ (\pi / \lambda_{ijk})^{3/2}$$

$$x\ (1 - \gamma_{ijk}/2)\ \text{Exp}(- \mu_k^{s.o\ (II)}\ (1 - \mu_k^{s.o\ (II)}/4\ \lambda_{ijk}) r^2) \qquad \text{... (III.4.7)}$$

and $A(J\ell)$ is given for the doublet satet ($S' = S = \frac{1}{2}$) by:

$$A_1(J\ell) = \frac{1}{3}\left[J(J + 1) - \ell(\ell + 1) - \frac{3}{4}\right] \qquad \text{... (III.4.8)}$$

and for the quartet state ($S' = S = 3/2$) by:

$$A_2(J\ell) = \frac{2}{3}\left[\ J(J + 1) - \ell(\ell + 1) - \frac{15}{4}\right] \qquad \text{... (III.4.9)}$$

(III.5.) THE QUADRATIC SPIN-ORBIT TERM

The direct term of the quadratic spin-orbit force $\underset{J\ell' M(s-s)}{\overset{Q\ S'}{D}}(r)$ is given in both cases ($s=\frac{1}{2}$ and $s=3/2$) by the following expression

$$\underset{J\ell' M(s-s)}{\overset{Q\ S'}{D}}(r) = \frac{4\ M\ r}{3\ \hbar^2} \sum_{\ell',S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m)$$

$$\times \int d\underline{R} \int d\Omega(\theta,\phi)\ \overset{*\ell'}{\underset{m'}{Y}}(\theta,\phi)\ \phi_s(R) \left\langle \chi^{S'}_{M-m'}(1,\overline{23}) \right| \sum_{=1}^{4} \Big[\frac{1}{4}(2W-h)_{\nu}$$

$$\times\, {}^{\nu}V_Q(\underline{r}_{12})\ \underline{L}_Q(12) \left| \chi^{S}_{M-m}(1,\overline{23}) \right\rangle + \frac{1}{4}(2b-m)_{\nu}\ {}^{\nu}V_Q(\underline{r}_{12})\ \underline{L}_Q(12) \left| \chi^{S}_{M-m}(2,\overline{13}) \right\rangle \Big]$$

$$\times\, \phi_s(R)\ \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\ \frac{1}{r}\ f^{S}_{J\ell M}(r) \qquad \ldots \quad (III.5.1)$$

where

$$\underline{L}_Q(12) = (\underline{\sigma}_1 \cdot \underline{\sigma}_2)\ \underline{L}^2_{12} - \underline{M}_{12} \qquad \ldots \quad (III.5.2)$$

and

$$\underline{M}_{12} = \frac{1}{2}\Big[(\underline{\sigma}_1 \cdot \underline{L}_{12})\ (\underline{\sigma}_2 \cdot \underline{L}_{12}) + (\underline{\sigma}_2 \cdot \underline{L}_{12})(\underline{\sigma}_1 \cdot \underline{L}_{12}) \Big]$$

$$\ldots \quad (III.5.3)$$

THE SPIN SIMPLIFICATION

(III.5.a.) THE DOUBLET STATE

It has been shown (Sribhibhadh, 1966) that the spin matrix elements in the direct interaction reduce to the following form:

$$< X^{\frac{1}{2}}_{M-m'}(1,\overline{23})\Big| \Big[\sum_{=1}^{4} (2W - h)_{\nu}\, {}^{\nu}V_Q(\underline{r}_{12})\, \underline{L}_Q(12) \Big|X^{\frac{1}{2}}_{M-m}(1,\overline{23})>$$

$$+ \sum_{=1}^{4} (2b - m)_{\nu}\, {}^{\nu}V_Q(\underline{r}_{12})\, \underline{L}_Q(12) \Big|X^{\frac{1}{2}}_{M-m}(2,\overline{13})> \Big] = \overset{Q\ (1)}{V}(\underline{r}_{12})$$

$$\times \Big[- \frac{4}{3} \underline{L}^2_{12} \Big] \delta(m',m) + \overset{Q\ (2)}{V}(\underline{r}_{12}) \Big[3\, \underline{L}^2_{12} \Big] \delta(m',m)$$

... (III.5.a.1)

where

$$\overset{Q\ (1)}{V}(\underline{r}_{12}) = \sum_{=1}^{4} \frac{1}{4}(2W - h + 2b - m)_{\nu}\, {}^{\nu}V_Q(\underline{r}_{12})$$

$$\times \sum_{k=1}^{2} \overset{Q\ (1)}{U_k} \, \mathrm{Exp}(- \overset{Q\ (1)}{\mu_k}\ \underline{r}^2_{12})$$ ... (III.5.a.2)

and

$$\overset{Q\ (2)}{V}(\underline{r}_{12}) = \sum_{=1}^{4} \frac{1}{4} (2b - m)_{\nu}\, {}^{\nu}V_Q(\underline{r}_{12}) = \sum_{k=1}^{2} \overset{Q\ (2)}{U_k} \, \mathrm{Exp}(- \overset{Q\ (2)}{\mu_k}\ \underline{r}^2_{12})$$

... (III.5.a.3)

we have also

$$\underline{L}_{12} = - \frac{3i}{2} (\underline{r} - \tfrac{1}{2} \underline{R})\wedge \frac{\partial}{\partial \underline{r}} - (\underline{r} - \tfrac{1}{2} \underline{R})\wedge \frac{\partial}{\partial \underline{R}}$$ ... (III.5.a.4)

Using (III.5.a.1) we get from (III.5.1)

$$\overset{Q}{D}_{J\ell' M(s-s)}(r) = \frac{4Mr}{3\hbar^2} \sum_{i,j=1}^{2} A_i\, A_j \sum_{\ell} \sum_{m',m} C_{\ell' \frac{1}{2}}(J\ M;m'\ M-m')$$

$$\times\, C_{\ell\frac{1}{2}}(J\ M;m\ M-m)\ \delta(m',m) \Big[\int d\underline{R} \int d\Omega(\theta,\phi)\ \mathrm{Exp}(-\alpha_i R^2)\ \overset{*}{Y}{}^{\ell'}_{m'}(\theta,\phi)$$

$$\times \overset{Q\ (1)}{V}(\underline{r}_{12}) \Big[- \frac{4}{3} \underline{L}^2_{12} \Big] \mathrm{Exp}(-\alpha_j R^2)\, Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\, f^{\frac{1}{2}}_{J\ell M}(r) + \int d\underline{R} \int d\Omega(\theta,\phi)$$

$$\times \, Exp(-\alpha_i R^2) \, \overset{*\ell'}{Y}_{m'}(\theta,\phi) \, \overset{Q}{V}{}^{(2)}(\underline{r}_{12}) \left[3 \, \underline{L}^2_{12} \right] Exp(-\alpha_j R^2) \, Y^{\ell}_{m}(\theta,\phi)$$

$$\times \, \frac{1}{r} \, f^{\frac{1}{2}}_{J\ell M}(r) \Big] \qquad \ldots \quad (III.5.a.5)$$

(III.5.b.) THE QUARTET STATE

The spin functions $|X^{S}_{M-m'}(1,\overline{23})\rangle$ in this case, need no simplification because they are symmetrical in 1,2 and 3.

Thus, the direct term is written as:

$$\overset{Q}{D}_{J\ell' M(s-s)}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m') \, C_{\ell 3/2}(J\ M;m\ M-m)$$

$$\times \, \delta(m',m) \int d\underline{R} \int d\Omega(\theta,\phi) \, \overset{*\ell'}{Y}_{m'}(\theta,\phi) \, \phi_s(R) \, \overset{Q}{V}{}^{(1)}(\underline{r}_{12}) \langle X^{3/2}_{M-m'}(1,\overline{23})|$$

$$\times \, \underline{L}^2_{12} \, |X^{3/2}_{M-m}(1,23)\rangle \, \phi_s(R) \, Y^{\ell}_{m}(\theta,\phi) \, \frac{1}{r} \, f^{3/2}_{J\ell M}(r) - \frac{4Mr}{3\hbar^2} \sum_{\ell} \sum_{m',m}$$

$$\times \, C_{\ell' 3/2}(J\ M;m'\ M-m') \, C_{\ell 3/2}(J\ M;m\ M-m) \int d\underline{R} \int d\Omega(\theta,\phi) \, \overset{*\ell'}{Y}_{m'}(\theta,\phi)$$

$$\times \, \phi_s(R) \, \overset{Q}{V}{}^{(1)}(\underline{r}_{12}) \langle X^{3/2}_{M-m'}(1,\overline{23})| \, \underline{M}_{12} \, |X^{3/2}_{M-m}(1,\overline{23})\rangle \, \phi_s(R) \, Y^{\ell}_{m}(\theta,\phi) \, \frac{1}{r}$$

$$\times \, f^{3/2}_{J\ell M}(r) \qquad \ldots \quad (III.5.b.1)$$

where $\underline{M}_{12}$ and $\overset{Q}{V}{}^{(1)}(\underline{r}_{12})$ were given in (III.5.3) and (III.5.a.2) respectively.

To solve equation (III.5.1), we consider the integrand involving the operator $\underline{L}^2_{12}$ in both the doublet and quartet states. Thus,

$$U^{Q\,(II)}_{\underline{L}_{12}}(r) = \sum_{i,j=1}^{2} A_i\, A_j \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M\text{-}m'\ M\text{-}m')\ \frac{4\ M}{3\hbar^2}$$

$$\times\ C_{\ell S}(J\ M;m\ M\text{-}m)\ \delta(S',S)\ \delta(m',m) \int d\underline{R} \int d\Omega\,(\theta,\phi)\ \mathrm{Exp}(-\alpha_i R^2)$$

$$\times\ V^{Q\,(II)}(\underline{r}_{12})\ \overset{*}{Y}{}^{\ell'}_{m'}(\theta,\phi)\ \underline{L}^2_{12}\ Y^{\ell}_{m}(\theta,\phi)\ \mathrm{Exp}(-\alpha_j R^2)\ \frac{1}{r}\ f^S_{J\ell M}(r)$$

... (III.5.4)

The operator $\underline{L}^2_{12}$ operates on the functions $Y^{\ell}_{m}(\theta,\phi)$ $\mathrm{Exp}(-\alpha_j R^2)\ \frac{1}{r}\ f^S_{J\ell M}(r)$ and we eliminate the function $\mathrm{Exp}(-\alpha_j R^2)$ first. Thus,

$$(i)^2\ \underline{L}^2_{12}\ \mathrm{Exp}(-\alpha_j R^2)\ Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) = \mathrm{Exp}(-\alpha_j R^2) \Big[-\frac{9}{4}\,\underline{L}^2$$

$$-\frac{9}{8}\left(i\ \underline{L}\cdot\underline{R}\wedge\frac{\partial}{\partial\underline{r}}\right) - \frac{9}{8}\left(i\ \underline{R}\wedge\frac{\partial}{\partial\underline{r}}\cdot\underline{L}\right) + \frac{9}{16}\left(\underline{R}\cdot\frac{\partial}{\partial\underline{r}}\right)\left(\underline{R}\cdot\frac{\partial}{\partial\underline{r}}\right)$$

$$-\frac{9}{16}\,R^2\left(\frac{\partial}{\partial\underline{r}}\cdot\frac{\partial}{\partial\underline{r}}\right) + \left(6\alpha_j r^2 - 3\alpha_j\ \underline{r}\cdot\underline{R} + \frac{3}{4}\right)\left(\underline{R}\cdot\frac{\partial}{\partial\underline{r}}\right) + \left(-6\alpha_j\ \underline{r}\cdot\underline{R}\right.$$

$$\left.+\ 3\alpha_j R^2 - \frac{3}{2}\right)\left(\underline{r}\cdot\frac{\partial}{\partial\underline{r}}\right) - 4\alpha_j^2(\underline{r}\cdot\underline{R})(\underline{r}\cdot\underline{R}) + \left(3\alpha_j\ R^2 - 4\alpha_j\ \underline{r}\cdot\underline{R} - 4\alpha_j r^2\right.$$

$$\left.+\ 4\alpha_j^2\ r^2 R^2\right) \Big]\ Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) \qquad \text{... (III.5.5)}$$

The other operations on the functions $Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r)$ are carried out in the following way (Edmonds, 1960; Rose, 1957; and Brink and Satchler, 1967). Thus,

$$\underline{L}^2\ Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) = \ell(\ell+1)\ Y^{\ell}_{m}(\theta,\phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) \qquad \text{... (III.5.6)}$$

$$(\underline{r}\cdot\frac{\partial}{\partial \underline{r}})\, \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\, \frac{1}{r}\, f^{S}_{J\ell M}(r) = (f^{S\,\prime}_{J\ell M}(r) - \frac{1}{r}\, f^{S}_{J\ell M}(r))\, \overset{\ell}{\underset{m}{Y}}(\theta,\phi) \qquad \ldots \quad (\text{III.5.7})$$

$$(\frac{\partial}{\partial \underline{r}}\cdot\frac{\partial}{\partial \underline{r}})\, \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\, \frac{1}{r}\, f^{S}_{J\ell M}(r) = (\frac{1}{r}\, f^{\prime\prime S}_{J\ell M}(r) - \frac{\ell(\ell+1)}{r^{3}}\, f^{S}_{J\ell M}(r))$$

$$\times\, \overset{\ell}{\underset{m}{Y}}(\theta,\phi) \qquad \ldots \quad (\text{III.5.8})$$

$$(\underline{R}\cdot\frac{\partial}{\partial \underline{r}})\, \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\, \frac{1}{r}\, f^{S}_{J\ell M}(r) = -\, R\, (4\pi/3)^{\frac{1}{2}} \sum_{\ell'',m'',q''} C_{\ell 1}(\ell'')$$

$$\times\, C_{\ell'' 1}(\ell m\,;\, m'' q'')\, \overset{1}{\underset{q}{Y''}}(\theta_R,\phi_R) \Big\{ \overset{\ell''}{\underset{m''}{Y}}(\theta,\phi)\, \frac{d}{dr} \Big[\frac{1}{r}\, f^{S}_{J\ell M}(r)\Big]$$

$$+ \Big[6\ell(\ell+1)(2\ell+1) \Big]^{\frac{1}{2}} W(\ell\, \ell''\,;\, 1\, 1\,;\, 1\, \ell)\, \overset{\ell''}{\underset{m''}{Y}}(\theta,\phi)\, \frac{1}{r^{2}}\, f^{S}_{J\ell M}(r) \Big\}$$

$$\ldots \quad (\text{III.5.9})$$

we also have,

$$(\underline{R}\cdot\frac{\partial}{\partial \underline{r}})(\underline{R}\cdot\frac{\partial}{\partial \underline{r}}) \Big[\overset{\ell}{\underset{m}{Y}}(\theta,\phi)\, \frac{1}{r}\, f^{S}_{J\ell N}(r) \Big] = \frac{4\pi}{3}\, R^{2} \sum_{\ell'',L_1} C_{\ell 1}(\ell'')$$

$$\times\, C_{\ell'' 1}(L_1) \Big\{ \frac{d^{2}}{dr^{2}} \Big[\frac{1}{r}\, f^{S}_{J\ell M}(r) \Big] + \Big[6\, \ell''(\ell''+1)(2\ell''+1) \Big]^{\frac{1}{2}}$$

$$\times\, W(\ell'' L_1\,;\, 1\, 1\,;\, 1\, \ell'')\, \frac{1}{r}\frac{d}{dr} \Big[\frac{1}{r}\, f^{S}_{J\ell M}(r) \Big] + \Big[6\ell(\ell+1)(2\ell+1) \Big]^{\frac{1}{2}}$$

$$\times\, W(\ell\, \ell''\,;\, 1\, 1\,;\, 1\, \ell)\, \frac{d}{dr} \Big[\frac{1}{r^{2}}\, f^{S}_{J\ell M}(r) \Big] + 6 \Big[\ell(\ell+1)(2\ell+1)$$

$$\times\, (\ell''+1)(2\ell''+1)\, \ell'' \Big]^{\frac{1}{2}} W(\ell\, \ell''\,;\, 1\, 1\,;\, 1\, \ell)\;\; W(\ell'' L_1\,;\, 1\, 1\,;\, 1\, \ell'')$$

$$\times\, \frac{1}{r^{3}}\, f^{S}_{J\ell M}(r) \Big\} \sum_{\nu,\mu,q,m''} C_{L_1 1}(\ell'' m''\,;\, \tau\, \mu)\, \overset{1}{\underset{q}{Y}}(\theta_R,\phi_R)\, \overset{1}{\underset{\mu}{Y}}(\theta_R,\phi_R)$$

$$\times \; \overset{1}{\underset{\nu}{Y}}(\theta,\phi) \qquad \ldots \quad (III.5.10)$$

Using the above results, we finally obtain for $\overset{Q\,(II)}{U_{\underline{L}_{12}}}(r)$

$$\overset{Q\,(II)}{U_{\underline{L}_{12}}}(r) = \sum_{\ell,S} \overset{Q\,(II)}{B_{\underline{L}_{12}}}(r) \Big[\psi_{ijk}(\ell^2+\ell)\, f^S_{J\ell M}(r) - (\tfrac{3}{2}\phi_{ijk} + \delta_{ijk}$$

$$\times (1 - \tfrac{3}{4}\gamma_{ijk}) + 4\,\alpha_j\,\eta_{ijk}\, r^2)\, f^S_{J\ell M}(r) + (\tfrac{3}{2}(1 + \gamma_{ijk} - \tfrac{3}{4}\gamma^2_{ijk})r$$

$$- \frac{3\alpha_i}{\lambda_{ijk}} r)\frac{d}{dr} f^S_{J\ell M}(r) - \frac{9}{16\,\lambda_{ijk}}\frac{d^2}{dr^2} f^S_{J\ell M}(r) \Big] \ldots \quad (III.5.11)$$

where

$$\overset{Q\,(II)}{B_{\underline{L}_{12}}}(r) = \sum_{i,j,k=1}^{2} A_i\, A_j\, \overset{Q\,(II)}{U_k}\, (\pi/\lambda_{ijk})^{3/2}\, \frac{4\,M}{3\hbar^2}$$

$$\times \operatorname{Exp}\Big[- \overset{Q\,(II)}{\mu_k} (1 - \frac{\overset{Q}{u_k}(II)}{4\,\lambda_{ijk}})\, r^2 \Big] \quad (II=1,2) \qquad \ldots \quad (III.5.12)$$

Again, the integrand involving the operator $\underline{M}_{12}$ is given by

$$\overset{Q\,(1)}{U_{\underline{M}_{12}}}(r) = - \frac{4Mr}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \sum_{\ell} \sum_{m',m} C_{\ell\,3/2}(J\;M;m'\;M-m')$$

$$\times\, C_{\ell 3/2}(J\;M;m\;M-m) \int_0^\infty dR\; R^2\, \operatorname{Exp}(-\alpha_i R^2)\, \overset{Q\,(1)}{V}(\underline{r}_{12}) \int d\Omega_R\; (\theta_R,\phi_R)$$

$$\times \int d\Omega(\theta,\phi)\, \overset{*\ell'}{\underset{m'}{Y}}(\theta,\phi) \langle \overset{3/2}{\underset{M-m'}{X}}(1,\overline{23}) |\, \underline{M}_{12}(\underline{r}^2_{12})\, | \overset{3/2}{\underset{M-m}{X}}(1,\overline{23}) \rangle$$

$$\times \operatorname{Exp}(-\alpha_j R^2)\, \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\, \frac{1}{r}\, \overset{3/2}{\underset{J\ell M}{f}}(r) \qquad \ldots \quad (III.5.13)$$

Operating by $\underline{M}_{12}$ on the function $\operatorname{Exp}(-\alpha_j R^2)\, \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\, \frac{1}{r}$ $\overset{3/2}{\underset{J\ell M}{f}}(r)$ we obtain:

$$\underline{M}_{12}(\underline{r}_{12})\ \mathrm{Exp}(-\alpha_j R^2)\ \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\ \frac{1}{r}\ f^{3/2}_{J\ell M}(r) = \mathrm{Exp}(-\alpha_j R^2)$$

$$\times \Big\{ \Big[\frac{9}{4}(\underline{\sigma}_1\cdot \underline{L})(\underline{\sigma}_2\cdot \underline{L}) + \frac{9}{8}(\underline{\sigma}_1\cdot \underline{L})\ (i\ \underline{\sigma}_2\cdot \underline{R}\wedge\frac{\partial}{\partial \underline{r}}) + \frac{9}{8}(i\ \underline{\sigma}_1\cdot\underline{R}\wedge\frac{\partial}{\partial \underline{r}})$$

$$\times (\underline{\sigma}_2\cdot \underline{L}) - \frac{9}{16}(i\ \underline{\sigma}_1\cdot \underline{R}\wedge\frac{\partial}{\partial \underline{r}})(i\ \underline{\sigma}_2\cdot \underline{R}\wedge\frac{\partial}{\partial \underline{r}}) - 3\alpha_j(i\ \underline{\sigma}_2\cdot \underline{r}\wedge \underline{R})$$

$$\times (\underline{\sigma}_1\cdot \underline{L}) + \frac{3}{2}\alpha_j(\underline{\sigma}_2\cdot \underline{r}\wedge \underline{R})(\underline{\sigma}_1\cdot \underline{R}\wedge\frac{\partial}{\partial \underline{r}}) - \frac{3}{4}(\underline{\sigma}_1\cdot \underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial \underline{r}})$$

$$+ \frac{3}{4}(\underline{\sigma}_2\cdot \underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial \underline{r}}) + \frac{3}{8}(\underline{\sigma}_1\cdot \underline{\sigma}_2)(\underline{R}\cdot\frac{\partial}{\partial \underline{r}}) - \frac{3}{8}(\underline{\sigma}_1\cdot\frac{\partial}{\partial \underline{r}})(\underline{\sigma}_2\cdot \underline{R})$$

$$+ \frac{2}{3}\alpha_j \Big[W_{12}(r^2) - W_{12}(\underline{r},\underline{R}) \Big] + \frac{3}{2}\alpha_j(\underline{\sigma}_1\cdot \underline{r}\wedge \underline{R})(\underline{\sigma}_2\cdot \underline{R}\wedge\frac{\partial}{\partial \underline{r}})$$

$$+ \frac{2}{3}\alpha_j\ (\underline{r}\cdot \underline{R} - 2r^2)\ (\underline{\sigma}_1\cdot \underline{\sigma}_2) - 4\ {}_j^{\,2}\ (\underline{\sigma}_1\cdot \underline{r}\wedge\underline{R})(\underline{\sigma}_1\cdot \underline{r}\wedge \underline{R}) \Big]\Big\}$$

$$\times \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\ \frac{1}{r}\ f^{3/2}_{J\ell M}(r) \qquad \ldots \quad \text{(III.5.14)}$$

All terms in (III.5.14) are then worked out separately using the results given in (III.5.7) to (III.5.10). Thus equation (III.5.13) is finally given by the following expression:

$${}^{Q}U^{(1)}_{\underline{M}_{12}}(r) = \sum_{\ell,L} \Big[{}^{Q}B^{(1)}_{\underline{M}_{12}}(r)\ H_1(\ell,L)\ \frac{d^2}{dr^2}\ f^{3/2}_{J\ell M}(r) + {}^{Q}B^{(2)}_{\underline{M}_{12}}(r)$$

$$\times \frac{d}{dr}\ f^{3/2}_{J\ell M}(r) + \ell(\ell+1)\ {}^{Q}B^{(3)}_{\underline{M}_{12}}(r)\ f^{3/2}_{J\ell M}(r) + {}^{Q}B^{(4)}_{\underline{M}_{12}}(r)\ f^{3/2}_{J\ell M}(r) \Big]$$

$$\times\ \delta(\ell', \ell) \qquad \ldots \quad \text{(III.5.15)}$$

where

$${}^{Q}B^{(1)}_{\underline{M}_{12}}(r) = \frac{15M}{\hbar^2}\ ({}^{Q}\mu^{(1)}_k\ r/2)^L\ (1/\lambda_{ijk})^{L/2}\ \frac{\Gamma((L+5)/2)}{\Gamma(L+3/2)} \sum_{i,j,k=1}^{2} A_i A_j$$

$$ {}^{Q}U_K^{(1)} (1/\lambda_{ijk})(\pi/\lambda_{ijk})^{3/2} \; \mathrm{Exp}(-{}^{Q}\mu_k^{(1)} (1-{}^{Q}\mu_k^{(1)}/4\lambda_{ijk})r^2) \quad \ldots \quad (III.5.16) $$

$$ {}^{Q}B^{(2)}_{\underline{M}_{12}}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \, {}^{Q}U_k^{(1)} (1/\lambda_{ijk})(\pi/\lambda_{ijk})^{3/2} $$

$$ \times \mathrm{Exp}(-{}^{Q}\mu_k^{(1)}(1-{}^{Q}\mu_k^{(1)}/4\lambda_{ijk})r^2) \Big\{ -\frac{5r^2}{4} \, {}^{Q}\mu_k^{(1)} - \frac{5}{4} \, {}^{Q}\mu_k^{(1)} + \frac{1}{2} + r\lambda_{ijk} $$

$$ + 5({}^{Q}\mu_k^{(1)} r/2)^L (1/\lambda_{ijk})^{L/2} \frac{\Gamma(\frac{1}{2}(L+5))}{\Gamma(L+3/2)} \Big[16\alpha_j H_4(\ell,L) + 3 H_2(\ell,L) \Big] \Big\} $$

$$ \ldots \quad (III.5.17) $$

$$ {}^{Q}B^{(3)}_{\underline{M}_{12}}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \, {}^{Q}U_k^{(1)} (\pi/\lambda_{ijk})^{3/2} (2-5r\,{}^{Q}\mu_k^{(1)}/4\lambda_{ijk}) $$

$$ \times \mathrm{Exp}(-{}^{Q}\mu_k^{(1)} (1-{}^{Q}\mu_k^{(1)}/4\lambda_{ijk})r^2) \quad \ldots \quad (III.2.18) $$

and

$$ {}^{Q}B^{(4)}_{\underline{M}_{12}}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \, {}^{Q}U_k^{(1)} (\pi/\lambda_{ijk})^{3/2} \Big\{ 5({}^{Q}\mu_k^{(1)} r/2)^L (1/\lambda_{ijk})^{L/2} $$

$$ \times \frac{\Gamma(\frac{1}{2}(L+5))}{\Gamma(L+3/2)} \Big[16(\alpha_j/\lambda_{ijk}) H_5(\ell,\ell) + 3 H_3(\ell,L) \Big] + 1 - (5\,{}^{Q}\mu_k^{(1)}/4\lambda_{ijk}) $$

$$ - (1/2r\lambda_{ijk}) + (r\alpha_j/2\lambda_{ijk}) + (4\alpha_j/3) \Big[2r^2 + (1/{}^{Q}\mu_k^{(1)}) $$

$$ - ({}^{Q}\mu_k^{(1)} r^2/4\lambda_{ijk}) \Big] A(\ell' 3/2 \,;\, \ell 3/2) \Big\} \quad \ldots \quad (III.5.19) $$

and where

$$ H_1(\ell,L) = \sum_{L_1,L_2} (-1)^L \hat{L}_1 \hat{L} \hat{L}_2^{-1} C_{\ell 1}(L_1) \, C_{\ell L}(L_2) \, C_{L_1 1}(L_2) \, C_{11}(L) $$

$$ \times W(\ell 1 \,;\, L_2 1 \,,\, L_1 L) \, W(1 1 \,;\, 1 1 \,;\, 1 L) \quad \ldots \quad (III.5.20) $$

$$ H_2(\ell,L) = \frac{1}{2} \sum_{L_1,L_2} \hat{L}_1 \hat{L}_2^{-1} \hat{L} \Big[\ell(\ell-1) - L_2(L_2+1) \Big] C_{\ell 1}(L_1) $$

$$\times\, C_{\ell L}(L_2)\, C_{L_1 1}(L_2)\, C_{11}(L)\, W(\ell\, 1\, ;\, L_2 1\, ;\, L_1\, L)\, W(1\,1\, ;\, 1\,1\, ;\, 1\, L)$$

... (III.5.21)

$$H_3(\ell,L) = \frac{1}{2}\sum_{L_1,L_2} (-1)^L\, \hat{L}_1\, \hat{L}_2^{-1}\, \hat{L}\Big\{L_1(L_1+1)\Big[L_2(L_2+1)+\ell(\ell+1)$$

$$- L_1(L_1+1)\Big] - \ell(\ell+1)\Big[2 + L_2(L_2+1)\Big]\Big\}\, C_{\ell 1}(L_1)\, C_{\ell L}(L_2)$$

$$\times\, C_{L_1 1}(L_2)\, C_{11}(L)\, W(\ell\, 1\, ;\, L_2 1\, ;\, L_1\, L)\, W(1\,1\, ;\, 1\,1\, ;\, 1\, L)$$

... (III.5.22)

$$H_4(\ell,L) = \sum_{L_1,L_2} (-1)^L\, \hat{L}_2\, \hat{L}\, C_{\ell 1}(L_1)\, C_{L_2 L}(L_1)\, C_{\ell 1}(L_2)\, C_{11}(L)$$

$$\times\, W(L_1 1\, ;\, L_2 1\, ;\, \ell\, 1)\, W(1\,1\, ;\, 1\,1\, ;\, 1\, L) \qquad \text{... (III.5.23)}$$

and

$$H_5(\ell,L) = \frac{1}{2}\sum_{L_1,L_2} (-1)^L\, \hat{L}_2\, \hat{L}\Big[\ell(\ell+1) - L_1(L_1+1)\Big]\, C_{\ell 1}(L_1)$$

$$\times\, C_{\ell_2 L}(L_1)\, C_{\ell 1}(L_2)\, C_{11}(L)\, W(L_1 1\, ;\, L_2 1\, ;\, \ell\, 1)\, W(1\,1\, ;\, 1\,1\, ;\, 1\, L)$$

... (III.5.24)

From equations (III.5.11) and (III.5.15), the direct term of the quadratic spin-orbit interaction is given in the doublet state by:

$$Q_{D_{J\ell' M(s-s)}}(r) = -\frac{4}{3}\, {}^{Q}U^{(1)}_{\underline{L}_{12}}(r) + 3\, {}^{Q}U^{(2)}_{\underline{L}_{12}}(r) \qquad \text{... (III.5.25)}$$

and in the quartet state by:

$$Q_{D_{J\ell' M(s-s)}}(r) = {}^{Q}U^{(1)}_{\underline{L}_{12}}(r) + {}^{Q}U^{(1)}_{\underline{M}_{12}}(r) \qquad \text{... (III.5.26)}$$

CHAPTER IV

THE ENERGY TERMS (s-s) INTERACTION

(IV.1.) THE W-KERNEL

The w-kernel is given in the doublet and quartet states by the following expression:

$$\underset{J\ell' M(s-s)}{W^{S'}}(r) = (4/3)^4 \frac{Mr}{\hbar^2} (E_p - E_d) \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')$$

$$\times\ C_{\ell S}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ \phi_S(u)\ \phi_S(V)\ \overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi)\ \langle \underset{M-m'}{X^{S'}}(1,\overline{23})\rangle^*$$

$$\times |\underset{M-m}{X^S}(2,\overline{13})\rangle\ \overset{\ell}{\underset{m}{Y}}(\theta',\phi')\ \frac{1}{r'}\ f^S_{J\ell M}(r') \qquad \ldots \quad (IV.1.1)$$

Summing over spins and expanding the functions $\phi_S(u)$ $\phi_S(V)$ in a series of spherical harmonics

$$\phi_S(u)\ \phi_S(V) = \sum_{n,p} p_n(r,r')\ \overset{n*}{\underset{p}{Y}}(\theta',\phi')\ \overset{n}{\underset{p}{Y}}(\theta,\phi) \qquad \ldots \quad (IV.1.2)$$

where

$$p_n(r,r') = 2\pi \int_{-1}^{+1} d\ \ p_n(\eta)\ \phi_S(u)\ \phi_S(V) \qquad \ldots \quad (IV.1.3)$$

hence (IV.1.1) becomes

$$\underset{J\ell' M(s-s)}{W^{S'}}(r) = (4/3)^4 \frac{Mr}{\hbar^2} (E_p - E_d) \sum_{\ell,S,n} \sum_{m',p} C_{\ell' S'}(J\ M;m'\ M-m')$$

$$\times\ C_{\ell S}(J\ M;m'\ M-m')\ \delta(S',S) \int_0^\infty r'\ dr'\ p_n(r,r')\ f^S_{J\ell M}(r')$$

$$\times \int d\Omega'(\theta',\phi') \; \overset{n_*}{\underset{p}{Y}}(\theta',\phi') \; \overset{\ell}{\underset{m}{Y}}(\theta',\phi') \int d\Omega(\theta,\phi) \; \overset{\ell'_*}{\underset{m'}{Y}}(\theta,\phi) \; \overset{n}{\underset{p}{Y}}(\theta,\phi) \qquad \ldots \text{(IV.1.4)}$$

Which after performing the angular integration and sum over all quantum numbers, with the exception of ℓ and S, finally becomes:

$$W^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell,S} \int_0^\infty dr' \; {}^{w}e_1(r.r') \; g(S) \; \delta(S',S) \; I_{\ell+\frac{1}{2}}(b_{ijk} rr')$$

$$\times \; \delta(\ell',\ell) \; f^S_{J\ell M}(r') \qquad \ldots \text{(IV.1.5)}$$

where

$${}^{w}e_1(r,r') = \frac{2\pi Mr}{\hbar^2} (E_p - E_d) \, (4/3)^4 \sum_{i,j=1}^{2} A_i A_j \, (2\pi/b_{ij} rr')^{\frac{1}{2}}$$

$$\times \; \mathrm{Exp}(- e_{ij} r^2 - f_{ij} r'^2) \qquad \ldots \text{(IV.1.6)}$$

(IV.2.) THE KINETIC ENERGY TERM

The kinetic energy term denoted by $T^{S'}_{J\ell' M(s-s)}(r)$ is given by:

$$T^{S'}_{J\ell' M(s-s)}(r) = {}^{(1)}T^{S'}_{J\ell' M(s-s)}(r) + {}^{(2)}T^{S'}_{J\ell' M(s-s)}(r) \qquad \ldots \text{(IV.2.1)}$$

where

$${}^{(1)}T^{S'}_{J\ell' M(s-s)}(r) = (4/3)^3 \, r \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M; m'\ M-m')$$

$$\times\, C_{\ell S}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ Y^{\ell'*}_{m'}(\theta,\phi)\ |X^{S'}_{M-m'}(1,\overline{23})\rangle \Big[\frac{1}{2}\nabla^2_{r'}$$

$$\times\, \phi_s(u)\ \phi_s(V) + \frac{1}{2}\nabla^2_r\ \phi_s(u)\ \phi_s(V) \Big]\ |X^S_{M-m}(2,\overline{13})\rangle\, Y^{\ell}_{m}(\theta',\phi')$$

$$\times\, \frac{1}{r'}\ f^S_{J\ell M}(r') \qquad \ldots \quad (IV.2.2)$$

Which after summing over spins becomes:

$$^{(1)}T^{S'}_{J\ell' M(s-s)}(r) = (4/3)^3\ r \sum_{\ell,S}\ \sum_{m',m}\ C_{\ell' S'}(J\ M;m'\ M-m')$$

$$\times\, C_{\ell S}(J\ M;m\ M-m)\ \delta(S',S)\,\delta(m',m)\ g(S) \int d\underline{r}'\ Y^{\ell'*}_{m'}(\theta,\phi)\ \frac{1}{2}\Big[\nabla^2_{r'}\ \phi_s(u)$$

$$\times\, \phi_S(V) + \nabla^2_r\ \phi_s(u)\ \phi_s(V)\Big]\ Y^{\ell}_{m}(\theta',\phi')\ \frac{1}{r'}\ f^S_{J\ell M}(r')$$

$$\ldots \quad (IV.2.3)$$

Operating on the functions $\phi_s(u)\ \phi_s(V)$ first by $\nabla^2_{r'}$ and then by ∇^2_r yield the following results:

$$\frac{1}{2}\nabla^2_{r'}\ \phi_s(u)\ \phi_s(V) = \phi_s(u)\ \phi_s(V)\Big[-\frac{3}{2}\ {}_1a_{ij} + \frac{1}{2}\ {}_1b^2_{ij}\ r^2$$

$$+ \frac{1}{2}\ {}_1a^2_{ij}\ r'^2 + {}_1a_{ij}\ {}_1b_{ij}\ \underline{r}\cdot\underline{r}'\Big] \qquad \ldots \quad (IV.2.4)$$

and

$$\frac{1}{2}\nabla^2_r\ \phi_s(u)\ \phi_s(V) = \phi_s(u)\ \phi_s(V)\Big[-\frac{3}{2}\ {}_2a_{ij} + \frac{1}{2}\ {}_2a^2_{ij}$$

$$+ {}_2a_{ij}\ {}_1b_{ij}\ \underline{r}\cdot\underline{r}'\Big] \qquad \ldots \quad (IV.2.5)$$

Combining the above two results we get:

$$\frac{1}{2}\left[\nabla^2_{r'}\ \phi_s(u)\ \phi_s(V) + \nabla^2_r\ \phi_s(u)\ \phi_s(V)\right] = \phi_s(u)\ \phi_s(V)$$

$$\times\left[-(15/4)\,{}_1b_{ij} + \frac{1}{2}\left({}_1b^2_{ij} + {}_2a^2_{ij}\right)r^2 + \frac{1}{2}\left({}_1a^2_{ij} + {}_1b^2_{ij}\right)r'^2\right.$$

$$\left. + \left({}_1a_{ij}\ {}_1b_{ij} + {}_2a_{ij}\ {}_1b_{ij}\right)\underline{r}\cdot\underline{r}'\right] \qquad \ldots \quad (IV.2.6)$$

Substituting (IV.2.6) into (IV.2.3) and summing over m.

$$\overset{(1)}{}T^{S'}_{J\ell' M(s-s)}(r) = (4/3)^3\, r \sum_{\ell,S}\ \sum_{m'}\ C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m'\ M-m')$$

$$\times\ g(S)\ \delta(S',S) \int_0^\infty dr'\ r' \int d\Omega'(\theta',\phi')\ d\Omega(\theta,\phi)\ Y^{\ell'*}_{m'}(\theta,\phi)\ \phi_s(u)$$

$$\times\left[-(15/4)\,{}_1b_{ij} + \frac{1}{2}\left({}_1b^2_{ij} + {}_2a^2_{ij}\right)r^2 + \frac{1}{2}\left({}_1a^2_{ij} + {}_1b^2_{ij}\right)r'^2\right.$$

$$\left. + \left({}_1a_{ij}\ {}_1b_{ij} + {}_2a_{ij}\ {}_2b_{ij}\right)\underline{r}\cdot\underline{r}'\right]\phi_s(V)\ Y^{\ell}_{m'}(\theta',\phi')\quad f^S_{J\ell M}(r')$$

$$\ldots \quad (IV.2.7)$$

Also, we have from (IV.2.1), the expression for $\overset{(2)}{}T^{S'}_{J\ell' M(s-s)}(r)$ which is given by:

$$\overset{(2)}{}T^{S'}_{J\ell' M(s-s)}(r) = -(4/3)^4\, r \sum_{\ell,S}\ \sum_{m',m}\ C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m)$$

$$\times \int d\underline{r}'\ d\Omega(\theta,\phi)\ \ Y^{\ell'*}_{m'}(\theta,\phi)\left[\frac{1}{2}\,\phi_s(V)\,\nabla^2_u\ \phi_s(u) + \frac{1}{2}\,\phi_s(u)\ \nabla^2_v\ \phi_s(V)\right]$$

$$\times\left\langle X^{S'}_{M-m'}(1,\overline{23})\middle|X^{S}_{M-m}(2,\overline{13})\right\rangle Y^{\ell}_{m}(\theta',\phi')\ \frac{1}{r'}\ f^S_{J\ell M}(r') \qquad \ldots \quad (IV.2.8)$$

After the spin summation is carried out, (IV.2.8) becomes:

$$ {}^{(2)}_{J\ell' M(s-s)}T^{S'}(r) = -(4/3)^4 \, r \sum_{\ell,S} \sum_{m'} C_{\ell' S'}(J\,M;m'\,M-m')\, C_{\ell S}(J\,M;m'M-m') $$

$$ \times\, g(S)\,\delta(S',S) \int d\underline{r}'\, d\Omega(\theta,\phi)\, Y^{\ell'*}_{m'}(\theta,\phi) \Big[\tfrac{1}{2}\,\phi_s(V)\,\nabla_u^2\,\phi_s(u) $$

$$ + \tfrac{1}{2}\,\phi_s(u)\,\nabla_v^2\,\phi_s(V) \Big]\, Y^{\ell}_{m'}(\theta',\phi')\,\frac{1}{r'}\, f^S_{J\ell M}(r') \qquad \ldots \quad (IV.2.9) $$

Again, operating on the functions $\phi_s(u)$ and $\phi_s(V)$ by the laplacian operators ∇_u^2 and ∇_v^2 . Thus,

$$ \nabla_u^2\,\phi_s(u) = \phi_s(u)\,(4\alpha_i^2\,u^2 - 6\alpha_i) \qquad \ldots \quad (IV.2.10) $$

and

$$ \nabla_v^2\,\phi_s(V) = \phi_s(V)\,(4\alpha_j^2\,V^2 - 6\alpha_j) \qquad \ldots \quad (IV.2.11) $$

Combining (IV.2.10) and (IV.2.11) we get

$$ \tfrac{1}{2} \Big[\phi_s(V)\nabla_u^2\,\phi_s(u) + \phi_s(u)\,\nabla_v^2\,\phi_s(V) \Big] = \phi_s(u)\,\phi_s(V) \Big[-\tfrac{27}{16} $$

$$ \times\, {}_1b_{ij} + {}_1d_{ij}\,r^2 + {}_2a_{ij}\,r'^2 + {}_3d_{ij}\,\underline{r}\cdot\underline{r}' \Big] \qquad \ldots \quad (IV.2.12) $$

Using (IV.2.12), in (IV.2.9), thus

$$ {}^{(2)}_{J\ell' M(s-s)}T^{S'}(r) = (4/3)^3 \sum_{\ell,S} \sum_{m'} C_{\ell' S'}(J\,M;m'\,M-m')\, C_{\ell S}(J\,M;m'\,M-m') $$

$$ \times\, g(S)\,\delta(S',S) \int_0^\infty r\,r'\,dr' \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi)\, Y^{\ell'*}_{m'}(\theta,\phi)\,\phi_s(u) $$

$$\times \left[(9/4)_1 b_{ij} - (4/3)_1 d_{ij}\, r^2 - (4/3)_2 d\, r'^2 - (4/3)_3 d_{ij}\, \underline{r}\cdot\underline{r}' \right]$$

$$\times\, \phi_s(V)\, Y^{\ell}_{m'}(\theta',\phi')\quad f^{S}_{J\ell M}(r') \qquad \ldots \quad (IV.2.13)$$

From (IV.2.7) and (IV.2.13), the total energy term $T^{S'}_{J\ell' M(s-s)}(r)$ is now given by:

$$T^{S'}_{J\ell' M(s-s)}(r) = (4/3)^3 \sum_{\ell,S} \sum_{m'} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m'\ M-m')$$

$$\times\, g(S)\,\delta(S',S) \int dr'\ rr'\ f^{S}_{J\ell M}(r') \int d\Omega'(\theta',\phi') \int d\Omega\,(\theta,\phi)\ Y^{\ell'*}_{m'}(\theta,\phi)$$

$$\times\, \phi_s(u) \left[-(3/2)_1 b_{ij} + W_{ij}\, r^2 + \Psi_{ij} r'^2 + \phi_{ij}\, \underline{r}\cdot\underline{r}' \right] \phi_s(V)\, Y^{\ell}_{m'}(\theta',\phi')$$

$$\ldots \quad (IV.2.14)$$

putting

$$\mathcal{T}(\underline{r},\underline{r}') = (4/3)^3\ \phi_s(u)\ \phi_s(V) \left[-(3/2)_1 b_{ij} + W_{ij} r^2 + \Psi_{ij}\, r'^2 \right.$$

$$\left. + \phi_{ij}\, \underline{r}\cdot\underline{r}' \right] \qquad \ldots \quad (IV.2.15)$$

and this can be expanded

$$\mathcal{T}(\underline{r},\underline{r}') = \frac{1}{rr'} \sum_{\mu,\nu} \mathcal{T}_{\nu}(r,r')\ Y^{\nu *}_{\mu}(\theta',\phi')\ Y^{\nu}_{\mu}(\theta,\phi) \qquad \ldots \quad (IV.2.16)$$

where

$$\mathcal{T}_{\nu}(r,r') = 2\pi \int_{-1}^{+1} d\eta\ p_{\nu}(\eta)\, \mathcal{T}(\underline{r},\underline{r}') \qquad \ldots \quad (IV.2.17)$$

Using (IV.2.16), (IV.2.14) can be written as:

$$T^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell,S,\nu} \sum_{m',\mu} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m'\ M-m')\ g(S)$$

$$\times\ \delta(S',S)\int_0^{\infty} dr'\,\mathcal{T}(r,r')\, f^{S}_{J\ell M}(r')\int d\Omega'(\theta',\phi')\, Y^{\nu *}_{\mu}(\theta',\phi')\, Y^{\ell}_{m'}(\theta',\phi')$$

$$\times \int d\Omega(\theta,\phi)\, Y^{\ell' *}_{m'}(\theta,\phi)\, Y^{\nu}_{\mu}(\theta,\phi) \qquad \ldots \quad (IV.2.18)$$

performing the angular integration part and then summing over ν, m', and μ, equation (IV.2.18) is further reduces to the following final form:

$$T^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell,S} \int_0^{\infty} dr'\; f^{S}_{J\ell M}(r')\; g(S)\,\delta(S',S)\Big[\, {}^{T}e_1^{(1)}(r,r')$$

$$\times\, I_{\ell+\frac{1}{2}}({}_1b'_{ij}\, rr') + {}^{T}e_1^{(2)}(r,r')\, I'_{\ell+\frac{1}{2}}({}_1b'_{ij}\, rr')\Big]\,\delta(\ell',\ell)$$

$$\ldots \quad (IV.2.19)$$

where

$${}^{T}e_1^{(1)}(r,r') = 2\pi rr' \sum_{i,j=1}^{2} A_i A_j\, \mathrm{Exp}(-e_{ij}\, r^2 - f_{ij}\, r'^2)$$

$$\times\, (2\pi/\, {}_1b_{ij}\, rr')^{\frac{1}{2}}\Big[-(3/2)\,{}_1b_{ij} - W_{ij}\, r^2 + \psi_{ij}\, r'^2 - \phi_{ij}\,/2\; {}_1b_{ij}\Big]$$

$$\ldots \quad (IV.2.20)$$

and

$${}^{T}e_1^{(2)}(r,r') = 2\pi rr' \sum_{i,j=1}^{2} A_i A_j\, \phi_{ij}\, (2\pi/\, {}_1b_{ij}\, rr')^{\frac{1}{2}}$$

$$\times\, \mathrm{Exp}(-\, e_{ij} r^2 - f_{ij}\, r'^2) \qquad \ldots \quad (IV.2.21)$$

CHAPTER V

THE EXCHANGE (s-s) INTERACTION TERMS

The exchange interactions of the central, tensor, spin-orbit and quadratic spin-orbit forces in the resulting integro-differential equations (I.1.4) are given below:

(V.1.) THE CENTRAL TERM

The central force term denoted by $^{c}E^{S'}_{J\ell' M(s-s)}(r)$ is given below by:

$$^{c}E^{S'}_{J\ell' M(s-s)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')$$

$$\times C_{\ell S}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ \phi_s(u)\ Y^{\ell'*}_{m'}(\theta,\phi)\ \langle X^{S'}_{M-m'}(1,\overline{23})| \sum_{\nu=1}^{4}$$

$$\times \left[\frac{1}{4}(2W - a)_{\nu}\ {}^{\nu}V_c(t)\ |X^{S}_{M-m}(2,\overline{13})\rangle + \frac{1}{4}(b - 2m)_{\nu}\ {}^{\nu}V_c(t)\,|X^{S}_{M-m}(1,\overline{23})\rangle \right]$$

$$\times Y^{\ell}_{m}(\theta',\phi')\ \phi_s(V)\ \frac{1}{r'}\ f^{S}_{J\ell M}(r') \quad \ldots \quad (V.1.1)$$

Summing over spins yields

$$^{c}E^{S'}_{J\ell' M(s-s)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{\ell,S} \sum_{m'} C_{\ell' S'}(J\ M;m'\ M-m')$$

$$\times C_{\ell S}(J\ M;m'\ M-m')\ \delta(S',S) \int d\underline{r}'\ d\Omega(\theta,\phi)\ Y^{\ell'*}_{m'}(\theta,\phi)\ \phi_s(u)\ {}^{c}V^{(II)}(t)$$

$$\times Y^{\ell}_{m'}(\theta',\phi')\ \phi_s(V)\ \frac{1}{r'}\ f^{S}_{J\ell M}(r') \qquad (II=3,4) \quad \ldots \quad (V.1.2)$$

where

$$ {}^{c}V(t) = \sum_{\nu=1}^{4} \frac{1}{4} \left[(b - 2m)_{\nu} + g(S)\ (2W - h)_{\nu} \right] {}^{\nu}V_{c}(t) $$

$$ = \sum_{k=1}^{2} {}^{c}U_{k}^{(II)}\ \mathrm{Exp}(- {}^{c}\mu_{k}^{(II)}\ t^{2}) \qquad \ldots \quad (V.1.3) $$

and $t = \frac{2}{3} (|\underline{r} - \underline{r}'|)$

Defining the function ${}^{c}Q^{(II)}(\underline{r},\underline{r}')$ by:

$$ {}^{c}Q^{(II)}(\underline{r},\underline{r}') = -(4/3)^{4} \frac{Mr}{\hbar^{2}} \phi_{s}(u)\ {}^{c}V^{(II)}(t)\ \phi_{s}(V) \qquad \ldots \quad (V.1.4) $$

which can be expanded

$$ {}^{c}Q^{(II)}(\underline{r},\underline{r}') = \sum_{\eta,\lambda} \frac{1}{rr'}\ {}^{c}p_{\lambda}^{(II)}(r,r')\ Y_{\eta}^{\lambda *}(\theta',\phi')\ Y_{\eta}^{\lambda}(\theta,\phi) \qquad \ldots \quad (V.1.5) $$

where

$$ {}^{c}p_{\lambda}^{(II)}(r,r') = 2\pi\ rr' \int_{-1}^{+1} dq\ p_{\lambda}(q)\ {}^{c}Q^{(II)}(\underline{r},\underline{r}')\ \left(q = \frac{\underline{r},\underline{r}'}{rr'}\right) \qquad \ldots \quad (V.1.6) $$

where $p_{\lambda}(q)$ is the Legendre polynomial.

Using (V.1.5) in (V.1.2) we get

$$ {}^{c}E^{S'}_{J\ell' M(s-s)}(r) = -(4/3)^{4} \frac{Mr}{\hbar^{2}} \sum_{\ell,S,} \sum_{m',m} C_{\ell' S'}(J\ M; m'\ M-m') $$

$$ C_{\ell S}(J\ M; m\ M-m) \int_{0}^{\infty} dr'\ {}^{c}p_{\lambda}^{(II)}(r,r')\ f^{S}_{J\ell M}(r')\ \delta(S',S)\ \delta(m',m) $$

$$x \int d\Omega(\theta,\phi)\, \overset{\ell'}{Y}{}^{*}_{m'}(\theta,\phi)\, \overset{\lambda}{Y}_{\eta}(\theta,\phi) \int d\Omega'(\theta',\phi')\, \overset{\lambda}{Y}{}^{*}_{\eta}(\theta',\phi')\, \overset{\ell}{Y}_{m}(\theta',\phi')$$

... (V.1.7)

Now, performing the angular integrations w.r. to $d\Omega(\theta,\phi)$ and $d\Omega'(\theta',\phi')$, and then summing over all quantum numbers, expression (V.1.7) for the exchange interaction of the central force, is finally given in the doublet and quartet states by:

$$c_{E\,J\ell'M(s-s)}^{S'}(\underline{r}) = \sum_{\ell,S} \int_{o}^{\infty} dr'\; c_{e_1}^{(II)}(r,r')\; I_{\ell+\frac{1}{2}}(C_{ijk}\, rr')\, \delta(S',S)$$

$$\times\ \delta(\ell',\ell)\ f^{S}_{J\ell M}(r') \qquad \ldots \quad (V.1.8)$$

where

$$c_{e_1}^{(II)}(r,r') = -(4/3)^3\, \frac{2\pi M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j\ \ c_{U_k}^{(II)} (2\pi / C_{ijk}\, rr')^{\frac{1}{2}}$$

$$x\ \mathrm{Exp}(-\, a_{ijk}\, r^2 - b_{ijk}\, r'^2) \qquad \ldots \quad (V.1.9)$$

and

$$a_{ijk} = \frac{4}{9}\,(\alpha_i + 4\alpha_j + \mu_k^{(II)}),$$

$$b_{ijk} = \frac{4}{9}\,(4\,\alpha_i + \alpha_j + \mu_k^{(II)}),$$

and

$$C_{ijk} = \frac{4}{9}\,(2\,\mu_k^{(II)} - 4\,\alpha_i - 4\alpha_j).$$

(V.2.) THE COULOMB TERM

The exchange term of the coulomb force $\overset{\text{coul}}{J\ell'} \overset{S'}{E}_{M(s-s)}(r)$ is given by:

$$\overset{\text{coul}}{J\ell'} \overset{S'}{E}_{M(s-s)}(r) = -(4/3)^4 \frac{3Mr}{2\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')$$

$$\times C_{\ell S}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ \phi_s(u)\ \overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi) \langle X^{S'}_{M-m'}(1,\overline{23})|$$

$$\times e^2/(|\underline{r}-\underline{r}'|)|X^{S}_{M-m}(2,\overline{13})\rangle \phi_s(V)\ \overset{\ell}{\underset{m}{Y}}(\theta',\phi')\ \frac{1}{r'}\ f^S_{J\ell M}(r') \qquad \ldots \quad (V.2.1)$$

Performing the spin summation, we get

$$\overset{\text{coul}}{J\ell'} \overset{S'}{E}_{M(s-s)}(r) = \sum_{\ell,S} \sum_{m'} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m'\ M-m')\ \delta(S',S)$$

$$\times \int_0^\infty dr'\ rr' \int d\Omega(\theta,\phi)\ d\Omega(\theta',\phi')\ \overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi)\ G(\underline{r},\underline{r}')\ \overset{\ell}{\underset{m'}{Y}}(\theta',\phi')$$

$$\times f^S_{J\ell M}(r') \qquad \ldots \quad (V.2.2)$$

where

$$G(\underline{r},\underline{r}') = -(4/3)^4 \frac{3Me^2}{2\hbar^2}\ g(S)\ \phi_s(u)\ 1/(|\underline{r}-\underline{r}'|)\ \phi_s(V) \qquad \ldots \quad (V.2.3)$$

The functuin $G(\underline{r},\underline{r}')$ can be expanded in series of spherical harmonics, Thus,

$$G(\underline{r},\underline{r}') = \sum_{n,p} \frac{1}{rr'}\ g(r,r')\ \overset{n*}{\underset{p}{Y}}(\theta',\phi')\ \overset{n}{\underset{p}{Y}}(\theta,\phi) \qquad \ldots \quad (V.2.4)$$

so that

$$g_n(r,r') = 2\pi rr' \int_{-1}^{+1} d\eta \, p_n(\eta) \, G(\underline{r},\underline{r}') \ldots \quad (V.2.5)$$

Using (V.2.4) in (V.2.2) and then summing over m', the coulomb exchange interaction is given in the doublet and quartet states by:

$$\overset{coul}{E}{}^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell,S} \int_0^\infty dr' \, (rr') \, \overset{coul}{e}_l(r,r') \, g(S) \, \delta(S',S)$$

$$\times \, \delta(\ell',\ell) \, f^S_{J\ell M}(r') \quad \ldots \quad (V.2.6)$$

where

$$\overset{coul}{e}_l(r,r') = -(4/3)^4 \frac{3\pi M e^2}{\hbar^2} \sum_{i,j=1}^{2} A_i A_j \, \mathrm{Exp}(-e_{ij}r^2 - f_{ij}r'^2)$$

$$\times \int_{-1}^{+1} d\eta \, (r^2 + r'^2 - 2rr'\eta)^{-\frac{1}{2}} \, p_\ell(\eta) \, \mathrm{Exp}(brr'\eta) \quad \ldots \quad (V.2.7)$$

(V.3.) THE TENSOR TERM

The exchange term of the tensor force denoted by

$t_E S'_{J\ell' M(s-s)}(r)$ is given below:

$$t_E S'_{J\ell' M(s-s)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{\ell, S} \sum_{m', m} C_{\ell' S'}(J\ M; m'\ M-m')$$

$$\times\ C_{\ell S}(J\ M; m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ \phi_s(u)\ \overset{\ell'}{Y}{}^{*}_{m'}(\theta,\phi) \langle X^{S'}_{M-m'}(1,\overline{23})|$$

$$\times \sum_{\nu=1}^{4} \frac{1}{4} (W - 2h + b - 2m)_\nu\ {}^{\nu}V_t(t)\ S_{12}(\underline{t}^2) |X^S_{M-m}(2,\overline{13})\rangle\ \phi_S(V)$$

$$\times\ \overset{\ell}{Y}_m(\theta',\phi')\ \frac{1}{r'}\ f^S_{J\ell M}(r') \qquad \ldots \quad (V.3.1)$$

The spin matrix elements can be evaluated by expressing them in terms of $Y^2_{m'-m}(\theta_t,\phi_t)$ spherical harmonic as follows:

$$\langle X^{S'}_{M-m'}(1,\overline{23})|\ S_{12}(\underline{t}^2)\ |X^S_{M-m}(2,\overline{13})\rangle = (4\pi/5)^{\frac{1}{2}}\ g(S',S)\ (-1)^{S+m}$$

$$\times\ C_{S' S}(2\ m'-m\ ; -m\ m')\ \overset{2}{Y}_{m'-m}(\theta_t,\phi_t) = (4\pi/5)^{\frac{1}{2}}\ g(S',S)\ (-1)^{S+M-m'}$$

$$\times\ C_{S' S}(2\ m'-m\ ;\ m'-M\ M-m)\ \frac{4}{9t^2} \Big[r^2\ \overset{2}{Y}_{m'-m}(\theta,\phi) + r'^2\ \overset{2}{Y}_{m'-m}(\theta',\phi')$$

$$-\ rr'\ (40\pi/3)^{\frac{1}{2}} \sum_{q,p} C_{11}(2\ m'-m\ ;\ qp)\ \overset{1}{Y}_q(\theta,\phi)\ \overset{1}{Y}_p(\theta',\phi') \Big]$$

$$\ldots \quad (V.3.2)$$

Using this result we then obtain from equation (V.3.1)

$$ {}^{t}E^{S'}_{J\ell' M(s-s)}(r) = -(4/3)^4 \frac{M}{\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M; m'\ M-m') $$

$$ \times C_{\ell S}(J\ M; m\ M-m)\ C_{S' S}(2\ m'-m\ ;\ m'-M,\ M-m)\ (-1)^{S+M-m'}\ g(S',S) $$

$$ \times (4\pi/5)^{\frac{1}{2}} \int_0^\infty dr'\ (rr') \int d\Omega'(\theta',\phi')\ \phi_s(u)\ Y^{\ell'*}_{m'}(\theta,\phi)\ {}^{t}V^{(4)}(t)\ \frac{4}{9t^2} $$

$$ \times \Big[r^2 Y^{2}_{m'-m}(\theta,\phi) + r'^2 Y^{2}_{m'-m}(\theta',\phi') - rr'(40\pi/3)^{\frac{1}{2}} \sum_{q,p} C_{11}(2m'-m;qp) $$

$$ \times Y^{1}_{q}(\theta,\phi)\ Y^{1}_{p}(\theta',\phi') \Big]\ \phi_s(V)\ Y^{\ell}_{m}(\theta',\phi')\ f^{S}_{J\ell M}(r') \qquad \ldots \quad (V.3.3) $$

Where ${}^{t}V^{(4)}(t)$ is the potential function given by

$$ {}^{t}V^{(4)}(t) = \sum_{\nu=1}^{4} \frac{1}{4}(w - 2h + b - 2m)_{\nu}\ {}^{\nu}V_t(t) = t^2 \sum_{k=1}^{2} {}^{t}U^{(4)}_{k} $$

$$ \times \operatorname{Exp}(-\ {}^{t}\mu^{(4)}_{k}\ t^2) \qquad \ldots \quad (V.3.4) $$

Expression (V.3.3) is further simplified as follows :

$$ {}^{t}E^{S'}_{J\ell' M(s-s)}(r) = \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M; m'\ M-m')\ C_{\ell S}(J\ M; m\ M-m) $$

$$ \times C_{S' S}(2\ m'-m;\ m'-M,\ M-m)\ (-1)^{S+M-m'}\ g(S',S)\ (4\pi/5)^{\frac{1}{2}} \int_0^\infty dr' $$

$$ \times f^{S}_{J\ell M}(r') \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi)\ Y^{\ell'*}_{m'}(\theta,\phi) \Big[\ {}^{t}U^{(1)}(\underline{r},\underline{r}')\ Y^{2}_{m'-m}(\theta,\phi) $$

$$ +\ {}^{t}U^{(2)}(\underline{r},\underline{r}')\ Y^{2}_{m'-m}(\theta',\phi') + (40\pi/3)^{\frac{1}{2}} \sum_{q,p} C_{11}(2,\ m'-m,\ qp)\ {}^{t}U^{(3)}(\underline{r},\underline{r}') $$

$$ \times Y^{1}_{q}(\theta,\phi)\ Y^{1}_{p}(\theta',\phi') \Big]\ Y^{\ell}_{m}(\theta',\phi') \qquad \ldots \quad (V.3.5) $$

where

$$\overset{t\,(I)}{U}(\underline{r},\underline{r}') = -(4/3)^4 \frac{M}{\hbar^2}\, \phi_s(u)\; \overset{t\,(4)}{V}(t)\, \phi_s(V)\, \frac{4}{9t^2} \left] \begin{array}{l} r^2 (I=1) \\ r'^2 (I=2) \\ -rr' (I=3) \end{array} \right. \qquad \ldots \quad (V.3.6)$$

The function $\overset{T\,(I)}{U}(\underline{r},\underline{r}')$ can also be expanded

$$\overset{t\,(I)}{U}(\underline{r},\underline{r}') = \sum_{L,\lambda} \overset{t\,(I)}{p}_L(r,r')\; \overset{L_*}{Y}_{\lambda}(\theta',\phi')\; \overset{L}{Y}_{\lambda}(\theta,\phi) \qquad \ldots \quad (V.3.7)$$

so that

$$\overset{t\,(I)}{p}_L(r,r') = 2\pi rr' \int_{-1}^{+1} d\eta\, p_L(\eta)\; \overset{t\,(I)}{U}(\underline{r},\underline{r}') \quad \left(\eta = \frac{\underline{r}\cdot\underline{r}'}{rr'}\right) \qquad \ldots \quad (V.3.8)$$

Using (V.3.7) in (V.3.5) and performing the angular integration, the sum over all quantum numbers (m',m and λ) may then be carried out, so that the exchange term of the tensor force is finally given in the quartet state by:

$$\overset{t\,S'}{E}_{J\ell' M(s-s)}(r) = \sum_{\ell} \int_0^{\infty} dr'\,(rr')\, f^S_{J\ell M}(r')\, A(\ell' 3/2\;;\;\ell 3/2)$$

$$\times \Big[\overset{t\,(1)}{e}_1(r,r')\; I_{\ell+\frac{1}{2}}(C_{ijk}\, rr) + \overset{t\,(2)}{e}_1(r,r')\; I_{\ell'+\frac{1}{2}}(C_{ijk} rr')$$

$$+ \overset{t\,(3)}{e}_1(r,r') \sum_L FF(\ell'\ell,L)\; I_{L+\frac{1}{2}}(C_{ijk}\, rr') \Big] \qquad \ldots \quad (V.3.9)$$

where

$$\overset{t\,(I)}{e}_1(r,r') = -(4/3)^4 \frac{8\pi M}{9\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j\; \overset{t\,(4)}{U}_k\; (2\pi/C_{ijk} rr')^{\frac{1}{2}}$$

$$\times \, \mathrm{Exp}(-a_{ijk}\, r^2 - b_{ijk}\, r'^2) \left] \begin{array}{l} r^2 \; (I=1) \\ r'^2 (I=2) \\ -rr' (I=3) \end{array} \right. \qquad \ldots \quad (V.3.10)$$

and

$$FF(\ell'\ell, L) = (-1)^L \, (150)^{\frac{1}{2}} \left[C_{1\ell}(L) \; C_{1\ell'}(L) \, / \, C_{\ell'\ell}(2) \right]$$

$$\times \, W(11 \; ; \; \ell'\ell \; ; \; 2 \; L) \qquad \ldots \quad (V.3.11)$$

The sum over L in equation (V.3.9) is limited by the Clebsch-Gordon Coefficients,so that $C_{1\ell}(L)$ and $C_{1\ell'}(L)$ satisfy the triangular inequality.

(V.4.) THE SPIN-ORBIT TERM

The term for the spin-orbit exchange interaction is given by:

$$\overset{s.o}{E}{}^{S'}_{J\ell' M(s-s)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{\ell, S} \; \sum_{m', m} C_{\ell' S'}(J \; M; m' \; M-m')$$

$$\times \, C_{\ell S}(J \; M; m \; M-m) \int d\underline{r}' \; d\,\Omega(\theta,\phi) \; Y^{\ell'*}_{m'}(\theta,\phi) \; \phi_s(u) \; \overset{s.o}{V}(t)$$

$$\times \left\langle X^{S'}_{M-m'}(1,\overline{23}) \right| \underline{S}_{12} \cdot \underline{L}_{12} \left| X^{S}_{M-m}(2,\overline{13}) \right\rangle \phi_s(V) \; Y^{\ell}_{m}(\theta',\phi') \; \frac{1}{r}$$

$$\times \; f^{S}_{J\ell M}(r') \qquad \ldots \quad (V.4.1)$$

The potential function $\overset{s.o}{V}(t)$ is given by:

$$\sum_{\nu=1}^{4} \frac{1}{4}(w - 2h + b - 2m)_{\nu} \overset{\nu}{V}_{s.o}(t) = \sum_{k=1}^{2} \overset{s.o\,(II)}{U_k} \; Exp(- \overset{s.o\,(II)}{\mu_k} \; t^2)$$

$$= \overset{s.o\,(II)}{V(t)} \qquad \ldots \quad (V.4.2)$$

and

$$\underline{S}_{12} \cdot \underline{L}_{12} = \frac{1}{2i} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \left[(\underline{r} - \underline{r}') \wedge \frac{\partial}{\partial \underline{r}} - (\underline{r} - \underline{r}') \wedge \frac{\partial}{\partial \underline{r}'} \right]$$

$$\ldots \quad (V.4.3)$$

Now, using (V.4.3) in (V.4.1) we get:

$$\overset{s.o\;S'}{E}_{J\ell' M(s-s)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'M-m')$$

$$\times\, C_{\ell S}(J\ M;m\ M-m) \int d\underline{r}' \int d\Omega(\theta,\phi)\, \overset{\ell'}{Y}{}^{*}_{m'}(\theta,\phi) \overset{s.o\,(II)}{V(t)}\; Exp(-\alpha_i u^2)$$

$$\times \langle X^{S'}_{M-m'}(1,\overline{23}) \Big| \left[\frac{1}{2i}(\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \left[(\underline{r} - \underline{r}') \wedge \frac{\partial}{\partial \underline{r}} - (\underline{r} - \underline{r}') \wedge \frac{\partial}{\partial \underline{r}'} \right] \right.$$

$$\left. \times\, Exp(-\alpha_j r^2) \right] \Big| X^{S}_{M-m}(2,\overline{13}) \rangle \overset{\ell}{Y}_m(\theta',\phi') \frac{1}{r'} f^{S}_{J\ell M}(r')$$

$$\ldots \quad (V.4.4)$$

In operating by $\frac{\partial}{\partial \underline{r}}$ and $\frac{\partial}{\partial \underline{r}'}$ on the functions $\phi_s(V)$ $\times \overset{\ell}{Y}_m(\theta',\phi') \frac{1}{r'} f^{S}_{J\ell M}(r')$ and $\phi_s(u) \overset{\ell'}{Y}{}^{*}_{m'}(\theta,\phi) \overset{s.o\,(II)}{V(t)}$, we first differentiate w.r.to $\underline{r}$

$$\int d\underline{r}'\; Exp(-\alpha_i u^2) \overset{s.o}{V(t)} \frac{1}{2i} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot (\underline{r} - \underline{r}') \wedge \frac{\partial}{\partial \underline{r}}$$

$$\times\, Exp(-\alpha_j V^2) \overset{\ell}{Y}_m(\theta',\phi') \frac{1}{r'} f^{S}_{J\ell M}(r')$$

obtaining $\frac{16}{3} \alpha_j \int d\underline{r}'\; Exp(-\alpha_i u^2) \overset{s.o\,(II)}{V(t)} \left[\frac{1}{2i} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \right.$

$$(\underline{r}' \wedge \underline{r}) \Big] \text{Exp}(-\alpha_j V^2) \overset{\ell}{\underset{m}{Y}}(\theta',\phi') \frac{1}{r'} f^{S}_{J\ell M}(r') \quad \ldots \quad (V.4.5)$$

Similarly, the term,

$$\int d\underline{r}' \text{ Exp}(-\alpha_i u^2) \overset{s.o\ (II)}{V(t)} \frac{1}{2i} (\underline{\sigma}_1 + \underline{\sigma}_2)\cdot(\underline{r} - \underline{r}')\wedge \frac{\partial}{\partial \underline{r}'}$$

$$\times \text{ Exp}(-\alpha_j V^2) \overset{\ell}{\underset{m}{Y}}(\theta',\phi') \frac{1}{r'} f^{S}_{J\ell M}(r')$$

Which by integrating by parts W.r. to $\underline{r}'$ and differentiating we obtain:

$$\frac{16}{3} \alpha_i \int d\underline{r}' \text{ Exp}(-\alpha_i u^2) \overset{s.o\ (II)}{V(t)} \Big[\frac{1}{2i} (\underline{\sigma}_1 + \underline{\sigma}_2)\cdot(\underline{r}' \wedge \underline{r}) \Big]$$

$$\times \text{ Exp}(-\alpha_j V^2) \overset{\ell}{\underset{m}{Y}}(\theta',\phi') \frac{1}{r'} f^{S}_{J\ell M}(r') \quad \ldots \quad (V.4.6)$$

(V.4.4) becomes, using (V.4.5) and (V.4.6)

$$\overset{s.o\ S'}{\underset{J\ell' M(s-s)}{,E}}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \overset{s.o\ (II)}{U_k} \frac{16}{3} (\alpha_i + \alpha_j) \sum_{\ell,S}$$

$$\times \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m) \int d\underline{r}' \int d\,\Omega(\theta,\phi)$$

$$\times \text{ Exp}(-\alpha_i u^2 - \alpha_j V^2) \overset{\ell'}{\underset{m'}{Y}}{}^{*}(\theta,\phi) \langle X^{S'}_{M-m'}(1,\overline{23}) | \frac{1}{2i} (\underline{\sigma}_1 + \underline{\sigma}_2)\cdot(\underline{r}' \wedge \underline{r})$$

$$\times \text{ Exp}(-C_{kij}\ \underline{r}\cdot\underline{r}') \, | X^{S}_{M-m}(2,\overline{13}) \rangle \overset{\ell}{\underset{m}{Y}}(\theta',\phi') \frac{1}{r'} f^{S}_{J\ell M}(r') = \sum_{\ell,S,L}$$

$$\times \sum_{m',m,p} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m) \int_0^\infty r'^2\, dr'$$

$$\times \overset{s,o\ (II)}{\underset{L}{p}}(r,r') \int d\,\Omega(\theta,\phi) \overset{\ell'}{\underset{m'}{Y}}{}^{*}(\theta,\phi) \overset{L}{\underset{p}{Y}}(\theta,\phi) \int d\,\Omega(\theta',\phi') \overset{L}{\underset{p}{Y}}{}^{*}(\theta',\phi')$$

$$x \langle X^{S'}_{M-m'}(1,\overline{23}) \,|\, \tfrac{1}{2}(\underline{\sigma}_1 + \underline{\sigma}_2)\cdot \underline{L}_{r'} \,|X^{S}_{M-m}(2,\overline{13})\rangle \, Y^{\ell}_{m}(\theta',\phi') \, \frac{1}{r'} \, f^{S}_{J\ell M}(r')$$

$$\ldots \quad (V.4.8)$$

Where use is made of the fact that

$$\frac{1}{2i}(\underline{\sigma}_1 + \underline{\sigma}_2)\cdot(\underline{r}'\wedge r)\,\mathrm{Exp}(-C_{kij}\,\underline{r}\cdot\underline{r}') = -\frac{1}{C_{kij}}\,\frac{1}{2i}(\underline{\sigma}_1 + \underline{\sigma}_2)\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'}$$

$$x\,\mathrm{Exp}(-C_{kij}\,\underline{r}\cdot\underline{r}') \quad \ldots \quad (V.4.9)$$

and

$$\overset{s.o}{p}_{L}(r,r') = 2\pi\int_{-1}^{+1} d\eta\, p_{L}(\eta)\, \overset{s,o\,(II)}{V}(\underline{r},\underline{r}') \quad \ldots \quad (V.4.10)$$

where

$$\overset{s.o}{V}(\underline{r},\underline{r}') = +(4/3)^4\,\frac{Mr}{\hbar^2}\sum_{i,j=1}^{2}\frac{16}{3C_{kij}}(\alpha_i+\alpha_j)\,\phi_s(u)\,\phi_s(V)$$

$$\ldots \quad (V.4.11)$$

We now consider the expression involving the operator $\underline{L}_{r'}$

$$\sum_{n,p}\int d\Omega(\theta,\phi)\, Y^{\ell'*}_{m'}(\theta,\phi)\, Y^{L}_{p}(\theta,\phi)\int d\Omega(\theta',\phi')\, Y^{L*}_{p}(\theta',\phi')$$

$$x \langle X^{S}_{M-m'}(1,\overline{23}) \,|\, \tfrac{1}{2}(\underline{\sigma}_1 + \underline{\sigma}_2)\cdot \underline{L}_{r'} \,|X^{S}_{M-m}(2,\overline{13})\rangle \, Y^{\ell}_{m}(\theta',\phi') \, \frac{1}{r'} \, f^{S}_{J\ell M}(r')$$

$$= \frac{1}{2}A(J\ell)\,\delta(S',S)\,\delta(\ell',\ell)\,\delta(m',m)\,\frac{1}{r'}\,f^{S}_{J\ell M}(r') \quad \ldots \quad (V.4.12)$$

Where $A(J\ell)$ was given in (III.4.8) and (III.4.9) respectively.

Using (V.4.12) and summing over m',m; expression (V.4.8) finally becomes:

$$\overset{s.o\;S'}{E}_{J\ell' M(s-s)}(r) \sum_{\ell,S}\int_{o}^{\infty} dr' \; \overset{s.o\,(II)}{e_1}(r,r')\,\frac{1}{2}A(J\ell)\,I_{e+\frac{1}{2}}(C_{kij}\,rr')$$

$$\times\, f^{S}_{J\ell M}(r')\,\delta(S',S)\,\delta(\ell',\ell) \qquad \ldots \quad (V.4.13)$$

where

$$\overset{s.o\,(II)}{e_1}(r,r') = -(4/3)^4\,\frac{2\pi\,Mrr'}{\hbar^2}\sum_{i,j.k=1}^{2}\frac{16}{3}\,\frac{(\alpha_i+\alpha_j)}{C_{kij}}\,A_i A_j$$

$$\times\, \overset{s.o\,(II)}{U_k}\,(2\pi/C_{kij}rr')^{\frac{1}{2}}\,\mathrm{Exp}(-\,a_{ijk}\,r^2 - b_{ijk}\,r'^2) \qquad \ldots \quad (V.4.14)$$

(V.5.) THE QUADRATIC SPIN-ORBIT TERM

The interaction due to the quadratic spin-orbit force is given in the doublet state by:

$$\overset{Q\;S'(II)}{E_{J\ell' M(s-s)}}(r) = -(4/3)^4\,\frac{Mr}{\hbar^2}\sum_{\ell}\sum_{m',m} C_{\ell'\frac{1}{2}}(J\;M;m'\;M-m')\;C_{\ell S}(J\;M;m\;M-m)$$

$$\times\int d\underline{r}'\;d\Omega(\theta,\phi)\;\phi_s(u)\;\overset{Q\,(II)}{V(t)}\;\overset{\ell'_*}{Y_{m'}}(\theta,\phi)\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\;(-\,4/3\;\underline{L}^2_{12})$$

$$\times\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle\,\overset{\ell}{Y_m}(\theta',\phi')\;\phi_s(V)\;\frac{1}{r'}\;f^{\frac{1}{2}}_{J\ell M}(r') - (4/3)^4\,\frac{Mr}{\hbar^2}\sum_{\ell}\sum_{m',m}$$

$$C_{\ell'\frac{1}{2}}(J\;M;m'\;M-m')\;C_{\ell\frac{1}{2}}(J\;M;m\;M-m)\int d\underline{r}'\;d\Omega(\theta,\phi)\;\phi_s(u)\;\overset{Q\,(II)}{V(t)}$$

$$\times\,\overset{\ell'_*}{Y_{m'}}(\theta,\phi)\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\,3\underline{L}^2_{12}\;|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle\,\overset{\ell'_*}{Y_{m'}}(\theta',\phi')\;\phi_s(V)\;\frac{1}{r'}$$

$$\times\, f^{\frac{1}{2}}_{J\ell M}(r') \qquad (II=3,4) \qquad \ldots \quad (V.5.1)$$

and in the quartet state it is given by:

$$\overset{Q\ S'(3)}{E}_{J\ell' M(s-s)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m')$$

$$\times C_{\ell 3/2}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ \phi_s(u)\ \overset{Q\ (3)}{V}(t)\ \overset{\ell'*}{Y}_{m'}(\theta,\phi)$$

$$\times \langle \overset{3/2}{X}_{M-m'}(1,\overline{23}) | \underline{L}_{12}^2 | \overset{3/2}{X}_{M-m}(2,\overline{13}) \rangle \overset{\ell}{Y}_m(\theta,\phi)\ \phi_s(V)\ \frac{1}{r'}\ \overset{3/2}{f}_{J\ell M}(r') + (4/3)^4$$

$$\times \frac{Mr}{\hbar^2} \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m')\ C_{\ell 3/2}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)$$

$$\times \overset{\ell'*}{Y}_{m'}(\theta,\phi)\ \overset{Q\ (3)}{V}(t)\ \phi_s(u) \langle \overset{3/2}{X}_{M-m}(1,\overline{23}) | \underline{Q}_{12}(\underline{t}^2) | \overset{3/2}{X}_{M-m}(2,\overline{13}) \rangle \phi_s(V)$$

$$\times \overset{\ell}{Y}_m(\theta',\phi')\ \frac{1}{r'}\ \overset{3/2}{f}_{J\ell M}(r') \qquad \ldots \quad (V.5.2)$$

The potential function $\overset{Q\ (II)}{V}(t)$ (II = 3,4), has already been defined in (III.5.a) and (III.5.b). Thus, from equation (V.5.1) and (V.5.2), we consider a general expression involving first the operator $\underline{L}_{12}^2$ and then the operator $\underline{Q}_{12}(\underline{t}^2)$ respectively. Thus,

$$\overset{Q\ S'(II)}{E}_{\underline{L}_{12}}(r) = \sum_{\ell,S} \sum_{m'} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m'\ M-m')\ \delta(S',S)$$

$$\times \int d\underline{r}'\ r\ d\Omega(\theta,\phi)\ \overset{\ell'*}{Y}_{m'}(\theta,\phi)\ \overset{Q\ (II)}{V}(t)\ \phi_s(u)\ \underline{L}_{12}^2\ \phi_s(V)\ \overset{\ell}{Y}_{m'}(\theta',\phi')$$

$$\times \frac{1}{r'}\ f^S_{J\ell M}(r') \qquad (II=3,4) \quad \ldots \quad (V.5.3)$$

where $\underline{L}_{12}^2$ is given by:

$$\underline{L}_{12}^2 = \left[(\underline{r} - \underline{r}') \wedge \frac{\vec{\partial}}{\partial \underline{r}'} \right] \cdot \left[(\underline{r} - \underline{r}') \wedge \frac{\vec{\partial}}{\partial \underline{r}} \right]$$

$$- \left[(\underline{r} - \underline{r}') \wedge \frac{\vec{\partial}}{\partial \underline{r}} \right] \cdot \left[\frac{\overleftarrow{\partial}}{\partial \underline{r}'} \wedge (\underline{r} - \underline{r}') \right]$$

$$- \left[\frac{\overleftarrow{\partial}}{\partial \underline{r}'} \wedge (\underline{r} - \underline{r}') \right] \cdot \left[\frac{\overleftarrow{\partial}}{\partial \underline{r}'} \wedge (\underline{r} - \underline{r}') \right]$$

$$- \left[\frac{\overleftarrow{\partial}}{\partial \underline{r}'} \wedge (\underline{r}-\underline{r}') \right] \cdot \left[(\underline{r}-\underline{r}') \wedge \frac{\vec{\partial}}{\partial \underline{r}} \right] \qquad \ldots \quad (V.5.4)$$

$$\overset{\ell'}{\underset{m'}{Y}}{}^{*}(\theta,\phi)\ \phi_s(u)\ \overset{Q\ (II)}{V}(t)\ \underline{L}^2_{12}\ \phi_s(V)\ \overset{\ell}{\underset{m}{Y}}(\theta',\phi')\ \frac{1}{r'}\ \underset{J\ell M}{f^S}(r') = \overset{\ell'}{\underset{m'}{Y}}{}^{*}(\theta,\phi)$$

$$x\ \phi_s(u)\ \overset{Q\ (II)}{V}(t) \Big[8\ {}_1g_{ij}\ r^2 r'^2 - 4\ {}_1\xi_{ijk}\ (r^2 + r'^2) + 6\ -{}_2\xi_{ijk} \underline{r}\cdot\underline{r}'$$

$$- 8\ {}_1g_{ij}\ (\underline{r}\cdot\underline{r}')^2 \Big]\ \phi_s(V)\ \overset{\ell}{\underset{m'}{Y}}(\theta,\phi)\ \frac{1}{r'}\ \underset{J\ell M}{f^S}(r') \qquad \ldots \quad (V.5.5)$$

Putting

$$\overset{Q\ (II)}{I}(\underline{r},\underline{r}') = \phi_s(u)\ \overset{Q\ (II)}{V}(t) \Big[8\ {}_1g_{ij}\ r^2\ r'^2 - 4\ {}_1\xi_{ijk}\ (r^2 + r'^2)$$

$$+ 6\ -\ {}_2\xi_{ijk}\ \underline{r}\cdot\underline{r}' - 8\ {}_1g_{ij}\ (\underline{r}\cdot\underline{r}')^2 \Big]\ \phi_s(V) \qquad \ldots \quad (V.5.6)$$

Using this result, enables us to write equation (V.5.3) in the following form:

$$\overset{Q\ S'(II)}{E}_{\underline{L}_{12}}(r) = \sum_{\ell,S} \sum_{m'} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m'\ M-m')\ \delta(S',S)$$

$$x \int dr'\ \underset{J\ell M}{f^S}(r') \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi)\ \overset{\ell'}{\underset{m'}{Y}}{}^{*}(\theta,\phi)\ \overset{Q\ (II)}{I}(\underline{r},\underline{r}')\ \overset{\ell}{\underset{m'}{Y}}(\theta',\phi')$$

$$\ldots \quad (V.5.7)$$

The function $\overset{Q\ (II)}{I}(\underline{r},\underline{r}')$ is again expanded

$$\overset{Q\ (II)}{I}(\underline{r},\underline{r}') = \frac{1}{rr'} \sum_{\mu,\nu} \overset{Q\ (II)}{\underset{\nu}{i}}(r,r')\ \overset{\nu}{\underset{\mu}{Y}}{}^{*}(\theta',\phi')\ \overset{\nu}{\underset{\mu}{Y}}(\theta,\phi) \qquad \ldots \quad (V.5.8)$$

where

$$ {}^{Q\,(II)}i(r,r') = 2\pi rr' \int_{-1}^{+1} d\eta \, p_n(\eta) \; {}^{Q\,(II)}I(\underline{r},\underline{r}') \qquad \ldots \quad (V.5.9)$$

Substituting (V.5.8) into (V.5.7), and integrating w.r.to the solid angles (θ',ϕ') and (θ,ϕ), and then summing over all magnetic quantum numbers (m', μ and ν), we finally obtain for ${}^{Q\,S\,(II)}E_{\underline{L}_{12}}(r)$ the following expression:

$$ {}^{Q\,S'(II)}E_{\underline{L}_{12}}(r) = \sum_{\ell,S} \int_0^\infty dr' \, f^S_{J\ell M}(r') \, \delta(S',S) \, \delta(\ell',\ell) \Big[\; {}^{1\,(II)}e_{\underline{L}_{12}}(r,r') $$

$$ \times \, I_{L+\frac{1}{2}}(C_{kij}\, rr') + {}^{2\,(II)}e_{\underline{L}_{12}}(r,r') \, I_{\ell+\frac{1}{2}}(C_{kij} rr') + {}^{3\,(II)}e_{\underline{L}_{12}}(r,r') $$

$$ \times \, I''_{\ell+\frac{1}{2}}(C_{kij} rr') \Big] \qquad (II=3,4) \qquad \ldots \quad (V.5.10)$$

where

$$ {}^{1\,(II)}e_{\underline{L}_{12}}(r,r') = 2\pi rr' \sum_{i,jk=1}^{2} A_i A_j \; {}^{Q\,(II)}U_k \; \mathrm{Exp}(-\,a_{ijk}\, r^2 - b_{ijk} r'^2) $$

$$ \times \Big[\, 8 \; {}_1g_{ij} \, r^2 r'^2 - 4 \; {}_1\xi_{ijk} \, (r^2 + r'^2) + 6 - (\, {}_2\xi_{ijk} / C_{kij}) $$

$$ + \, (6 \; {}_1g_{ij} \, / \, C^2_{kij}) \Big] \qquad \ldots \quad (V.5.11)$$

$$ {}^{2\,(II)}e_{\underline{L}_{12}}(r,r') = 2\pi rr' \sum_{i,j,k=1}^{2} A_i A_j \; {}^{Q\,(II)}U_k \; \mathrm{Exp}(-\,a_{ijk}\, r^2 - b_{ijk} r'^2) $$

$$ \times \Big[\; {}_2\xi_{ijk} - (12 \, / \, C_{kij}) \Big] \qquad \ldots \quad (V.5.12)$$

and

$$ {}^{3}e^{(II)}_{\underline{L}_{12}}(r,r') = 16\pi rr' \sum_{i,j,k=1}^{2} A_i A_j \; {}^{Q}U_k^{(II)} \; {}_{1}g_{ij} $$

$$ \times \, \mathrm{Exp}(-\, a_{ijk}\, r^2 - b_{ijk}\, r'^2) \qquad \ldots \quad (V.5.13) $$

$I_\lambda(X)$ is the modified Bessel function of the first kind of order λ and is defined as:

$$ I_\lambda(X) = (i)^{-\lambda} \; J_\lambda(iX) \qquad \ldots \quad (V.5.14) $$

and $I'_\lambda(X)$ and $I''_\lambda(X)$ denote the first and second derivatives w.r. to X.

Similar procedure is also applied to calculate the expression containing the operator $\underline{Q}_{12}(\underline{t}^2)$. Thus,

$$ {}^{Q}E^{S'(3)}_{J\ell' M(s-s)}(r) = \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M; m'\ M-m')\; C_{\ell S}(J\ M; m\ M-m) \int_0^\infty dr' $$

$$ \times\, (rr'^2) \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi)\; Y^{\ell'*}_{m'}(\theta,\phi)\; \phi_s(u)\; {}^{Q}V^{(3)}(t) \langle X^{S'}_{M-m'}(1,\overline{23})| $$

$$ \times\, \underline{Q}_{12}(\underline{t}^2)\, |X^{S}_{M-m}(2,\overline{13})\rangle\, \phi_s(V)\, Y^{\ell}_{m}(\theta,\phi)\, \frac{1}{r'}\, f^{S}_{J\ell M}(r') \qquad \ldots \quad (V.5.15) $$

where

$$ \underline{Q}_{12}(\underline{t}^2) = \frac{1}{2}\Big[(\underline{\sigma}_1 \cdot \underline{L}_{12})(\underline{\sigma}_2 \cdot \underline{L}_{12}) + (\underline{\sigma}_2 \cdot \underline{L}_{12})(\underline{\sigma}_1 \cdot \underline{L}_{12}) \Big] $$

$$ = -\Big[\underline{\sigma}_1 \cdot (\underline{r} - \underline{r}') \wedge \Big(\frac{\vec{\partial}}{\partial \underline{r}} - \frac{\vec{\partial}}{\partial \underline{r}'}\Big) \Big]\Big[\underline{\sigma}_2 \cdot (\underline{r} - \underline{r}') \wedge \Big(\frac{\vec{\partial}}{\partial \underline{r}} - \frac{\vec{\partial}}{\partial \underline{r}'}\Big) \Big] $$

$$ = -\Big[\underline{\sigma}_1 \cdot (\underline{r} - \underline{r}') \wedge \frac{\vec{\partial}}{\partial \underline{r}} \Big]\Big[\underline{\sigma}_2 \cdot (\underline{r} - \underline{r}') \wedge \frac{\vec{\partial}}{\partial \underline{r}} \Big] $$

$$+ \left[\underline{\sigma}_1 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}} \right] \left[\underline{\sigma}_2 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}'} \right]$$

$$+ \left[\underline{\sigma}_1 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}'} \right] \left[\underline{\sigma}_2 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}} \right]$$

$$+ \left[\underline{\sigma}_1 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}'} \right] \left[\underline{\sigma}_2 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}'} \right] \qquad \ldots \quad (V.5.16)$$

Thus, the first part of (V.5.16) is

$$- \overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi)\ {}^{Q\,(3)}V(t)\ \phi_s(u) \left[\underline{\sigma}_1 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}} \right] \left[\underline{\sigma}_2 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}} \right]$$

$$\times\ \phi_s(V)\ \overset{\ell}{\underset{m}{Y}}(\theta',\phi')\ \frac{1}{r'}\ f^{S}_{J\ell M}(r') = \overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi)\ {}^{Q\,(3)}V(t)\ \phi_s(u) \Big[- (16/3)^2\ \alpha_j^2$$

$$\times\ (\underline{\sigma}_1 \cdot \underline{r}'\wedge \underline{r})(\underline{\sigma}_2 \cdot \underline{r}'\wedge \underline{r}) - \frac{16}{9}\ \alpha_j\ r'^2\ S_{12}(\underline{r}'^2) + \frac{16}{9}\ \alpha_j(\underline{r}\cdot\underline{r}')$$

$$\times\ S_{12}(\underline{r}',\underline{r}) - \frac{32}{9}\ \alpha_j\ (\underline{\sigma}_1 \cdot \underline{\sigma}_2)(\underline{r}\cdot\underline{r}') + \frac{32}{9}\ \alpha_j(\underline{\sigma}_1 \cdot \underline{\sigma}_2)\ r'^2 \Big]$$

$$\times\ \phi_s(V)\ \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\ \frac{1}{r'}\ f^{S}_{J\ell M}(r') \qquad \ldots \quad (V.5.17)$$

The second part of (V.5.16)

$$\overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi)\ {}^{Q\,(3)}V(t)\ \phi_s(u) \left[\underline{\sigma}_1 \cdot (\underline{r} - \underline{r}')\wedge \frac{\vec{\partial}}{\partial \underline{r}} \right] \left[\frac{\overleftarrow{\partial}}{\partial \underline{r}'}\wedge (\underline{r} - \underline{r}') \cdot \underline{\sigma}_2 \right]$$

$$\times\ \phi_s(V)\ \overset{\ell}{\underset{m'}{Y}}(\theta',\phi')\ \frac{1}{r'}\ f^{S}_{J\ell M}(r') = \overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi)\ {}^{Q\,(3)}V(t)\ \phi_s(u) \Big[-(16/3)^2$$

$$\times\ \alpha_i\ \alpha_j\ (\underline{\sigma}_1 \cdot \underline{r}'\wedge \underline{r})(\underline{\sigma}_2 \cdot \underline{r}'\wedge \underline{r}) - \frac{8}{27}\ (-2\alpha_i + 4\alpha_j + {}^{Q(3)}u_k)\ r^2$$

$$\times\ S_{12}(\underline{r}^2) - \frac{8}{27}(-2\alpha_j + 4\alpha_i + {}^{Q(3)}u_k)\ r'^2\ S_{12}(\underline{r}'^2) + \frac{16}{27}\ (\alpha_i + \alpha_j + {}^{Q(3)}u_k)$$

$$\times (\underline{r}\cdot\underline{r}')\, S_{12}(\underline{r},\underline{r}') + \frac{16}{27}\left(-2\alpha_i + 4\alpha_j + \mu_k^{Q(3)}\right)(\underline{\sigma}_1\cdot\underline{\sigma}_2)\, r^2$$

$$-2(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\underline{r}')\Big]\, \phi_s(V)\, Y^{\ell}_{m}(\theta',\phi')\, \frac{1}{r'}\, f^{S}_{J\ell M}(r') \quad \ldots \quad (V.5.18)$$

The third part of (V.5.16)

$$Y^{*\ell'}_{m'}(\theta,\phi)\, V^{Q(3)}(t)\, \phi_s(u)\left[\frac{\overleftarrow{\partial}}{\partial\underline{r}'}\wedge(\underline{r}-\underline{r}')\cdot\underline{\sigma}_1\right]\left[\underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\wedge\frac{\overrightarrow{\partial}}{\partial\underline{r}}\right]$$

$$\times\, \phi_s(V)\, Y^{\ell}_{m}(\theta',\phi')\, \frac{1}{r'}\, f^{S}_{J\ell M}(r') = Y^{*\ell'}_{m'}(\theta,\phi)\, V^{Q(3)}(t)\, \phi_s(u)\Big[-(16/3)^2$$

$$\times\, \alpha_i\,\alpha_j(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})\Big]\, \phi_s(V)\, Y^{\ell}_{m}(\theta',\phi')\, \frac{1}{r'}\, f^{S}_{J\ell M}(r')$$

$$\ldots \quad (V.5.19)$$

and the fourth part of (V.5.16) is

$$-Y^{*\ell'}_{m'}(\theta,\phi)\, V^{Q(3)}(t)\, \phi_s(u)\left[\frac{\overleftarrow{\partial}}{\partial\underline{r}}\wedge(\underline{r}-\underline{r}')\cdot\underline{\sigma}_1\right]\left[\frac{\partial}{\partial\underline{r}'}\wedge(\underline{r}-\underline{r}')\cdot\underline{\sigma}_2\right]$$

$$\times\, \phi_s(V)\, Y^{\ell}_{m}(\theta',\phi')\, \frac{1}{r'}\, f^{S}_{J\ell M}(r') = Y^{*\ell'}_{m'}(\theta,\phi)\, V^{Q(3)}(t)\, \phi_s(u)\Big[-(16/3)^2\alpha_i^2$$

$$\times\, (\underline{\sigma}_1\cdot\underline{r}'\wedge r)(\underline{\sigma}_2\cdot r'\wedge r) + (16/9)\,\alpha_i(\underline{r}\cdot\underline{r}')\, S_{12}(\underline{r},\underline{r}') - (16/9)\,\alpha_i r^2\, S_{12}(\underline{r}^2)$$

$$-(32/9)\,\alpha_i(\underline{\sigma}_1\cdot\underline{\sigma}_2)\,(\underline{r}\cdot\underline{r}') + \frac{32}{9}\,\alpha_i(\underline{\sigma}_1\cdot\underline{\sigma}_2)\, r^2\Big]\, \phi_s(V)\, Y^{\ell}_{m}(\theta',\phi')\, \frac{1}{r'}$$

$$f^{S}_{J\ell M}(r') \quad \ldots \quad (V.5.20)$$

Collecting all terms we obtain:

$$Y^{*\ell'}_{m'}(\theta,\phi)\, V^{Q(3)}(t)\, \phi_s(u)\Big[-9\, {}_1b^2_{ijk}\,(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r}) - {}_3\xi_{ijk}$$

$$\times \left[r^2 S_{12}(\underline{r}^2) + r'^2 S_{12}(\underline{r}'^2) - 2(\underline{r}\cdot\underline{r}') S_{12}(r,\underline{r}') \right]$$

$$+ \left[2\ {}_3\xi_{ijk}(r^2 + r'^2) - 2 \right] (\underline{\sigma}_1 \cdot \underline{\sigma}_2) - {}_4\xi_{ijk}(\underline{r}\cdot\underline{r}')(\underline{\sigma}_1\cdot\underline{\sigma}_2) \Big]$$

$$\times \phi_s(V) \overset{\ell}{\underset{m}{Y}}(\theta',\phi') \frac{1}{r'} f^S_{J\ell M}(r') \qquad \ldots \quad (V.5.21)$$

Using (V.5.21) we then obtain from (V.5.15)

$$E^{S'(3)}_{\underline{Q}_{12}}(r) = - \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m) \int_0^\infty dr'$$

$$\times rr' \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi) \overset{\ell'^*}{\underset{m'}{Y}}(\theta,\phi)\ \phi_s(u)\ \overset{Q\ (3)}{V}(t) \langle X^{S'}_{M-m'}(1,\overline{23})|$$

$$\times \Big\{ {}_3\xi_{ijk} \left[r^2 S_{12}(\underline{r}^2) + r'^2 S_{12}(r'^2) - 2(\underline{r}\cdot\underline{r}') S_{12}(\underline{r},\underline{r}') \right]$$

$$+ \left[2 - 2\ {}_3\xi_{ijk}(r^2 + r'^2) \right] (\underline{\sigma}_1 \cdot \underline{\sigma}_2) + {}_4\xi_{ijk}(\underline{r}\cdot\underline{r}')(\underline{\sigma}_1 \cdot \underline{\sigma}_2)$$

$$+ 9\ {}_1b^2_{ijk}\ (\underline{\sigma}_1 \cdot \underline{r}' \wedge \underline{r})(\underline{\sigma}_2 \cdot \underline{r}' \wedge \underline{r}) \Big\} |X^S_{M-m}(2,\overline{13})\rangle \phi_s(V) \overset{\ell}{\underset{m}{Y}}(\theta',\phi')$$

$$\times f^S_{J\ell M}(r') \qquad \ldots \quad (V.5.22)$$

The analysis for $\overset{Q\ S'(3)}{E}_{\underline{Q}_{12}}(r)$ in the above equation follows the same course, and the result is finally given by:

$$\overset{Q\ S'(3)}{E}_{\underline{Q}_{12}}(r) = \sum_{\ell} \int_0^\infty dr'\ f^S_{J\ell M}(r') \Big\{ A(\ell' 3/2\ ;\ \ell 3/2) \Big[\overset{1\ (3)}{e}_{\underline{Q}_{12}}(r,r')$$

$$\times I_{\ell+\frac{1}{2}}(C_{kij}\ rr') + \overset{2\ (3)}{e}_{\underline{Q}_{12}}(r,r')\ I_{\ell'+\frac{1}{2}}(C_{kij}\ rr') - \overset{3\ (3)}{e}_{\underline{Q}_{12}}(r,r')$$

$$\times \sum_{L} FF(\ell' \ell;L)\left(-1 + \frac{2L+1}{rr'}\right) I_{L+\frac{1}{2}}(C_{kij}\, rr') \Big] + {}^{4\,(3)}e_{Q_{12}}(r,r')$$

$$\times I_{\ell+\frac{1}{2}}(C_{kij} rr') + {}^{5\,(3)}e_{Q_{12}}(r,r')\left(-1 + \frac{2\ell+1}{rr'}\right) I_{\ell+\frac{1}{2}}(C_{kij}\, rr')$$

$$+ {}^{6\,(3)}e_{Q_{12}}(r,r') \sum_{L} H(\ell,L)\, I_{L+\frac{1}{2}}(C_{kij}\, rr') \Big\} \qquad \ldots \quad (V.5.23)$$

where

$${}^{1\,(3)}e_{Q_{12}}(r,r') = -2\pi \sum_{i,j,k=1}^{2} A_i A_j\, {}^{Q\,(3)}U_k\; {}_3\xi_{ijk}\, (2\pi/C_{kij} rr')^{\frac{1}{2}}$$

$$\times \operatorname{Exp}(-a_{ijk}\, r^2 - b_{ijk}\, r'^2) \begin{bmatrix} r^3\, r'(I=1) \\ r\, r'^3 (I=2) \end{bmatrix} \qquad \ldots \quad (V.5.24)$$

$${}^{3\,(3)}e_{Q_{12}}(r,r') = -2\pi\, rr' \sum_{i,j,k=1} A_i A_j\, {}^{Q\,(3)}U_k\, ({}_3\xi_{ijk}/\, C_{kij})$$

$$\times (2\pi/C_{kij} rr')^{\frac{1}{2}} \operatorname{Exp}(-a_{ijk}\, r^2 - b_{ijk}\, r'^2) \qquad \ldots \quad (V.5.25)$$

$${}^{4\,(3)}e_{Q_{12}}(r,r) = -2\pi\, rr' \sum_{i,j,k=1}^{2} A_i A_j\, {}^{Q\,(3)}U_k\, (2\pi/C_{kij} rr')^{\frac{1}{2}}$$

$$\times \left[2 - 2\, \xi_{ijk}(r^2 + r'^2)\right] \operatorname{Exp}(-a_{ijk}\, r^2 - b_{ijk}\, r'^2) \qquad \ldots \quad (V.5.26)$$

$${}^{5\,(3)}e_{Q_{12}}(r,r') = -2\pi\, rr' \sum_{i,j,k=1}^{2} A_i A_j\, {}^{Q\,(3)}U_k\, \frac{1}{C_{kij}}\, (2\pi/C_{kij} rr')^{\frac{1}{2}}$$

$$\times {}_4\xi_{ijk}\; \operatorname{Exp}(-a_{ijk} r^2 - b_{ijk} r'^2) \qquad \ldots \quad (V.5.27)$$

and

$$e^{6\,(3)}_{Q_{12}}(r,r') = -\,18\pi\, r^2 r'^2 \sum_{i,j,k=1}^{2} A_i A_j \, U^{Q\,(3)}_k \, b^2_{ijk} \, (2\pi/C_{kij} rr')^{\frac{1}{2}}$$

$$\times \, \mathrm{Exp}(-\,a_{ijk} r^2 - b_{ijk} r'^2) \qquad \ldots \quad (V.5.28)$$

also

$$H(\ell;L) = \sum_{L'} (-1)^{L'} \left[\frac{20}{3} - \frac{5\,L'(L'+1)}{3} \right] C^{2}_{11}(L)\, C^{2}_{L'\ell}(L) \qquad \ldots \quad (V.5.29)$$

Thus, from (V.5.10) and (V.5.23), we can write the exchange interaction term of the quadratic spin-orbit in the doublet state as

$$\overset{Q\;S'}{E}_{J\ell'M(s-s)}(r) = -(4/3)^4 \frac{M}{\hbar^2} \left[-\frac{4}{3}\, \overset{Q\;S'(3)}{E}_{L_{12}}(r) + 3\, \overset{Q\;S'(4)}{E}_{L_{12}}(r) \right] \qquad \ldots \quad (V.5.30)$$

and in the quartet state it is given by

$$\overset{Q\;S'}{E}_{J\ell'M(s-s)}(r) = -(4/3)^4 \frac{M}{\hbar^2} \left[\overset{Q\;S'(3)}{E}_{L_{12}}(r) - \overset{Q\;S'(3)}{E}_{Q_{12}}(r) \right] \ldots \quad (V.5.31)$$

CHAPTER VI

DIRECT (s-D)-INTERACTION TERMS

The (s-D) -terms are derived from expressions containing a single tensor (from the deuteron D-state function), and the analysis follows that for the tensor (s-s) term very closely. Due to this tensor operator, the only contribution is being in the quartet state.

(VI.1.) THE CENTRAL TERM

The central interaction term is given by:

$$
\begin{aligned}
{}^{c}D^{S'}_{J\ell' M(s\text{-}D)}(r) &= \frac{4M}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M\text{-}m')\ C_{\ell S}(J\ M;m\ M\text{-}m) \\
&\times \int d\underline{R}\ d\Omega(\theta,\phi)\ Y^{\ell' *}_{m'}(\theta,\phi)\ \phi_s(R) < X^{S'}_{M\text{-}m'}(1,\overline{23}) | \sum_{=1}^{4} \frac{1}{4} \Big[(2w-h)_\nu \\
&\times {}^{\nu}V_c(\underline{r}_{12})\ S_{23}(\underline{R}^2)\ |X^{S}_{M\text{-}m}(1,\overline{23})> + (2b-m)_\nu\ {}^{\nu}V_c(\underline{r}_{12})\ S_{13}(\underline{R}^2) \\
&\times |X^{S}_{M\text{-}m}(2,\overline{13})> \Big]\ Y^{\ell}_{m}(\theta,\phi)\ \phi_D(R)\ f^{S}_{J\ell M}(r) = \frac{4M}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} \\
&\times C_{\ell' S'}(J\ M;m'\ M\text{-}m')\ C_{\ell S}(J\ M;m\ M\text{-}m) \int d\underline{R}\ d\Omega(\theta,\phi)\ Y^{\ell}_{m}(\theta,\phi)\ \phi_s(R) \\
&\times < X^{S'}_{M\text{-}m'}(1,\overline{23}) |\ S_{23}(\underline{R}^2)\ {}^{c}V^{(2)}(\underline{r}_{12})\ |X^{S}_{M\text{-}m}(1,\overline{23})>\ Y^{\ell}_{m}(\theta,\phi)\ \phi_D(R)\ f^{S}_{J\ell M}(r)
\end{aligned}
\qquad \text{... (VI.1.1)}
$$

where

$$
{}^{c}V^{(2)}(\underline{r}_{12}) = \sum_{=1}^{4} \frac{1}{4} \Big[(2w-h)_\nu + (2b-m)_\nu \Big]\ {}^{\nu}V_c(\underline{r}_{12})
$$

$$= \sum_{k=1}^{2} {}^{c}U_k^{(2)} \, \mathrm{Exp}(- {}^{c}\mu_k^{(2)} \, \underline{r}_{12}^2) \qquad \ldots \quad (VI.1.2$$

The matrix elements of the tensor operator $S_{23}(\underline{R}^2)$ are now expressed in terms of C.G. coefficients and $Y^2_{m'-m}(\theta_R,\phi_R)$ harmonics (Bransden, Smith, and Tate, 1958; Blatt and Weiskopf, 1962). Thus,

$$\langle X^{S'}_{M-m'}(1,\overline{23})| \; S_{23}(\underline{R}^2) \; |X^{S}_{M-m}(1,\overline{23})\rangle = (-1)^{S+m} \, (4\pi/5)^{\frac{1}{2}} \, g(S',S)$$

$$\times \, C_{S'S}(2,\, m-m';\, m'\, m) \, Y^{2}_{m-m'}(\theta_R,\phi_R) \qquad \ldots \quad (VI.1.3)$$

and the potential function ${}^{c}V(\underline{r}_{12})$ is also expanded in spherical harmonics as follows:

$${}^{c}V(\underline{r},\underline{R}) = \sum_{\ell'',m''} {}^{c}p^{(2)}_{\ell''}(r,R) \; Y^{\ell''}_{m''}(\theta_R,\phi_R) \; Y^{\ell''}_{m''}(\theta,\phi) \qquad \ldots \quad (VI.1.4)$$

where

$${}^{c}p^{(2)}_{\ell''}(r,R) = 2\pi \int_{-1}^{+1} d\mu \; p_{\ell''}(\mu) \; {}^{c}V^{(2)}(\underline{r},\underline{R}) \qquad \ldots \quad (VI.1.5)$$

where $p_{\ell''}(\mu)$ is the legendre polynomial.

Using (VI.1.3) and (VI.1.4) in (VI.1.1) we get

$${}^{c}D^{S'}_{J\ell' M(s-D)}(r) \doteq \frac{4M}{3\hbar^2} \sum_{\ell,\ell'',S} \; \sum_{m',m,m''} C_{\ell' S'}(J\, M; m'\, M-m')$$

$$\times \, C_{\ell S}(J\, M; m\, M-m) \; g(S',S) \; C_{S'S}(2,\, m-m';\, m' m) \; (4\pi/5)^{\frac{1}{2}} \int d\Omega_R(\theta_R,\phi_R)$$

$$\times \; Y^{\ell''*}_{m''}(\theta_R,\phi_R) \; Y^{2}_{m-m'}(\theta_R,\phi_R) \int d\Omega(\theta,\phi) \; Y^{\ell'*}_{m'}(\theta,\phi) \; Y^{\ell''}_{m''}(\theta,\phi) \; Y^{\ell}_{m}(\theta,\phi)$$

$$\times \sum_{i,j=1}^{2} A_i A_j' \int_0^\infty dR\, R^4\, \text{Exp}(-(\alpha_i + \alpha_j)R^2)\; {}^{c\,(2)}p_{\ell''}(r,R)\; f^{S}_{J\ell M}(r) \qquad \ldots \text{(VI.1.6)}$$

Integrating the angular part, and applying the rules for the sum of four C.G. coefficients (Rose, 1957), enables us to extend the analysis and carry out the integration w.r. to dR, which finally leaves the direct interaction term in the following form:

$$ {}^{c\,S'}D_{J\ell' M(s-D)}(r) = \sum_{\ell} {}^{c\,(2)}B_1(r)\; A_{\ell'\ell}(3/2,3/2)\; f^{S}_{J\ell M}(r) \qquad \ldots \text{(VI.1.7)}$$

where

$$ {}^{c\,(2)}B_1(r) = \frac{4M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j' \; {}^{c\,(2)}U_k \; \gamma'^{\,2}_{ijk}\, (\pi/X_{ijk})^{3/2}$$

$$\times\, \text{Exp}(-({}^{c\,(2)}\mu_k - \lambda'_{ijk}\, \gamma^{2}_{ijk})r^2) \qquad \ldots \text{(VI.1.8)}$$

(VI.2.) THE COULOMB TERM

The term for the coulomb force is given by:

$$ {}^{coul\,S'}D_{J\ell' M(s-D)}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell,S} \sum_{m,m'} C_{\ell' S'}(J\,M;m'\,M-m')\; C_{\ell S}(J\,M;m\,M-m)$$

$$\times \int d\underline{R}\; d\Omega(\theta,\phi)\; Y^{\ell' *}_{m'}(\theta,\phi)\; \phi_s(R) \langle X^{S'}_{M-m'}(1,\overline{23}) | \frac{e^2}{(|\underline{r}-\tfrac{1}{2}\underline{R}|)}\; S_{23}(\underline{R}^2)$$

$$\times\, | X^{S}_{M-m}(2,\overline{13}) \rangle\, Y^{\ell}_{m}(\theta,\phi)\; \phi_D(R)\; \frac{1}{r}\; f^{S}_{J\ell M}(r) \qquad \ldots \text{(VI.2.1)}$$

We define the function $\overset{coul}{V}(|\underline{r} - \tfrac{1}{2}\underline{R}|) = \dfrac{e^2}{(|\underline{r} - \tfrac{1}{2}\underline{R}|)}$

which is expanded. Thus

$$\overset{coul}{V}(|\underline{r} - \tfrac{1}{2}\underline{R}|) = \sum_{n,p} \overset{coul}{B}_n(r,R)\, Y_p^{*n}(\theta_R,\phi_R)\, Y_p^{n}(\theta,\phi) \qquad \ldots \quad (VI.2.2)$$

where

$$\overset{coul}{B}_n(r,R) = 2\pi \int_{-1}^{+1} d\mu\, p_n(\mu)\, \overset{coul}{V}(|\underline{r} - \tfrac{1}{2}\underline{R}|) \qquad \ldots \quad (VI.2.3)$$

Using (VI.2.2) in (VI.2.1) and adopting the same procedure, used in evaluating the central term, we finally get

$$\overset{coul}{\underset{J\ell' M(s-D)}{\overset{S'}{D(r)}}} = \sum_{\ell} \overset{coul}{B}_2(r)\, A(\ell' 3/2\, ;\, \ell 3/2)\, \underset{J\ell M}{\overset{3/2}{f(r)}} \ldots \quad (VI.2.4)$$

where

$$\overset{coul}{B}_2(r) = \frac{M e^2}{4\hbar^2 r^3} \sum_{i,j=1}^{2} A_i A'_j \frac{1}{(\alpha_i + \alpha'_j)^2} (\pi/(\alpha_i + \alpha'_j))^{3/2} \qquad \ldots \quad (VI.2.5)$$

(VI.3.) THE TENSOR TERM

The direct term of the tensor force in the doublet and quartet states is given by:

$$ {}^{t\ S'}D_{J\ell' M(s-D)}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m) $$

$$ \times\int d\underline{R}\ d\Omega(\theta,\phi)\ Y^{\ell'*}_{m'}(\theta,\phi)\ \phi_s(R)\ {}^{t\ (II)}V(\underline{r}_{12}) < X^S_{M-m'}(1,\overline{23})|S_{12}(\underline{r}^2_{12}) $$

$$ \times|X^S_{M-m}(1,\overline{23})> Y^{\ell}_{m}(\theta,\phi)\ \phi_D(R)\ \frac{1}{r}\ f^S_{J\ell M}(r) \qquad \ldots \quad (VI.3.1) $$

where

$$ {}^{t\ (II)}V(\underline{r}_{12}) = \sum \frac{1}{4}(2w - h + 2b - m)_\nu\ {}^\nu V_t(\underline{r}_{12}) $$

$$ = S_{12}(\underline{r}^2_{12}) \sum_{k=1}^{2} {}^{t\ (II)}U_k\ \mathrm{Exp}(-{}^{t\ (II)}\mu_k\ \underline{r}^2_{12}) $$

The spin matrix elements of the double operators $S_{12}(\underline{r}^2_{12})$ and $S_{23}(\underline{R}^2)$ can be reduced to a simple form, and we consider two distinct cases (i.e. the doublet and quartet states, in which $S=\frac{1}{2}$ and $S=3/2$ respectively).

(VI.3.2) THE DOUBLET STATE

We write

$$ <X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\ S_{12}(\underline{r}^2_{12})\ S_{23}(\underline{R}_2)\ {}^{t\ (1)}V(\underline{r}_{12})\ \phi_D(R)|X^{\frac{1}{2}}_{M-m}(1,\overline{23})> $$

$$ = \sum_{k,j=1}^{2} {}^{t\ (1)}U_k\ A'_j\ \mathrm{Exp}(-{}^{t\ (1)}\mu_k\ \underline{r}^2_{12} - \alpha_j R^2) $$

$$ \times<X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\ W_{12}(\underline{r}^2_{12})\ W_{23}(\underline{R}^2)|X^{\frac{1}{2}}_{M-m}(1,\overline{23})> \qquad \ldots \quad (VI.3.2a) $$

where

$$W_{ij}(\underline{A},\underline{B}) = 3(\underline{\sigma}_1 \cdot \underline{A})(\underline{\sigma}_j \cdot \underline{B}) - (\underline{\sigma}_i \cdot \underline{\sigma}_j)(\underline{A}\cdot\underline{B}) \quad \ldots \quad (VI.3.2b)$$

The spin elements of the double operotors $W_{12}(\underline{r}_{12}^2)$ and $W_{23}(\underline{R}^2)$ are further reduced. Thus,

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})| W_{12}(\underline{r}_{12}^2)\, W_{23}(\underline{R}^2) |X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle = \langle X^{\frac{1}{2}}_{M-m'}(1,23)|$$

$$\times \Big[- 3R^2\, (i\, \underline{\sigma}_1 \cdot \underline{r}\wedge\underline{R}) + 6(i\, \underline{\sigma}_1 \cdot \underline{r}\wedge\underline{R})(\underline{r}\cdot\underline{R}) + 2\, r^2R^2 + 4R^2(\underline{r}\cdot\underline{R})$$

$$- 6(\underline{r}\cdot\underline{R})(\underline{r}\cdot\underline{R}) - R^4 \Big] |X^{\frac{1}{2}}_{M-m}(1,23)\rangle \quad \ldots \quad (VI.3.2c)$$

Using (VI.3.2c) and putting

$$\overset{t\ (1)}{V}(\underline{r},\underline{R}) = \frac{4M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j'\ \mathrm{Exp}(- \overset{t\ (1)}{\mu_k}\ \underline{r}_{12}^2) \Big[- 3R^2(i\ \underline{\sigma}_1\cdot\underline{r}\wedge\underline{R})$$

$$+ 6(i\ \underline{\sigma}_1 \cdot \underline{r}\wedge\underline{R})(\underline{r}\cdot\underline{R}) + 2\, r^2R^2 + 4R^2(\underline{r}\cdot\underline{R}) - 6(\underline{r}\cdot\underline{R})(\underline{r}\cdot\underline{R}) - R^4 \Big]$$

$$\times\ \mathrm{Exp}(-(\alpha_i + \alpha_j')R^2) \quad \ldots \quad (VI.3.3)$$

Then from (VI.3.1) we get:

$$\overset{t\ S'}{D}_{J\ell' M(s-D)}(r) = \int_0^\infty R^2\, dR\ \ d\Omega_R(\theta_R,\phi_R) \int d\Omega(\theta,\phi)\ \overset{\ell'}{Y}{}^*_{m'}(\theta,\phi)\ V(\underline{r},\underline{R})$$

$$\ldots \quad (VI.3.4)$$

The function $\overset{t\ (1)}{V}(r,R)\ Y^*_{\mu}(\theta_R,\phi_R)$ may now be expanded

$$\overset{t\ (1)}{V}(\underline{r},\underline{R}) = \sum_{\lambda,\mu} \overset{t\ (1)}{V}(r,R)\ \overset{\lambda}{Y}{}^*_{\mu}(\theta_R,\phi_R)\ \overset{\lambda}{Y}_{u}(\theta,\phi) \quad \ldots \quad (VI.3.5)$$

where

$$\overset{t}{V}\overset{(1)}{}(r,R) = 2 \int_{-1}^{+1} d\mu \; p_{\lambda}(\mu) \; \overset{t}{V}\overset{(1)}{}(\underline{r},\underline{R}) \qquad \ldots \quad (VI.3.6)$$

Using (VI.3.5) and performing the integration over $d\Omega(\Theta,\phi)$ and dR, then from (VI.3.4) we finally obtain:

$$\overset{t}{D}\overset{S'}{}_{J\ell' M(s-D)}(r) = \sum_{\ell} \overset{t}{B}\overset{(1)}{}_2(r) \; f^{\frac{1}{2}}_{J\ell M}(r)\,\delta(\ell',\ell) \qquad \ldots \quad (VI.3.7)$$

where

$$\overset{t}{B}\overset{(1)}{}_2(r) = \frac{4M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i A'_j \; \overset{T}{U}\overset{(1)}{}_k \; (\pi/\lambda'_{ijk})^{3/2} \; Exp(-\overset{T}{\mu}\overset{(1)}{}_k \, (1-\frac{\overset{T}{\mu}\overset{(1)}{}_k}{4\lambda'_{ijk}})r^2)$$

$$x\left[-\frac{15}{4\lambda^2_{ijk}} + 10\,\frac{\gamma'_{ijk}}{\lambda'_{ijk}}\,(1-\tfrac{1}{2}\,\gamma'_{ijk})\, r^2 - 4\,\gamma'^2_{ijk}\,(1-\tfrac{1}{2}\,\gamma'_{ijk})^2\, r^2 \right]$$

$$\ldots \quad (VI.3.8)$$

<u>(VI.3.9) THE QUARTET STATE</u>

The matrix elements of the operators $W_{12}(\underline{r}^2_{12})$ and $W_{23}(\underline{R}^2)$ are written in the following way

$$< X^{3/2}_{M-m'}(1,\overline{23})|\; W_{12}(\underline{r}^2_{12})\; W_{23}(\underline{R}^2)|X^{3/2}_{M-m}(1,\overline{23})> = < X^{3/2}_{M-m'}(1,\overline{23})|$$

$$x\left[3(i\;\underline{\sigma_1}\cdot\underline{r}\wedge\underline{R})\; W_{23}(\underline{r},\underline{R}) - \frac{3}{2}\,(i\;\underline{\sigma_1}\cdot\underline{r}\wedge\underline{R})\; W_{23}(\underline{R}^2) - R^2\; W_{23}(\underline{r}^2)\right.$$

$$+ \frac{1}{4}\,(R^2 - 4\,r^2 - 2\,\underline{r}\cdot\underline{R})\; W_{23}(\underline{R}^2) - \frac{1}{2}\,(R^2 - 6\underline{r}\cdot\underline{R})\; W_{23}(\underline{r},\underline{R})$$

$$+ \left[3(\underline{r}\cdot\underline{R})(\underline{r}\cdot\underline{R}) - r^2R^2 + \frac{1}{2}\,R^4 - 2\,R^2(\underline{r}\cdot\underline{R}) \right] + 3(\underline{r}\cdot\underline{R})(i\;\underline{\sigma_1}\cdot\underline{r}\wedge\underline{R})$$

$$- \frac{3}{2} R^2 (i\, \underline{\sigma}_1 \cdot \underline{r} \wedge \underline{R}) \Big] \Big| X^{3/2}_{M-m} (1,\overline{23}) \Big\rangle \qquad \ldots \quad (VI.3.9a)$$

substituting(VI.3.9a) into (VI.3.1) and working out all terms involved, the following expression for the direct interaction in the quartet state was finally obtained:

$$\overset{t}{D}{}^{S'}_{J\ell' M(s-D)}(r) = \sum_{\ell} \overset{t}{B}{}^{(2)}_{2}(r)\, f^{3/2}_{J\ell M}(r)\, \delta(\ell',\ell) \qquad \ldots \quad (VI.3.10)$$

where

$$\overset{t}{B}{}^{(2)}_{2}(r) = \frac{4M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j'\, \overset{t}{U}{}^{(2)}_{k} (\pi / \lambda'_{ijk})^{3/2}$$

$$\times \mathrm{Exp}(- \overset{t}{\mu}{}^{(2)}_{k} (1 - \frac{\overset{t}{\mu}{}^{(2)}_{k}}{4\lambda'_{ijk}})) \Big[A(\ell' 3/2\ ;\ \ell 3/2) \Big[\gamma'^2_{ijk} (1 - \tfrac{1}{2} \gamma'^2_{ijk}) r^4$$

$$- \frac{7}{4} \frac{\gamma_{ijk}}{\lambda'_{ijk}} (1 - \tfrac{1}{2} \gamma'_{ijk}) r^2 \Big] + 2 \gamma'^2_{ijk} (1 - \tfrac{1}{2} \gamma'_{ijk})^2 r^4 - \frac{5r^2}{\lambda'_{ijk}}$$

$$\times \gamma'_{ijk} (1 - \tfrac{1}{2} \gamma'_{ijk}) + \frac{15}{8\lambda^2_{ijk}} \Big] \qquad \ldots \quad (VI.3.11)$$

(VI.4.) THE SPIN-ORBIT TERM

The expression representing the spin-orbit interaction is given below by:

$$\overset{s.o}{D}{}^{S'}_{J\ell' M(s-D)}(r) = \frac{4Mr}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m)$$

$$\times \int d\underline{R}\; d\Omega(\theta,\phi)\; \phi_S(R)\; \overset{\ell'*}{\underset{m'}{Y}}(\theta,\phi) < X^{S'}_{M-m'}(1,\overline{23}) \Big|^{s.o\,(II)} V(|\underline{r} - \tfrac{1}{2}\underline{R}|)$$

$$\times \left[\tfrac{1}{4}(\underline{\sigma}_1 + \underline{\sigma}_2).\overleftrightarrow{L}_{(12)} S_{23}(R^2) \right] |X^S_{M-m}(1,\overline{23})> \phi_D(R)\; \overset{\ell}{\underset{m}{Y}}(\theta,\phi)\; \frac{1}{r}\, f^S_{J\ell M}(r)$$

$$(II = 1,2) \quad \ldots \quad (VI.4.1)$$

Where $S_{23}(\underline{R}^2)$ is a tensor operator defined in

(I.2.6) and $\overleftrightarrow{\underline{L}}_{(12)} = \overrightarrow{\underline{L}}_{12} - \overleftarrow{\underline{L}}_{12}$. ... (VI.4.2)

also

$$\overrightarrow{\underline{L}}_{12} = \frac{1}{i}(\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \left(\frac{3}{2}\frac{\overrightarrow{\partial}}{\partial \underline{r}} - \frac{\overrightarrow{\partial}}{\partial \underline{R}}\right) \quad \ldots \quad (VI.4.3)$$

and

$$\overleftarrow{\underline{L}}_{12} = \frac{1}{i}\left(\frac{3}{2}\frac{\overleftarrow{\partial}}{\partial \underline{r}} - \frac{\overleftarrow{\partial}}{\partial \underline{R}}\right) \wedge (\underline{r} - \tfrac{1}{2}\underline{R}) \quad \ldots \quad (VI.4.4)$$

We represent the factors $\phi_S(R)\; V(|\underline{r} - \tfrac{1}{2}\underline{R}|)\; \phi_D(R)$ by Gaussian functions. Thus

$$\sum_{i,j=1}^{2} A_i A'_j \left(-\frac{1}{4}\right) \mathrm{Exp}(-\alpha_i R^2)\; V^{s.o(1)}(|\underline{r} - \tfrac{1}{2}\underline{R}|) \left[(\underline{\sigma}_1 + \underline{\sigma}_2).(\overrightarrow{\underline{L}}_{12} - \overleftarrow{\underline{L}}_{12})\right]$$

$$\times W_{23}(\underline{R}^2)\, \mathrm{Exp}(-\alpha'_j R^2) = \sum_{i,j=1}^{2} A_i A'_j \left(-\frac{3}{4}\right) \mathrm{Exp}(-\alpha_i R^2)\; V^{s.o}(|\underline{r} - \tfrac{1}{2}\underline{R}|)$$

$$\times \left[i\,(\underline{\sigma}_1 + \underline{\sigma}_2).(\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\overrightarrow{\partial}}{\partial \underline{r}} - \frac{1}{3}\, i(\underline{\sigma}_1 + \underline{\sigma}_2).(\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\overrightarrow{\partial}}{\partial \underline{R}} \right.$$

$$\left. + \frac{1}{3}\, i(\underline{\sigma}_1 + \underline{\sigma}_2).\frac{\overleftarrow{\partial}}{\partial \underline{R}} \wedge (\underline{r} - \tfrac{1}{2}\underline{R}) \right] W_{23}(\underline{R}^2)\, \mathrm{Exp}(-\alpha_j R^2)$$

$$\ldots \quad (VI.4.4)$$

Evaluating the above expression leads to the following terms:

$$(-\tfrac{3}{4})\ \phi_s(R)\ \overset{s.o\ (II)}{V}(|\underline{r} - \tfrac{1}{2}\underline{R}|)\ \phi_D(R)\Big[\ S_{23}(\underline{R}^2)(\underline{\sigma}_1\cdot\underline{L}) + \frac{3}{R^2}$$

$$\times\ (\underline{\sigma}_3\cdot\underline{R})(\underline{R}\cdot\underline{L}) + \frac{3}{R^2}(i\ \underline{L}\wedge\underline{R}\cdot\underline{\sigma}_2)(\underline{\sigma}_3\cdot\underline{R}) - (\underline{o}_3\cdot\underline{L})$$

$$+\ (i\ \underline{L}\cdot\underline{\sigma}_2\wedge\underline{\sigma}_3) + (\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_3\cdot\underline{R}) + \frac{1}{2}(\underline{\sigma}_2\cdot\underline{R})(\underline{\sigma}_3\cdot\frac{\partial}{\partial\underline{r}}) - \frac{1}{2}$$

$$\times\ S_{23}(\underline{R}^2)(\underline{R}\cdot\frac{\partial}{\partial\underline{r}}) - \frac{1}{2}(\underline{R}\cdot\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_2\cdot\underline{\sigma}_3) + \frac{1}{2}(i\ \underline{\sigma}_3\cdot\underline{R}\wedge\frac{\partial}{\partial\underline{r}}) - \frac{1}{2}$$

$$\times\ S_{23}(\underline{R}^2)(i\ \underline{\sigma}_1\cdot\underline{R}\wedge\frac{\partial}{\partial\underline{r}}) + \frac{2}{3}(i\ \underline{\sigma}_1\cdot\underline{r}\wedge\underline{R})\ S_{23}(\underline{R}^2) - \frac{2}{3}\alpha'_j$$

$$\times\ (i\ \underline{\sigma}_3\cdot\underline{r}\wedge\underline{R}) + \frac{1}{3R^2}(i\ \underline{\sigma}_1\wedge\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_3\cdot\underline{R}) - \frac{1}{6R^2}(i\ \underline{R}\cdot\underline{\sigma}_1\wedge\underline{\sigma}_2)$$

$$\times\ (\underline{\sigma}_3\cdot\underline{R}) + \frac{1}{3R^2}(i\ \underline{r}\cdot\underline{\sigma}_1\wedge\underline{\sigma}_3)(\underline{\sigma}_2\underline{R}) - \frac{1}{6R^2}(i\underline{R}\cdot\underline{\sigma}_1\wedge\underline{\sigma}_3)(\underline{\sigma}_2\cdot\underline{R})$$

$$+\ \frac{1}{3R^2}(i\ \underline{\sigma}_3\cdot\underline{r}\wedge\underline{R}) - \frac{1}{3R^2}(\frac{2}{3}\alpha'_j R^2 + \frac{2}{3})\ W_{23}(\underline{r},\underline{R}) - \frac{1}{9R^2}(\underline{r},\underline{R})(\underline{\sigma}_2\cdot\underline{\sigma}_3)$$

$$+\ \frac{2}{9}(\alpha'_j R^2 + 2\alpha_i + \frac{3}{2})\ S_{23}(\underline{r},\underline{R}) + \frac{1}{3}(\underline{\sigma}_2\cdot\underline{\sigma}_3) + \frac{2}{3R^2}(i\ \underline{\sigma}_2\cdot\underline{r}\wedge\underline{R})$$

$$+\ \frac{2}{3}\alpha_i(i\ \underline{\sigma}_3\cdot\underline{r}\wedge\underline{R}) - \frac{2}{3}\ {}_i(i\ \underline{\sigma}_1\cdot\underline{r}\wedge\underline{R})\ S_{23}(\underline{R}^2) - \frac{2}{9}\alpha_i(\underline{r}\cdot\underline{R} - R^2)$$

$$\times\ S_{23}(\underline{R}^2)\ \Big] \qquad \ldots \quad (VI.4.5)$$

We now consider two distinct cases (namely, the doulet and quartet states):

(VI.4.6) THE DOUBLET CASE

Proceeding with the analysis, we make use of the fact that the spin functions in this case help to reduce various products of equation (VI.4.5) as follows:

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\, S_{23}(\underline{R}^2)(\underline{\sigma}_1\cdot\underline{L})\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle = \frac{4}{3}\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,\underline{\sigma}_1\cdot\underline{L}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\, W_{23}(\underline{R}^2)(\underline{\sigma}_1\cdot\underline{L})\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle = \frac{4R^2}{3}\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,\underline{\sigma}_1\cdot\underline{L}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\,(\underline{\sigma}_1\wedge\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_3\cdot\underline{B})\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle = -\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,\underline{\sigma}_1\cdot\underline{A}\wedge\underline{B}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

$$= 0 \text{ if } \underline{A} = \underline{B}$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\,(\underline{\sigma}_2\wedge\underline{\sigma}_3\cdot\underline{A})(\underline{\sigma}_2\cdot\underline{B})\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle = -\langle X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})|\,\underline{\sigma}_1\cdot\underline{A}\wedge\underline{B}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

$$= 0 \text{ if } \underline{A} = \underline{B}$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\,\underline{\sigma}_1\cdot\underline{L}\,|X^{\frac{1}{2}}_{M-m'}(1,\overline{23})\rangle = -\frac{1}{3}\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,\underline{\sigma}\cdot\,\underline{L}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\,\underline{\sigma}_3\cdot\underline{L}\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle = \frac{2}{3}\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,\underline{\sigma}_1\cdot\,\underline{L}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

and finally

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|\,(\underline{\sigma}_2\cdot\,\underline{A})\,(\underline{\sigma}_3\cdot\,\underline{B})\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle$$
$$= -\underline{A}\cdot\underline{B} - \frac{2}{3}\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,i\underline{\sigma}_1\cdot\underline{A}\wedge\underline{B}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

Using the above results, all terms in (IV.4.5) were calculated. Thus, the direct spin-orbit interaction term in the doublet state is finally given by the following expression

$$\overset{s.o\ S'}{D}_{J\ell' M(s-D)}(r) = \sum_{\ell} \overset{s.o\ (1)}{B_2}(r)\, A_{J\ell}\, f^{\frac{1}{2}}_{J\ell M}(r)\, \delta(\ell',\ell) \quad \ldots \quad (VI.4.6)$$

where

$$\overset{s.o\ (1)}{U_4}(r) = \frac{M\ \pi^{3/2}}{4\ \hbar^2} \sum_{i,j,k=1}^{2} A_i A'_j \overset{s.o\ (1)}{U_k} \lambda^{-5/2}_{ijk}$$

$$\times \left[\overset{s.o\ (1)}{\mu_k} (1 - \tfrac{1}{2}\gamma'_{ijk})\, r^2 - \tfrac{5}{2} \right] Exp(-(\overset{s.o\ (1)}{\mu_k} - \lambda'_{ijk}\gamma'_{ijk})r^2)$$

$$\ldots \quad (VI.4.7)$$

(VI.4.8) THE QUARTET CASE

Starting from equations (VI.4.1) and (VI.4.5), the direct interaction term of the spin-orbit force is finally given by:

$$\overset{s.o\ S'}{D}_{J\ell' M(s-D)}(r) = \sum_{\ell} \left[\overset{s.o\ 1}{B_2}(r)\, A_{J\ell}\, \delta(\ell',\ell) + \overset{s.o\ 2}{B_2}(r)\, A(\ell' 3/2;\ell 3/2) \right.$$

$$\left. + \overset{s.o\ 3}{B_2}(r)\, E_1(\ell' 3/2;\ell 3/2) \right] f^{3/2}_{J\ell M}(r) \quad \ldots \quad (VI.4.8.1)$$

where

$$\overset{s.o\ 1}{B_2}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \overset{s.o}{U_k} (\pi/\lambda'_{ijk})^{3/2} \left[\frac{7}{8} \frac{\gamma'_{ijk}}{\lambda'_{ijk}} \right.$$

$$\left. - \frac{1}{2}(1-\tfrac{1}{2}\gamma'_{ijk})\, \gamma'_{ijk}\, r^2 \right] Exp(-\overset{s.o}{\mu_k} r^2 + \frac{\overset{s.o\ 2}{\mu}\ r^2}{4})$$

$$\ldots \quad (VI.4.8.2)$$

$$\overset{s.o\ 2}{B_2}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A'_j \overset{s.o}{U_k} (\alpha_i + \alpha'_j) \frac{\gamma'_{ijk}}{\lambda'_{ijk}} (\pi/\lambda'_{ijk})^{3/2}$$

$$\times \, \mathrm{Exp}\left(- \overset{s.o}{\mu_k} r^2 + \frac{\overset{s.o}{\mu_k}{}^2 r^2}{4}\right) \quad \ldots \quad (VI.4.8.3)$$

and

$$\overset{s.o}{B_2}{}^3(r) \frac{Mr^2}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j' \overset{s.o}{\mu_k} \gamma'^2_{ijk} (1 - \tfrac{1}{2} \gamma'_{ijk})$$

$$\times \, (\pi / \lambda'_{ijk})^{3/2} \, \mathrm{Exp}\left(- \overset{s.o}{\mu_k} r^2 + \frac{\overset{s.o}{\mu_k}{}^2 r^2}{4_{ijk}}\right) \quad \ldots \quad (VI.4.8.4)$$

we also have

$$E_1(\ell 3/2; \ell 3/2) = 40 \left(\frac{\ell(\ell+1)(2\ell'+1)}{15} \right)^{\frac{1}{2}} (-1)^{\ell} (2\ell+1) \, C_{\ell\ell'}(2)$$

$$\times \, W(\ell 3/2; \ell 3/2; J2) \, W(\ell 3/2; \ell 3/2; J1) \quad \ldots \quad (VI.4.8.5)$$

CHAPTER VII

THE ENERGY TERMS (s-D) INTERACTION

The contribution of both the W-, and the kinetic energy terms in the integro-differential equations are given below:

(VII.1.) THE W-KERNEL

This kernel contributes in the quartet state only and is given by the following expression:

$$W^{S'}_{J\ell' M(s-D)}(r) = (4/3)^4 \frac{Mr}{\hbar^2} (E_p - E_d) \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m')$$

$$\times\ C_{\ell 3/2}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ Y^{\ell' *}_{m'}(\theta,\phi)\ \phi_s(u) \langle X^{3/2}_{M-m'}\ 1,\overline{23})|$$

$$\times\ S_{13}(\underline{V}^2)|X^{3/2}_{M-m}(1,\overline{23})\rangle\ \phi_D(V)\ Y^{\ell}_{m}(\theta',\phi')\ \frac{1}{r'}\ f^{3/2}_{J\ell M}(r') \quad \ldots \quad (VII.1.1)$$

After working out the spin elements of the tensor $S_{13}(\underline{r}^2)$ and then performing the angular integration and the sums over all magnetic quantum numbers one obtains:

$$W^{S'}_{J\ell' M(s-D)}(r) = \sum_{\ell} \int_0^{\infty} dr'\ A(\ell' 3/2;\ell 3/2)\ f^{3/2}_{J\ell M}(r') \Big[\ {}^{w\,1}e_2(r,r')$$

$$\times\ I_{\ell+\frac{1}{2}}(b'_{ij}\ rr') + {}^{w\,2}e_2(r,r')\ I_{\ell'+\frac{1}{2}}(b'_{ij}\ rr') + \sum_{L} {}^{w\,3}e_2(r,r')$$

$$\times\ FF(\ell'\ell;L)\ I_{L+\frac{1}{2}}(b'_{ij}\ rr')\ \Big] \quad \ldots \quad (VII.1.2)$$

where

$$ {}^{w\,1}e_2(r,r') = (4/3)^4 \frac{32\pi M}{9\hbar^2} \; r^3 r' (E_p - E_d) \sum_{i,j=1}^{2} A_i A_j' $$

$$ \times\ (2\pi/b_{ij}'\,rr')^{\frac{1}{2}}\ \mathrm{Exp}(-\ e_{ij}'\ r^2 - f_{ij}'\ r'^2) \qquad \ldots \quad (\mathrm{VII.1.3}) $$

$$ {}^{w\,2}e_2(r,r') = (4/3)^4 \frac{8\pi M}{9\hbar^2} \; rr'^3 (E_p - E_d) \sum_{i,j=1}^{2} A_i A_j' \ (2\pi/b_{ij}'\ rr')^{\frac{1}{2}} $$

$$ \times\ \mathrm{Exp}(-\ e_{ij}'\ r^2 - f_{ij}'\ r'^2) \qquad \ldots \quad (\mathrm{VII.1.4}) $$

and

$$ {}^{w\,3}e_2(r,r') = (4/3)^4 \frac{16\pi M}{9\hbar^2} \ (rr')^2 \ (E_p - E_d) \sum_{i,j=1}^{2} A_i A_j' $$

$$ \times\ (2\pi/b_{ij}'\ rr')^{\frac{1}{2}}\ \mathrm{Exp}(-\ e_{ij}'\ r^2 - f_{ij}'\ r'^2) \qquad \ldots \quad (\mathrm{VII.1.5}) $$

(VII.2.) THE KINETIC ENERGY TERM

This is given in the quartet state only by the following expression:

$$ {}_{T}{}^{S'}{}_{J\ell' M(s-D)}(r) = {}^{(1)}{}_{T}{}^{S'}{}_{J\ell' M(s-D)}(r) + {}^{(2)}{}_{T}{}^{S'}{}_{J\ell' M(s-D)}(r) \qquad \ldots \quad (\mathrm{VII.2.1}) $$

where

$$ {}^{(1)}{}_{T}{}^{S'}{}_{J\ell' M(s-D)}(r) = (4/3)^3 \int d\underline{r}'\ r \int d\Omega(\theta,\phi) \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'M-M') $$

$$\times\, C_{\ell 3/2}(J\ M;m\ M-m)\ Y_{m'}^{\ell'*}(\theta,\phi) < X_{M-m'}^{3/2}(1,\overline{23}) \big| \tfrac{1}{2}(\nabla_{r'}^{2} + \nabla_{r}^{2})$$

$$\times \Big[\phi_s(u)\ S_{13}(V^2)\ \phi_D(V) \Big] \big| X_{M-m}^{3/2}(2,\overline{13}) > Y_{m}^{\ell}(\theta,\phi)\ \frac{1}{r'}\ f_{J\ell M}^{3/2}(r')$$

... (VII.2.2)

Which after operating by $\nabla_{r'}^2$ and ∇_r^2 becomes

$$(1)\ S_{J\ell' M(s-D)}^{'T}(r) = (4/3)^4 \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m')\ C_{\ell 3/2}(J\ M;m\ M-m)$$

$$\times \int_0^{\infty} r' r\, dr' \int d\Omega(\theta,\phi) \int d\Omega'(\theta',\phi')\ \phi_s(u)\ Y_{m'}^{\ell'*}(\theta,\phi)\left(1/3V^2\right)$$

$$\times < X_{M-m'}^{3/2}(1,\overline{23}) \big| \Big[(10\alpha_i^{2}\ u^2 + 10\alpha_j'^{2}\ V^2 + 16\alpha_i\ \alpha_j'\ \underline{u}\cdot\underline{V} - 15\alpha_i - 35\alpha_j')$$

$$\times\, W_{13}(\underline{V}^2) - 16\alpha_i\ W_{13}(\underline{u},\underline{V}) \Big] \big| X_{M-m}^{3/2}(2,\overline{13}) > \phi_D(V)\ Y_{m}^{\ell}(\theta',\phi')\ f_{J\ell M}^{3/2}(r')$$

... (VII.2.3)

and

$$(2)\ S_{J\ell' M(s-D)}^{'T}(r) = -(4/3)^4 \sum_{\ell} C_{\ell' 3/2}(J\ M;m'\ M-m')\ C_{\ell 3/2}(J\ M;m\ M-m)$$

$$\times \int r\, d\underline{r}'\ d\Omega(\theta,\phi)\ Y_{m'}^{\ell'*}(\theta,\phi) < X_{M-m'}^{3/2}(1,\overline{23}) \big| \Big[\tfrac{1}{2} \Big[\nabla_u^2\ \phi_s(u)\Big]$$

$$\times\, S_{13}(\underline{V}^2)\ \phi_D(V) + \tfrac{1}{2}\ \phi_s(u) \Big[\nabla_V^2\ S_{13}(\underline{V}^2)\ \phi_D(V)\Big]\Big] \big| X_{M-m}^{3/2}(2,\overline{13}) >$$

$$\times\, Y_{m}^{\ell}(\theta',\phi')\ \frac{1}{r'}\ f_{J\ell M}^{3/2}(r') = -(4/3)^4 \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m')$$

$$\times\, C_{\ell 3/2}(J\ M; m\ M-m) \int_0^\infty dr'\ (rr') \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi)\ \phi_s(u)$$

$$\times\, Y^{\ell'*}_{m'}(\theta,\phi)\ \frac{1}{V^2} \langle X^{3/2}_{M-m'}(1,\overline{23}) \big| (2\alpha_i^2 u^2 + 2\alpha_j'^2 V^2 - 3\alpha_i - 7\alpha_j')\ W_{13}(\underline{V}^2)$$

$$\times\, \big| X^{3/2}_{M-m}(2,\overline{13}) \rangle\ Y^{\ell}_{m}(\theta',\phi')\ \phi_D(V)\ f^{3/2}_{J\ell M}(r') \qquad \ldots \quad (VII.2.4)$$

From (VII.2.3) and (VII.2.4), the total kernel is finally written as:

$$T^{S'}_{J\ell' M(s-D)}(r) = \sum_{\ell} \int_0^\infty dr'\ (rr')\ f^{3/2}_{J\ell M}(r')\ A(\ell' 3/2;\ell 3/2) \Big[\ {}^{T1}e_2(r,r')$$

$$\times\, I_{\ell+\frac{1}{2}}(b'_{ij}\ rr) + {}^{T2}e_2(r,r')\ I_{\ell+3/2}(b'_{ij}\ rr') + {}^{T1}e_3(r,r')\ I_{\ell'+\frac{1}{2}}(b'_{ij} rr')$$

$$+\ {}^{T2}e_3(r,r')\ I_{\ell'+3/2}(b'_{ij}\ rr') + \sum_{L} FF(\ell',\ell;L) \Big[\ {}^{T1}e_4(r,r')$$

$$\times\, I_{n+\frac{1}{2}}(b'_{ij} rr) + {}^{T2}e_4(r,r')\ I_{n+3/2}(b'_{ij}\ rr')\ \Big]\Big] \qquad \ldots \quad (VII.2.5)$$

where

$${}^{T1}e_2(r,r') = (4/3^5\ 2 \sum_{i,j=1}^{2} A_i A'_j\ (2\pi/{}_1b'_{ij}\ rr')^{\frac{1}{2}}$$

$$\times\, \mathrm{Exp}(-\ e'_{ij} r^2 - f'_{ij}\ r'^2) \Big[\ W'_{ij}\ r^2 + \Psi'_{ij}\ r'^2 - \frac{56}{9}\alpha_i - \frac{56}{9}\alpha'_j$$

$$+\ 16\ \frac{\phi'_{ij}}{{}_1b'_{ij}}\ (\frac{2\ell+1}{2} - rr')\ \Big] \qquad \ldots \quad (VII.2.6)$$

$${}^{T2}e_2(r,r') = (4/3)^5\ 32 \sum_{i,j=1}^{2} A_i A'_j\ (2\pi/{}_1b'_{ij} rr')^{\frac{1}{2}}$$

$$\times\, \mathrm{Exp}(-\ e'_{ij}\ r^2 - f'_{ij}\ r'^2)\ \frac{\phi'_{ij}}{{}_1b'_{ij}} \qquad \ldots \quad (VII.2.7)$$

$$T_{e_3}^{1}(r,r') = (4/3)^5\, 2 \sum_{i,j=1}^{2} A_i A_j \,(2\pi/{}_1b'_{ij}rr')^{\frac{1}{2}}\, \mathrm{Exp}(-e'_{ij}r^2 - f'_{ij}\, r^2)$$

$$\times \left[W'_{ij}\, r^2 + \psi'_{ij}\, r'^2 - \frac{39}{9}\alpha_i - \frac{14}{9}\,\alpha'_j + 4\,\frac{\phi'_{ij}}{{}_1b'_{ij}} \left(\frac{2\ell'+1}{2} - rr'\right)\right]$$

... (VII.2.8)

$$T_{e_3}^{2}(r,r') = (4/3)^5\, 8 \sum_{i,j=1}^{2} A_i A_j \,\frac{\phi'_{ij}}{{}_1b'_{ij}}\, (2\pi/{}_1b'_{ij}\, rr')^{\frac{1}{2}}$$

$$\times\ \mathrm{Exp}(-e'_{ij}r^2 - f'_{ij}r'^2)$$ ... (VII.2.9)

$$T_{e_4}^{1}(r,r') = (4/3)^5\, 2 \sum_{i,j=1}^{2} A_i A_j \,(2\pi/{}_1b'_{ij}rr')^{\frac{1}{2}}$$

$$\times\ \mathrm{Exp}(-e'_{ij}r^2 - f'_{ij}\, r'^2) \left[W'_{ij}r^2 + \psi'_{ij}\, r'^2 - \frac{104}{9}\alpha_i - \frac{56}{9}\,\alpha'_j \right.$$

$$\left. + \frac{16}{{}_1b'_{ij}}\, \phi'_{ij} \left(\frac{2L+1}{2} - rr' \right) \right]$$ ... (VII.2.10)

and

$$T_{e_4}^{2}(r,r') = (4/3)^5\, 32 \sum_{i,j=1}^{2} A_i A_j \,\frac{\phi'_{ij}}{{}_1b'_{ij}}\, (2\pi/{}_1b'_{ij}rr')^{\frac{1}{2}}$$

$$\times\ \mathrm{Exp}(-e'_{ij}\, r^2 - f'_{ij}\, r'^2)$$ ... (VII.2.11)

CHAPTER VIII

THE EXCHANGE TERMS (s-D) INTERACTION

(VIII.1.) THE CENTRAL TERM

The exchange interaction of the central force $E^{c\,S'}_{J\ell' M(s-D)}(r)$ is given by:

$$E^{c\,S'}_{J\ell' M(s-D)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M; m'\ M-m')$$

$$\times\ C_{\ell S}(J\ M; m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi)\ \phi_s(u)\ Y^{\ell'*}_{m'}(\theta,\phi) < X^{S'}_{M-m'}(1,\overline{23})|$$

$$\times \sum_{\upsilon} \frac{1}{4} (W - 2h + b - 2m)_{\upsilon}\ {}^{\upsilon}V_c(t)\ S_{13}(\underline{V}^2)\ |X^{S}_{M-m}(2,\overline{13})> \phi_D(V)$$

$$\times\ Y^{\ell}_{m}(\theta',\phi')\ \frac{1}{r'}\quad f^{S}_{J\ell M}(r') \qquad \ldots \quad (VIII.1.)$$

The spin matrix elements in (VIII.1.1) are evaluated by expressing them in terms of $Y^2_{m',m}(\theta_v,\phi_v)$ harmonics,

The (θ_v,ϕ_v) are then written in terms of the polar angles of $\underline{V} = \frac{2}{3}(\underline{r}' + 2\underline{r})$, (Bransden, Smith and Tate, 1958), thus, we have

$$<X^{S'}_{M-m'}(1,\overline{23})|\,S_{13}(\underline{V}^2)\,|X^{S}_{M-m}(2,\overline{13})> = \overset{-1}{g}(S) \quad (4\pi/5)^{\frac{1}{2}}\ (-1)^{S+M-m'}$$

$$\times\ g(S',S)\ C_{S' S}(2, m'-m;\ m'-M,\ M-m')\ \frac{4}{9V^2} \Big[\ 4r^2\ Y^2_{m'-m}(\theta,\phi) + r'^2\ Y^2_{m',m}(\theta,\phi)$$

$$+ 2\, rr' \, (40\pi/3)^{\frac{1}{2}} \sum_{\eta,\xi} C_{11}(2,m'-m;\xi\eta) \, \overset{1}{Y}_{\eta}(\theta',\phi') \, \overset{1}{Y}_{\xi}(\theta,\phi) \Big] \qquad \ldots \text{(VIII.1.2)}$$

We now define the function $\overset{c\ (I)}{Q}(\underline{r},\underline{r}')$, (I=1,2,3)

$$\overset{c\ (I)}{Q}(\underline{r},\underline{r}') = -(4/3)^4 \frac{M}{\hbar^2} \, \phi_s(u) \, {}^{c}V(t) \, \phi_D(V) \, 4/9V^2$$

$$\left[\begin{array}{ll} 4\, r^2 & (I=1) \\ r'^2 & (I=2) \\ 2\, rr' & (I=3) \end{array} \right. \qquad \ldots \text{(VIII.1.3)}$$

These can also be expanded in harmonics

$$\overset{c\ (I)}{Q}(\underline{r},\underline{r}') = \frac{1}{rr'} \sum_{L,p} \overset{c\ (I)}{p_L}(r,r') \, \overset{L*}{Y}_{p}(\theta',\phi') \, \overset{L}{Y}_{p}(\theta,\phi) \qquad \ldots \text{(VIII.1.4)}$$

where

$$\overset{c\ (I)}{p_L}(r,r') = 2\pi\, rr' \int_{-1}^{+1} d\eta \, P_L(\eta) \, \overset{c\ (I)}{Q}(\underline{r},\underline{r}') \qquad \ldots \text{(VIII.1.5)}$$

Where $p_L(\eta)$ is the legendre polynomial of order L.

Using (VIII.1.2) and (VIII.1.4), and performing the angular integration and then sums over all magnetic quantum numbers, expression (VIII.1.) finally becomes:

$$\overset{c\ 3/2}{E}_{J\ell' M(s-D)}(r) = \sum_{\ell} \int_0^{\infty} dr' \, (rr') \, A(\ell' 3/2;\ell 3/2) \Big[\overset{c\ 1}{e_2}(r,r')$$

$$\times\, I_{\ell+\frac{1}{2}}(C'_{ijk}rr') + \overset{c\ 2}{e_2}(r,r') \, I_{\ell'+\frac{1}{2}}(C'_{ijk}rr') + \overset{c\ 3}{e_2}(r,r') \sum_{L}$$

$$\times\, FF(\ell'\ell;L) \, I_{L+\frac{1}{2}}(C'_{ijk}rr') \Big] \qquad \ldots \text{(VIII.1.6)}$$

where

$$ {}^{c}e_{2}^{I}(r,r') = -\frac{8\pi M}{9\hbar^2}(4/3)^4 \sum_{i,j,k=1}^{2} A_i A_j \, {}^{c(4)}U_k (2\pi/C' rr')^{\frac{1}{2}} $$

$$ \mathrm{Exp}(-a'_{ijk}\, r^2 - b'_{ijk} r'^2) \left[\begin{array}{ll} 4r^2 & (I=1) \\ r'^2 & (I=2) \\ 2rr' & (I=3) \end{array} \right. \qquad \ldots \quad (VIII.1.7) $$

and $FF(\ell';L)$ has been defined previously .

(VIII.2.) THE COULOMB TERM

This is given by:

$$ {}^{coul}E^{S'}_{J\ell' M(s-D)}(r) = -(4/3)^4 \frac{Me^2 r}{\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m') $$

$$ \times\, C_{\ell S}(J\ M;m\ M-m) \int d\underline{r}' \int d\Omega(\theta,\phi)\, Y^{\ell' *}_{m'}(\theta,\phi)\, \phi_s(u) $$

$$ \times \langle X^{S'}_{M-m'}(1,\overline{23}) |\, S_{13}(\underline{V}^2)\, | X^{S}_{M-m}(2,\overline{13}) \rangle \frac{1}{t}\, \phi_D(V)\, Y^{\ell}_{m}(\theta',\phi')\, \frac{1}{r'}\, f^{S}_{J\ell M}(r') $$

$$ = \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\ M;m'\ M-m')\, C_{\ell S}(J\ M;m\ M-m)\, C_{S' S}(2,m'-m;m'-M,M-m) $$

$$ \times\, g(S',S)\, (-1)^{S+M-m'}\, (4\pi/5)^{\frac{1}{2}} \int_0^\infty dr'\, (rr')\, f^{S}_{J\ell M}(r') \int d\Omega(\theta,\phi) $$

$$ \times \int d\Omega'(\theta',\phi')\, Y^{\ell'}_{m'}(\theta,\phi) \Big[G^{(1)}(\underline{r}.\underline{r}')\, Y^{2}_{m'-m}(\theta,\phi) + G^{(2)}(\underline{r},\underline{r}')\, Y^{2}_{m'-m}(\theta',\phi') $$

$$ + (40\pi/3)^{\frac{1}{2}} \sum_{p,q} C_{11}(2,m'-m;p\ q)\, G^{(3)}(\underline{r},\underline{r}')\, Y^{1}_{p}(\theta,\phi)\, Y^{1}_{q}(\theta',\phi') \Big] $$

$$ \times\, Y^{\ell}_{m}(\theta',\phi') \qquad \ldots \quad (VIII.2.1) $$

where

$$\overset{(I)}{G}(\underline{r},\underline{r}') = -(4/3)^4 \frac{Me^2}{h^2} \phi_s(u) \frac{1}{t} \phi_D(V)\, 4/9V^2 \left[\begin{array}{ll} 4r^2 & (I=1) \\ r'^2 & (I=2) \\ 2rr' & (I=3) \end{array}\right. \quad \ldots \quad (VIII.2.2)$$

The $\overset{(I)}{G}(\underline{r},\underline{r}')$ can be expanded

$$\overset{(I)}{G}(r,\underline{r}') = (rr')^{-1} \sum_{\lambda,L} \overset{(I)}{g_L}(r,r') \overset{*L}{Y_\lambda}(\theta',\phi') \overset{L}{Y_\lambda}(\theta,\phi) \quad \ldots \quad (VIII.2.3)$$

so that

$$\overset{(I)}{g_L}(r,r') = 2\pi rr' \int_{-1}^{+1} d\eta\, P_L(\eta)\, \overset{(I)}{G}(\underline{r},\underline{r}') \quad \ldots \quad (VIII.2.4)$$

Using (VIII.2.4) in (VIII.2.1), the angular integration and sums over m', m and are then carried out. Thus,

$$E_{J\ell' M(s-D)}(r) = \sum_{\ell} \int_0^\infty dr'\, A(\ell' 3/2;\ell 3/2)\, f(r') \Big[\overset{coul\,1}{e_2}(r,r') + \overset{coul\,2}{e_2}(r,r')$$

$$\times \sum_L FF(\ell'\ell\,;\,L)\Big] \quad \ldots \quad (VIII.2.5)$$

where

$$\overset{coul\,1}{e_2}(r,r') = -(4/3)^4 \frac{16\pi Me^2}{3\hbar^2} r^3 rr' \sum_{i,j=1}^{2} A_i A_j'\, Exp(-e_{ij}' r^2 - f_{ij}' r'^2)$$

$$\times \int_{-1}^{+1} d\ \ P_\ell(\eta)(r^2+r'^2-2\underline{r}\cdot\underline{r}')^{-\frac{1}{2}} Exp(b_{ij}'\,\underline{r}\cdot\underline{r}') \quad \ldots \quad (VIII.2.6)$$

$$\overset{coul\,2}{e_2}(r,r') = -(4/3)^4 \frac{4\pi Me^2}{3\hbar^2} r'^3 r \sum_{i,j=1}^{2} A_i A_j'\, Exp(-e_{ij}' r^2 - f_{ij}' r'^2)$$

$$\times \int_{-1}^{+1} d\ \ P_{\ell'}(\eta)\, (r^2+r'^2-2\underline{r}\cdot\underline{r}')^{-\frac{1}{2}} Exp(b_{ij}'\underline{r}\cdot\underline{r}') \quad \ldots \quad (VIII.2.7)$$

$$\overset{coul\,3}{e_2}(r,r') = -(4/3)^4 \frac{8\pi M e^2}{3\hbar^2} r^2 r'^2 \sum_{i,j=1}^{2} A_i A_j'\, Exp(-e_{ij}' r^2 - f_{ij}' r'^2)$$

$$\times \int_{-1}^{+1} d\eta \, P_L(\eta) \, (r^2 + r'^2 - 2\underline{r}\cdot\underline{r}')^{-\frac{1}{2}} \, \mathrm{Exp}(b'_{ij}\underline{r}\cdot\underline{r}') \quad \ldots \quad (\mathrm{VIII.2.8})$$

(VIII.3.) THE TENSOR TERM

This term is given by

$$\overset{t}{E}{}^{S'}_{J\ell' M(s-D)}(r) = -(4/3)^4 \frac{M}{h^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\,M;m'\,M-m')$$

$$\times\, C_{\ell S}(J\,M;m\,M-m) \int_0^\infty dr' \,(rr') \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi) \overset{*}{Y}{}^{\ell'}_{m'}(\theta,\phi)$$

$$\times\, \phi_s(u) \langle X^{S'}_{M-m'}(1,\overline{23}) | \overset{t\,(II)}{V(t)} \, S_{12}(t^2) \, S_{13}(V^2) \, \phi_D(V) | X^{S}_{M-m}(1,\overline{23}) \rangle$$

$$\times\, Y^{\ell}_{m}(\theta',\phi') \, f^{S}_{J\ell M}(r') \quad \ldots \quad (\mathrm{VIII.3.1})$$

where

$$\overset{t\,(II)}{V(t)} = \sum_{\nu} \frac{1}{4} (W - 2h + b - 2m)_{\nu}^{\nu} V_T(t) = t^2 \sum_{k=1}^{2} \overset{t\,(II)}{U_k}$$

$$\times\, \mathrm{Exp}(- \overset{t\,(II)}{\mu_k} t^2) \quad \ldots \quad (\mathrm{VIII.3.2})$$

The spin matrix elements of the tensor operators $S_{12}(t^2)$ and $S_{13}(V^2)$ are simplified for the doublet and quartet states separetely as follows:

(VIII.3.a) THE DOUBLET STATE

We have

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23}) | \overset{t\,(3)}{V(t)} \, S_{12}(t^2) \, S_{13}(V^2) \, \phi_D(V) \, | X^{\frac{1}{2}}_{M-m}(2,\overline{13}) \rangle$$

$$= \sum_{j,k=1}^{2} A_j' \, {}^{t}U_k^{(3)}(t) \, \mathrm{Exp}(- {}^{t}\mu_k^{(3)} t^2 - \alpha_j' V^2) \, \langle X^{\frac{1}{2}}_{M-m'} (1,\overline{23}) | W_{12}(t^2)$$

$$\times W_{13}(\underline{V}^2) | X^{\frac{1}{2}}_{M-m} (2,\overline{13}) \rangle = - \frac{16}{81} \sum_{j,k=1}^{2} A_j' \, {}^{t}U_k^{(3)} \, \mathrm{Exp}(- {}^{t}\mu_k^{(3)} t^2 - \alpha_j' V^2)$$

$$\times \langle X^{\frac{1}{2}}_{M-m'} (1,\widehat{23}) | \Big[(16\, r^4 - 34\, r^2 r'^2 + 4\, r'^4) - (16\, r^2 - 3\, r'^2)$$

$$\times (\underline{r}\cdot\underline{r}') + 22(\underline{r}\cdot\underline{r}')(\underline{r}\cdot\underline{r}') + 18(2\, r^2 - r'^2 - \underline{r}\cdot\underline{r}')(i\, \underline{\sigma}_1 \cdot \underline{r} \wedge \underline{r}')$$

$$\times | X^{\frac{1}{2}}_{M-m} (1,\widetilde{23}) \rangle \qquad \ldots \quad (\mathrm{VIII.3.a.1})$$

Substituting (VIII.3.a.1) into (VIII.3.1) we obtain

$${}^{t}E_{J\ell' M(s-D)}(r) = +(4/3)^4 \, (2/3)^4 \, \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j' \, {}^{t}U_k^{(3)} \int_0^{\infty} dr'$$

$$\times (rr') \, \mathrm{Exp}(- a_{ijk}' r^2 - b_{ijk}' r'^2) \, f^{\frac{1}{2}}_{J\ell M}(r') \sum_{\ell} \sum_{m',m}$$

$$\times C_{\ell' \frac{1}{2}}(J\ M; m'\ M-m') \, C_{\ell \frac{1}{2}}(J\ M; m\ M-m) \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi)$$

$$\times Y^{\ell' *}_{m'}(\theta,\phi) \langle X^{\frac{1}{2}}_{M-m} (1,\widetilde{23}) | \Big[(16\, r^4 - 34\, r^2 r'^2 + 4\, r'^4) - (16\, r^2 - 3\, r'^2)$$

$$\times (\underline{r}\cdot\underline{r}') + 22(\underline{r}\cdot\underline{r}')(\underline{r}\cdot\underline{r}') + 18(2\, r^2 - r'^2 - \underline{r}\cdot\underline{r}')(i\, \underline{\sigma}_1 \cdot \underline{r} \wedge \underline{r}') \Big]$$

$$\times | X^{\frac{1}{2}}_{M-m} (1,\widetilde{23}) \rangle \, Y^{\ell}_{m}(\theta',\phi') \, \mathrm{Exp}(C_{kij}' \, \underline{r}\cdot\underline{r}') \qquad \ldots \quad (\mathrm{VIII.3.a.2})$$

The above terms are all worked out, and we only qoute the result.

$$ {}^{t}E_{J\ell' M(s-D)}(r) = \sum_{\ell} \int_{0}^{\infty} dr' \, (rr') \, {}^{t}e_2^{(1)}(r,r') \, f^{\frac{1}{2}}_{J\ell M}(r') $$

$$ \times \Big\{ \Big[(16\, r^4 - 34\, r^2 r'^2 + 4\, r'^4) + \frac{(16\, r^2 - 3\, r'^2)}{C'_{kij}} + \frac{22}{C'^2_{kij}} \Big] $$

$$ \times I_{\ell+\frac{1}{2}}(C'_{kij}\, rr')\, \delta(\ell',\ell) + \Big[(16\, r^3 r' - 3\, r'^3 r + 44\, \frac{rr'}{C'_{kij}}) $$

$$ \times I'_{\ell+\frac{1}{2}}(C'_{kij}\, rr') + 22\, r^2 r'^2\, I''_{\ell+\frac{1}{2}}(C'_{kij}\, rr') \Big] \delta(\ell',\ell) + \sum_{\lambda} $$

$$ \times F_1(\ell'\ell\, ;\, \tfrac{1}{2}\lambda) \Big[(2\, r^2 - r'^2 + 1)\, I_{\lambda+\frac{1}{2}}(C'_{kij} rr') - rr'\, I'_{\lambda+\frac{1}{2}}(C'_{kij} rr') \Big] \Big\} $$

... (VIII.3.a.3)

where

$$ {}^{t}e_2^{(1)}(r,r') = + (4/3)^4\, (2/3)^4\, \frac{2\pi M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A'_j\, {}^{t}U_k^{(3)} $$

$$ \times (2\pi / C'_{kij}\, rr')^{\frac{1}{2}}\, \mathrm{Exp}(- a'_{ijk}\, r^2 - b'_{ijk}\, r'^2) $$ ... (VIII.3.a.4)

and $$ F_1(\ell'\ell\, ;\, \tfrac{1}{2}\lambda) = 2(-1)^{\ell-J+\frac{1}{2}}\, \hat{\ell}\, C_{\ell' 1}(\lambda)\, W(\ell' 1\, ;\, \ell\, 1\, ;\, 1\, \lambda) $$

$$ \times W(\ell' \tfrac{1}{2}\, ;\, \ell\, \tfrac{1}{2},\, 1J) $$ ... (VIII.3.a.5)

(VIII.3.b.) THE QUARTET STATE

The spin products in this case are written as follows:

$$< \underset{M-m'}{\overset{3/2}{X}}(1,\overline{23})| \overset{t\ (4)}{V}(t)\ S_{12}(t^2)\ S_{13}(V^2)\ \phi_D(V)|\underset{M-m}{\overset{3/2}{X}}(2,\overline{13})>$$

$$= (2/3)^4 \sum_{i,j,k=1}^{2} A_i A_j' \overset{t\ (4)}{U_k} \text{Exp}(- \overset{t\ (4)}{\mu_k} t^2 - \alpha_j' V^2) < \underset{M-m'}{\overset{3/2}{X}}(1,\overline{23})|$$

$$\times \Big\{ \Big[18\ W_{13}(r^2) - 2\ W_{13}(r'^2) - 2\ W_{13}(\underline{r},\underline{r}') \Big] (i\ \underline{\sigma}_2 \cdot \underline{r} \wedge \underline{r}')$$

$$+ (4\ r^2 + 11\ r'^2 - 2\ \underline{r}\cdot\underline{r}')\ W_{13}(r^2) + (-\ 11\ r^2 + r'^2 + \underline{r}\cdot\underline{r}')$$

$$\times W_{13}(r'^2) + (-\ 2\ r^2 + r'^2 + 19\ \underline{r}\cdot\underline{r}')\ W_{13}(\underline{r},\underline{r}') + (18r^2 - 9r'^2 - 9\underline{r}\cdot\underline{r}')$$

$$\times (i\ \underline{\sigma}_2 \cdot \underline{r} \wedge \underline{r}') - (8\ r^2 - 4\ r'^2 - 11)(\underline{r}\cdot\underline{r}') + (8\ r^4 + 2r'^4 - 17r^2 r'^2) \Big]$$

$$\times |\underset{M-m}{\overset{3/2}{X}}(1,\overline{23})> \qquad \ldots \quad (\text{VIII.3.b.1})$$

Using (VIII.3.b.1), in (VIII.3.1) the exchange term of the tensor force is finally written in the quartet state as:

$$\overset{t}{E}_{J\ell' M(s-D)}(r) = \sum_{\ell} \int_0^{\infty} dr'\ (rr')\ \overset{t\ (2)}{e_2}(r,r')\ \overset{3/2}{f}_{J\ell M}(r')$$

$$\times \Big\{ \Big[(8\ r^4 - 17\ r^2 r'^2 - 2\ r'^4) - \frac{1}{2C'_{kij}} (8\ r^2 - 4\ r'^2 - 11)$$

$$\times (2\ell - 1) \Big] I_{\ell+\frac{1}{2}}(C' rr') + A(\ell' 3/2;\ \ell\ 3/2) \Big[\Big\{ 22r^2 + 11r'^2$$

$$- \frac{(2\ell-1)}{C'_{kij}} \Big\} I_{\ell+\frac{1}{2}}(C'_{kij}\ rr') - \Big\{ 11\ r^2 - 10\ r'^2 - \frac{(2\ell'-1)}{2C'_{kij}} \Big\}$$

$$\times I_{\ell'+\frac{1}{2}}(C'_{kij}\,rr') + \sum_{L} FF(\ell'\ell;L)\Big\{ r'^2 - 2\,r^2 - 9\,rr' + \frac{19}{2C'_{kij}}$$

$$\times (2L+1)\Big\} I_{L+\frac{1}{2}}(C'_{kij}\,rr')\Big] + A(\ell' 3/2\ ;\ \ell 3/2)\Big[rr'\ I_{\ell'+3/2}(C'_{kij}rr')$$

$$- 2\,rr'\ I_{\ell+3/2}(C'_{kij}\,rr') + 19\,rr' \sum_{L} FF(\ell'\ell;L)\ I_{L+3/2}(C'_{kij}\,rr')\Big]$$

$$- (8\,r^2 - 4\,r'^2 - 11)(rr')\ I_{\ell+3/2}(C'_{kij}rr') + 12/7 \sum_{L}$$

$$\times F_5(\ell'\ell\ ;\ 3/2L)\Big[\ (2\,r^2 - r'^2)\ I_{L+\frac{1}{2}}(C'_{kij}rr') - \frac{(2L-1)}{2\ C'_{kij}}$$

$$\times I_{L+\frac{1}{2}}(C'_{kij}\,rr') - rr'\ I_{L+3/2}(C'_{kij}\,rr')\Big]\Big\} \qquad \ldots \quad \text{(VIII.3.b.2)}$$

where

$$e_2^{t\,(2)}(r,r') = -\ (4/3)^4\ (2/3)^4\ \frac{2\pi\ M}{h^2} \sum_{i,j,k=1}^{2} A_i A'_j\ U_k^{t\,(4)}$$

$$\times \operatorname{Exp}(-\ a'_{ijk}\ r^2 - b'_{ijk}\ r'^2) \qquad \ldots \quad \text{(VIII.3.b.3)}$$

and

$$F_5(\ell'\ell\ ;\ 3/2\ L) = 21(10)^{\frac{1}{2}}\ \hat{\ell}\ (-1)^{\ell-J+3/2}\ C_{\ell' 1}(L)\ C_{\ell 1}(L)$$

$$\times W(\ell' 1\ ;\ \ell 1\ ;\ 1L)\ W(\ell' 3/2\ ;\ \ell\ 3/2\ ;\ 1J) \qquad \ldots \quad \text{(VIII.3.b.4)}$$

(VIII.4.) THE SPIN-ORBIT TERM

This is given by the following expression:

$$\overset{s.o}{}E^{S'}_{J\ell' M(s-D)}(r) = -(4/3)^4 \frac{Mr}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(JM;m'M-m')$$

$$\times C_{\ell S}(J\,M;m\,M-m)\int d\underline{r}'\; d\,\Omega(\theta,\phi)\; \mathrm{Exp}(-\alpha_i u^2)\; \overset{\ell'}{Y}{}^{*}_{m'}(\theta,\phi) \langle X^{S'}_{M-m'}(1,\overline{23})|$$

$$\times \frac{1}{4} \sum_{\nu} (W - 2h + b - 2m)_{\nu}\, {}^{\nu}V_{s.o}(t) \left[\, \underline{S}_{12} \cdot \underline{L}_{12} \,\right] W_{13}(\underline{V}^2)$$

$$\times \mathrm{Exp}(-\alpha'_j V^2)\, |X^{S}_{M-m}(2,\overline{13})\rangle\, \overset{\ell}{Y}_{m}(\theta',\phi')\, \frac{1}{r'}\, f^{S}_{J\ell M}(r') = -(4/3)^4 \frac{Mr}{\hbar^2}$$

$$\times \sum_{i,j,k=1}^{2} A_i A_j \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\,M;m'\,M-m')\; C_{\ell S}(J\,M;m\,M-m) \int d\underline{r}'$$

$$\times \int d\,\Omega(\theta,\phi)\; \mathrm{Exp}(-\alpha_i u^2)\; \overset{s.o}{V}(t)\; \overset{\ell'}{Y}{}^{*}_{m'}(\theta,\phi)\, \langle X^{S'}_{M-m'}(1,\overline{23})|\, (\underline{S}_{12} \cdot \underline{L}_{12})$$

$$\times W_{13}(\underline{V}^2)\, |X^{S}_{M-m}(2,\overline{13})\rangle\; \mathrm{Exp}(-\alpha'_j V^2)\; \overset{\ell}{Y}_{m}(\theta',\phi')\; \frac{1}{r'}\; f^{S}_{J\ell M}(r') \qquad \ldots \text{(VIII.4.1)}$$

where

$$\underline{L}_{12} = -\,i\,(\underline{r}-\underline{r}') \wedge \left(\frac{\partial}{\partial \underline{r}} - \frac{\partial}{\partial \underline{r}'} \right) \qquad \ldots \text{(VIII.4.2)}$$

and

$$\underline{S}_{12} = \frac{1}{2}(\underline{\sigma}_1 + \underline{\sigma}_2) \qquad \ldots \text{(VIII.4.3)}$$

We also have

$$\phi_s(u)\; \overset{s.o}{V}(t)\; (\underline{S}_{12} \cdot \underline{L}_{12})\; S_{13}(\underline{V}^2)\; \phi_D(V) = \phi_s(u)\; \overset{s.o}{V}(t)\; \frac{1}{2i}$$

$$\times \left[(\underline{\sigma}_1 + \underline{\sigma}_2)\cdot(\underline{r}-\underline{r}')\wedge \frac{\overrightarrow{\partial}}{\partial \underline{r}} - \frac{\overleftarrow{\partial}}{\partial r'} \wedge (\underline{r}-\underline{r}')\cdot(\underline{\sigma}_1 + \underline{\sigma}_2) \right] \underline{S}_{13}(\underline{V}^2)$$

$$\times\ \phi_D(V) = \sum_{i,j,k=1}^{2} A_i A_j \ {}^{s.o}U_k \ \mathrm{Exp}(-\ a'_{ijk} r^2 - b'_{ijk}\ r'^2 + C'_{ijk}\ \underline{r}\cdot\underline{r}')$$

$$\times \left[3\ {}_1b'_{ij} \left\{ \left[4\ W_{13}(\underline{r}^2) + W_{13}(r'^2) + 4\ W_{13}(\underline{r},\underline{r}') \right] (i\ \underline{\sigma}_2\cdot\underline{r}\wedge\underline{r}') \right.\right.$$

$$\left. + 6\ {}_1b'_{ij} \left[(r'^2 + 2\underline{r}\cdot\underline{r}')\ W_{13}(r^2) - \frac{1}{2}(2r^2 + \underline{r}\cdot\underline{r}')\ W_{13}(r'^2) \right] \right\}$$

$$- 3\ {}_1b'_{ij}\ (4\ r^2 - 2\ \underline{r}\cdot\underline{r}')(\underline{\sigma}_1\cdot\ \underline{r})(\underline{\sigma}_3\cdot\ \underline{r}') - 3\ {}_1b'_{ij}\ (8r^2 - r'^2 + 2\underline{r}\cdot\underline{r}')$$

$$\times\ (\underline{\sigma}_1\cdot\ \underline{r}')(\underline{\sigma}_3\cdot\ \underline{r}) + 3\ {}_1b'_{ij}\ (4\ r^2 - r'^2)(\underline{\sigma}_1\cdot\ \underline{\sigma}_3)(\underline{r}\cdot\underline{r}')$$

$$- 3\ {}_1b'_{ij}\ (4\ r^2 + r'^2 + 4\ \underline{r}\cdot\underline{r}')(i\ \underline{\sigma}_3\cdot\ \underline{r}\wedge\underline{r}') - 12\ W_{13}(\underline{r}^2)$$

$$+ 6\ W_{13}(\underline{r}'^2) - 6(\underline{\sigma}_1\cdot\ \underline{r})(\underline{\sigma}_3\cdot\ \underline{r}') + 24(\underline{\sigma}_1\cdot\ \underline{r}')(\underline{\sigma}_3\cdot\ \underline{r})$$

$$+ 42(i\ \underline{\sigma}_3\cdot\ \underline{r}\wedge\underline{r}') - 6(\underline{\sigma}_1\cdot\ \underline{\sigma}_3)(\underline{r}\cdot\underline{r}') - (i\ \underline{\sigma}_1\wedge\underline{\sigma}_2\cdot\ \underline{r})$$

$$\times \left\{ 12\ \underline{\sigma}_3\cdot\ \underline{r} - 6\ \underline{\sigma}_3\cdot\ \underline{r}' \right\} + (i\ \underline{\sigma}_1\wedge\ \underline{\sigma}_2\cdot\ \underline{r}') \left\{ 12\ \underline{\sigma}_3\cdot\ \underline{r} - 6\ \underline{\sigma}_3\cdot\underline{r}' \right\}$$

$$+ (i\ \underline{\sigma}_2\wedge\ \underline{\sigma}_3\cdot\ \underline{r}) \left\{ 12\ \underline{\sigma}_1\cdot\ \underline{r} - 6\ \underline{\sigma}_1\cdot\ \underline{r}' \right\} - (i\ \underline{\sigma}_2\wedge\ \underline{\sigma}_3\cdot\ r')$$

$$\left. \times \left\{ 12\ \underline{\sigma}_1\cdot\ \underline{r} - 6\ \underline{\sigma}_1\cdot\ \underline{r}' \right\} \right] \qquad \ldots \quad (\text{VIII.4.4})$$

The spin simplification is again treated in two distinct cases as follows:

(a) THE DOUBLET CASE

The following results are quoted for further use

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|(\underline{\sigma}_1\cdot\underline{A})(i\,\underline{\sigma}_2\wedge\underline{\sigma}_3\cdot\underline{B})|X^{\frac{1}{2}}_{M-m}(2,\overline{13})\rangle$$

$$= +\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,\underline{A}\cdot\underline{B}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle - \langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|(i\,\underline{\sigma}_1\cdot\underline{A}\,\underline{B})|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle,$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|S_{13}(\underline{A}\,,\underline{B})(i\,\underline{\sigma}_2\cdot\underline{r}\wedge\underline{r}')|X^{\frac{1}{2}}_{M-m}(2,\overline{13})\rangle$$

$$= -\frac{2}{3}(\underline{A}\cdot\underline{B})\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|(i\,\underline{\sigma}_1\cdot\underline{r}\wedge\underline{r}')|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle,$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|(i\,\underline{\sigma}_1\wedge\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_3\cdot\underline{B})|X^{\frac{1}{2}}_{M-m}(2,\overline{13})\rangle$$

$$= \langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,\underline{A}\cdot\underline{B}\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle,$$

$$\langle X^{\frac{1}{2}}_{M-m'}(1,\overline{23})|(i\,\underline{\sigma}_2\cdot\underline{r}\wedge\underline{r}')|X^{\frac{1}{2}}_{M-m}(2,\overline{13})\rangle$$

$$= \frac{1}{6}\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,i\,\underline{\sigma}_1\cdot\underline{r}\wedge\underline{r}'\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

$$\langle X^{\frac{1}{2}}_{M-m}(1,\overline{23})|\,i\,\underline{\sigma}_3\cdot\underline{r}\wedge\underline{r}'\,|X^{\frac{1}{2}}_{M-m}(1,\overline{23})\rangle$$

$$= -\frac{1}{6}\langle X^{\frac{1}{2}}_{M-m'}(1,\widetilde{23})|\,i\,\underline{\sigma}_1\cdot\underline{r}\wedge\underline{r}'\,|X^{\frac{1}{2}}_{M-m}(1,\widetilde{23})\rangle$$

The vectors $\underline{A}$ and $\underline{B}$ are either $\underline{r}$ or/and r'. With the help of the above results, the spin products in the doublet state reduce to the following form

$$\left\langle X^{\frac{1}{2}}_{M-m}(1,\overline{23})\right|\phi_s(u)\ \overset{s.o}{V}(t)\ (\underline{S}_{12}\cdot\underline{L}_{12})\ \underline{S}_{13}(\underline{V}^2)\ \phi_D(V)\left|X^{\frac{1}{2}}_{M-m}(2,\overline{13})\right\rangle$$

$$=\sum_{i,j,k=1} A_i A'_j\ \overset{s.o}{U}_k\ \mathrm{Exp}(-\ a'_{ijk}r^2 -\ b'_{ijk}\ r'^2 +\ C'_{kij}\ \underline{r}\cdot\underline{r}')$$

$$\mathrm{x}\ \left\{\left[\frac{1}{2}\ {}_1b'_{ij}\ (4\ r^2 + r'^2 + 4\ \underline{r}\cdot\underline{r}')\ -5\ \right]\right.$$

$$\mathrm{x}\ \left\langle X^{\frac{1}{2}}_{M-m'}(1,\tilde{23})\right|\ i\ \underline{\sigma}_1\cdot\ \underline{r}\ \ \underline{r}'\left|X^{\frac{1}{2}}_{M-m}(1,\tilde{23})\right\rangle \qquad \ldots\ (\mathrm{VIII.4.5})$$

putting $\overset{s.o}{V}(\underline{r},\underline{r}') = -(4/3)^4\ \frac{M}{\hbar^2}\ (rr')\sum_{i,j,k=1}^{2} A_i A'_j\ \overset{s.o}{U}_k$

$$\mathrm{x}\ \mathrm{Exp}(-\ a'_{ijk}\ r^2 -\ {}_1b'_{ij}\ r^2 +\ C'_{kij}\ \underline{r}\cdot\underline{r}')\left[\frac{1}{2}\ {}_1b'_{ij}(4\ r^2 + r'^2 + 4\underline{r}\cdot\underline{r}')-5\ \right]$$

$$\ldots\ (\mathrm{VIII.4.6})$$

Which can be expanded in harmonics

$$\overset{s.o}{V}(\underline{r},\underline{r}') = \frac{1}{rr'}\ \sum_{L,n}\ \overset{s.o}{p}_L(r,r')\ \overset{L*}{\underset{n}{Y}}(\theta',\phi')\ \overset{L}{\underset{n}{Y}}(\theta,\phi) \ldots\ (\mathrm{VIII.4.7})$$

so that

$$\overset{s.o}{p}_L(r,r') = 2\pi\ rr'\int_{-1}^{+1} d\eta\ p_L(\eta)\ \ \overset{s.o}{V}(\underline{r},\underline{r}') \qquad \ldots\ (\mathrm{VIII.4.8})$$

Before the angular integration is carried out, the spin matrix elements are expanded as follows:

$$\left\langle X^{\frac{1}{2}}_{M-m'}(1,\tilde{23})\right|i\ \underline{\sigma}_1\cdot\ \underline{r}\wedge\underline{r}'\left|X^{\frac{1}{2}}_{M-m}(1,\tilde{23})\right\rangle = (3/2)^{\frac{1}{2}}\ \frac{8\pi\ rr'}{9}\ \sum_{\lambda,p}$$

$$\mathrm{x}\ C_{11}\ (1\ \lambda+\ p\ ;\ \ \lambda)\ C_{\frac{1}{2}1}\ (1\ M-m;\ M-m',-\lambda-\ p)\ \overset{1}{\underset{-\lambda}{Y}}(\theta',\phi')\ \overset{1}{\underset{-p}{Y}}(\theta,\phi)$$

$$\ldots\ (\mathrm{VIII.4.9})$$

Substituting (VIII.4.7) and (VIII.4.9) in (VIII.4.1) and performing the spherical integration and sums over all magnetic quantum numbers (m', m, n, λ and p), the exchange term of the spin-orbit force is finally given in the doublet state by:

$$ {}^{s.o}{}_{J\ell'M(s-D)}^{\ S'}E(r) = \sum_{\ell,L} \int_0^\infty dr' \ {}^{s.o}e_2(r,r') \, F_1(\ell'\ell;\tfrac{1}{2}L) \, f^{\frac{1}{2}}_{J\ell M}(r') $$

$$ \times \Big[\Big\{ \tfrac{1}{2} \, {}_1b'_{ij}(4\, r^2 + \frac{2(2L-1)}{C_{kij}} + r^2) - 5 \Big\} I_{L+\frac{1}{2}}(C'_{kij} rr') $$

$$ + 2 \, {}_1b'_{ij} \, rr' \, I_{L+3/2}(C'_{kij} \, rr' \Big] \qquad \ldots \quad (\text{VIII.4.10}) $$

where

$$ {}^{s.o}e_2(r,r') = -(4/3)^4 \, \frac{2M\pi\, rr'}{h^2} \sum_{i,j,k=1}^{2} A_i A'_j \, {}^{s.o(2)}U_k $$

$$ \times \, (2\pi / C'_{kij} \, rr')^{\frac{1}{2}} \, \text{Exp}(- a'_{ijk} \, r^2 - b'_{ijk} \, r'^2) \qquad \ldots \quad (\text{VIII.4.11}) $$

and

$$ F_1(\ell'\ell;\tfrac{1}{2}\, L) = (-1)^{\ell - J + \frac{1}{2}} \, (4(2\ell+1))^{\frac{1}{2}} \, C_{\ell' 1}(L) \, C_{\ell 1}(L) \, W(\ell' 1;\ell 1;1L) $$

$$ \times \, W(\ell' \tfrac{1}{2};\ell \tfrac{1}{2};\, 1J) \qquad \ldots \quad (\text{VIII.4.12}) $$

(b) THE QUARTET CASE

From (VIII.4.1), the integral for the exchange interaction in the quartet state is given by:

$$\underset{J\ell' M(s-D)}{\overset{s.o\ S'}{E}}(r) = -(4/3)^4 \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A'_j \ \overset{s.o}{U_k} \sum_{\ell} \sum_{m',m}$$

$$\times\ C_{\ell' 3/2}(J\ M;m'\ M-m')\ C_{\ell 3/2}(J\ M;m\ M-m) \int dr'\ (rr')\ \mathrm{Exp}(-a'_{ijk} r^2$$

$$-\ b'_{ijk} r'^2 + C'_{kij}\ \underline{r},\underline{r}') \int d\Omega'(\theta',\phi') \int d\Omega(\theta,\phi)\ \overset{\ell'}{Y}{}^{*}_{m'}(\theta,\phi)$$

$$\times \left\langle \overset{3/2}{\underset{M-m'}{X}}(1,\overline{23}) \middle| \underline{OS} \middle| \overset{3/2}{\underset{M-m}{X}}(1,\overline{23}) \right\rangle \overset{\ell}{\underset{m}{Y}}(\theta',\phi')\ \overset{3/2}{\underset{J\ell M}{f}}(r') \qquad \ldots \quad (VIII.4.13)$$

where

$$\underline{OS} = 3\ {}_1b'_{ij} \left[4\ W_{13}(\underline{r}^2) + W_{13}(\underline{r}'^2) + 4\ W_{13}(\underline{r},\underline{r}') \right] (i\ \underline{\sigma}_2 \cdot \underline{r} \wedge \underline{r}')$$

$$+ \left[6\ {}_1b'_{ij}\ (r'^2 + 2\ \underline{r}\cdot\underline{r}') - 12 \right] W_{13}(\underline{r}^2) + \left[-\ 3\ {}_1b'_{ij}\ (2r^2 + \underline{r}\cdot\underline{r}') + 6 \right]$$

$$\times\ W_{13}(\underline{r}'^2) + \left[-\ 3\ {}_1b'_{ij} (4\ r^2 - r'^2) + 6 \right] W_{13}(\underline{r},\underline{r}') + 42 (i \underline{\sigma}_2 \cdot \underline{r} \wedge \underline{r}')$$

$$\ldots \quad (VIII.4.14)$$

Using (VIII.4.14), finally we obtain from (VIII.4.13)

$$\underset{J\ell' M(s-D)}{\overset{s.o\ S'}{E}}(r) = \sum_{\ell} \int_0 dr'\ rr'\ \overset{s.o}{e_2}(r,r')\ \overset{3/2}{\underset{J\ell M}{f}}(r') \Big\{ A(\ell' 3/2;\ell 3/2)$$

$$\times \Big[12\ {}_1b'_{ij}\ r^2\ I_{\ell+\frac{1}{2}}(C'_{kij}\ rr') + \Big\{ 6\ {}_1b'_{ij} (r'^2 + \frac{2\ell-1}{C'_{kij}})\ r^2 - 12\ r^2 \Big]$$

$$\times\ I_{\ell+\frac{1}{2}}(C'_{kij}\ rr') + \Big\{ -\ {}_1b'_{ij} \Big[6\ r^2 r'^2 + \frac{3}{2C'_{kij}}\ (2\ell' - 1)\ r'^2 \Big]$$

$$- 6\, r'^2 \Big\} I_{\ell'+\frac{1}{2}}(C'_{kij}\, rr') - 3\, {}_1b'_{ij}\, r'^2\, I_{\ell'+3/2}(C'_{kij}\, rr') \Big]$$

$$+ \sum_{L} \Big[A(\ell' 3/2; \ell 3/2) \Big\{ - 3\, {}_1b'_{ij}(4\, r^2 - r'^2) rr' + 6\, rr' \Big\}$$

$$\times FF(\ell'\ell;L) \Big\{ \frac{2L-1}{2C'_{kij}}\, I_{L+\frac{1}{2}}(C'_{kij}\, rr') + I_{L+3/2}(C'_{kij}\, rr') \Big\}$$

$$+ 4\, F_5(\ell'\ell;3/2\ L)\, I_{\ell+\frac{1}{2}}(C'_{kij}\, rr') \Big] \Big] \qquad \ldots \quad (VIII.4.15)$$

where

$$^{s.o}e_2(r,r') = -(4/3)^4\, \frac{2\pi M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A'_j\, {}^{s.o}U_k\, (2\pi/C'_{kij}\, rr')^{\frac{1}{2}}$$

$$\times\ Exp(- a'_{ijk}\, r^2 - b'_{ijk}\, r'^2) \qquad \ldots \quad (VIII.4.16)$$

$$F_5(\ell'\ell;3/2L) = 21\, (10)^{\frac{1}{2}}\, \hat{\ell}\, (-1)^{\ell'-J+3/2}\, C_{\ell' 1}(L)\, C_{\ell 1}(L)\, W(\ell' 1;\ell 1;1L)$$

$$\times\ W(\ell' 3/2\ \ell 3/2;\ 1J) \qquad \ldots \quad (VIII.4.17)$$

and

$$FF(\ell'\ell;L) = -\, (30)^{\frac{1}{2}}\, \hat{\lambda}' \frac{C_{\lambda 1}(L)\, C_{\lambda 1}(L)\, W(1\lambda;\ 1\lambda';L2)}{C_2(\lambda')} \qquad \ldots \quad (VIII.4.18)$$

It has to be noted that in the forgoing analysis, we made use of the condensed notation for $\hat{\ell} = (2\ell+1)^{\frac{1}{2}}$, $\hat{\lambda}' = (2\lambda'+1)^{1/2}$ and $C_{\ell'\ell}(L) = C_{\ell'\ell}(L\ 0;00)$.

CHAPTER IX

DIRECT AND EXCHANGE (D-s)-INTERACTION TERMS

The formulation of the direct and exchange (D-s)-terms is similar to that of the (s-D)-terms, but in the integrands the factors containing the tensor operator (from the deuteron D-state function) are now written in the reverse order.

Since these operators are Hermitian the results will be exactly the same as these of the (s-D)-terms, with only i and j as well as r and r' in theexchange terms interchanged.

(IX.1.) THE CENTRAL DIRECT TERM

This term is given by

$$ {}^{c}D^{S'}_{J\ell' M(D-s)}(r) = \frac{4\,M}{3\hbar^2} \sum_{\ell} \sum_{m',m} C_{\ell 3/2}(J\,M;m'\,M-m')\, C_{\ell 3/2}(J\,M;m\,M-m) $$

$$ \times \int d\underline{R}\, d\Omega(\theta,\phi) \left[\phi_D(R)\, S_{23}(\underline{R}^2)\, Y^{\ell}_{m'}(\theta,\phi)\, |X^{S'}_{M-m'}(1,\overline{23})\rangle \right]^{*} V^{(2)}_{c}(\underline{r}_{12}) $$

$$ \times |X^{S}_{M-m}(1,\overline{23})\rangle\, \phi_s(R)\, Y^{\ell}_{m}(\theta,\phi)\, f^{3/2}_{J\ell M}(r) = \sum_{\ell} {}^{c}B_3(r)\, A(\ell' 3/2\,;\,\ell\,3/2) $$

$$ \times f^{3/2}_{J\ell M}(r) \qquad \ldots \quad (IX.1.1) $$

where

$$ {}^{c}B_3(r) = \frac{4\,M}{3\hbar^2} \sum_{i,j,k=1}^{2} A'_i A_j\, {}^{c}U^{(2)}_{k}\, \gamma^{2}_{ijk}\, (\pi/ {}''_{ijk})^{3/2} $$

$$ \times \mathrm{Exp}(-({}^{c}\mu^{(2)}_{k} - \lambda''_{ijk}\, \gamma''^{2}_{ijk})r^2) \qquad \ldots \quad (IX.1.2) $$

(IX.2.) THE CENTRAL EXCHANGE TERM

The exchange term of the central force is given by

$$ {}^{c}E^{S'}_{J\ell' M(D-s)}(r) = -(4/3)^4 \frac{M r}{\hbar^2} \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M; m'\ M-m') $$

$$ \times C_{\ell 3/2}(J\ M; m\ M-m) \int d\underline{r}'\ d\Omega(\Theta,\phi) \Big[\phi_D(u)\ S_{23}(u^2)\ Y^{\ell'}_{m'}(\Theta,\phi) $$

$$ \times |X^{S'}_{M-m'}(1,\overline{23})\rangle \Big]^{*}\ {}^{c}V^{(4)}(t)\ |X^{S}_{M-m}(1,\overline{23})\rangle\ \phi_s(V)\ Y^{\ell}_{m}(\Theta',\phi')\ \frac{1}{r'}\ f^{3/2}_{J\ell M}(r') $$

$$ = \sum_{\ell} \int_0^{\infty} dr'\ (rr')\ A(\ell' 3/2\ ;\ \ell\ 3/2)\ {}^{c}e_3(r',r)\ f^{3/2}_{J\ell M}(r') $$

$$ \times \Big[r^2\ I_{\ell+\frac{1}{2}}(C''_{kij}\ r'r) + 4\ r'^2\ I_{\ell'+\frac{1}{2}}(C''_{kij}\ r'r) + 2rr' \sum_{L} FF(\ell\ell';L) $$

$$ \times I_{L+\frac{1}{2}}(C''_{kij}\ r'r) \Big] \qquad \ldots \quad (IX.2.1) $$

where

$$ {}^{2}e_3(r',r) = -\frac{8\pi M}{9h^2}(4/3)^4 \sum_{i,j,k=1}^{2} A'_i A_j\ {}^{c}U^{(4)}_k\ (2\pi/\ C''_{kij}\ rr')^{\frac{1}{2}} $$

$$ \times \mathrm{Exp}(-\ a''_{ijk}\ r'^2 - b''_{ijk}\ r^2) $$

(IX.3.) THE COULOMB DIRECT TERM

The direct term of the coulomb force is given below by:

$$ {}^{coul}{}_{J\ell' M(D-s)}^{S'}D(r) = \frac{4\,M}{3\hbar^2} \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m')\ C_{\ell 3/2}(J\ M;m\ M-m) $$

$$ \times \int d\underline{R}\ d\Omega(\theta,\phi) \left[\phi_D(R)\ S_{23}(\underline{R}^2)\ Y_{m'}^{\ell'}(\theta,\phi) \left|X_{M-m'}^{S'}(1,\overline{23})\right> \right]^* \frac{e^2}{r_{12}} $$

$$ \times \left|X_{M-m}^{S}(1,\overline{23})\right> \phi_s(R)\ Y_m^{\ell}(\theta,\phi)\ f_{J\ell M}^{S}(r) = \sum_{\ell} {}^{coul}B_3(r)\ A(\ell' 3/2;\ell 3/2) $$

$$ \times\ f_{J\ell M}^{3/2}(r) \qquad \ldots \quad (IX.3.1) $$

where

$$ {}^{coul}B_3(r) = \frac{M\,e^2}{4\hbar^2 r^3} \sum_{i,j=1} A_i'\ A_j \frac{1}{(\alpha_i' + \alpha_j)^2} \left(\pi/(\alpha_i' + \alpha_j)\right)^{3/2} $$

$$ \ldots \quad (IX.3.2) $$

(IX.4.) THE COULOMB EXCHANGE TERM

The (D-s)-term of the coulomb force is given by the following expressions:

$$ {}^{coul}{}_{J\ell' M(D-s)}^{S'}E(r) = -(4/3)^4 \frac{M\,e^2 r}{\hbar^2} \sum_{\ell} \sum_{m',m} C_{\ell' 3/2}(J\ M;m'\ M-m') $$

$$ \times\ C_{\ell 3/2}(J\ M;m\ M-m) \int d\underline{r}'\ d\Omega(\theta,\phi) \left[\phi_D(u)\ S_{23}(\underline{u}^2)\ Y_{m'}^{\ell'}(\theta,\phi) \right. $$

$$ \times \left. \left|X_{M-m'}^{S'}(1,\overline{23})\right> \right]^* \frac{1}{t} \left|X_{M-m}^{S}(2,\overline{13})\right> \phi_s(V)\ Y_m^{\ell}(\theta',\phi')\ \frac{1}{r'}\ f_{J\ell M}^{3/2}(r') $$

$$ = \sum_{\ell} \int_0^{\infty} dr'\ A(\ell 3/2\ ;\ \ell' 3/2) \left[{}^{coul\ 1}e_3(r',r) + {}^{coul\ 2}e_3(r',r) \right. $$

$$+ \; e_3^{coul\,3}(r',r) \sum_L FF(\ell\ell';L) \Big] \qquad \text{(IX.4.1)}$$

where

$$e_3^{coul\,1}(r',r) = -(4/3)^4 \frac{16\pi M e^2}{3\hbar^2} r'^3 r \sum_{i,j=1}^{2} A_j A_i' \, Exp(-e_{ji}'' r'^2 - f_{ji}'' r^2)$$

$$\times \int_{-1}^{+1} d\eta \, P_{\ell'}(\eta) \, (r^2 + r'^2 - 2\underline{r}.\underline{r}')^{-\frac{1}{2}} \, Exp(b_{ji}'' \, \underline{r}.\underline{r}') \; \ldots \qquad \text{(IX.4.2)}$$

$$e_3^{coul\,2}(r',r) = -(4/3)^4 \frac{4\pi M e^2}{3\hbar^2} r^3 r' \sum_{i,j=1}^{2} A_j A_i' \, Exp(-e_{ji}'' r'^2 - f_{ji}'' r^2)$$

$$\times \int_{-1}^{+1} d\eta \, P_{\ell}(\eta)(r^2 + r'^2 - 2\underline{r}.\underline{r}')^{-\frac{1}{2}} \, Exp(b_{ji}'' \underline{r}.\underline{r}') \quad \ldots \qquad \text{(IX.4.3)}$$

and

$$e_3^{coul\,3}(r',r) = -(4/3)^4 \frac{8\pi M e^2}{3\hbar^2} r^2 r'^2 \sum_{i,j=1}^{2} A_j A_i' \, Exp(-e_{ji}'' r'^2$$

$$- f_{ji}'' r^2) \int_{-1}^{+1} d\eta \, P_L(\eta)(r^2 + r'^2 - 2\underline{r}.\underline{r}')^{-\frac{1}{2}} Exp(b_{ji}'' \underline{r}.\underline{r}') \ldots \qquad \text{(IX.4.4)}$$

(IX.5.) THE TENSOR DIRECT TERM

This is given for both cases ($s=\frac{1}{2}$ and $s=3/2$) by:

$$D^{T\,S'}_{J\ell' M(D-s)}(r) = \frac{4\,M}{3\hbar^2} \sum_{\ell,S} \sum_{m',m} C_{\ell' S'}(J\,M;m'\,M-m')\, C_{\ell S}(J\,M;m\,M-m)$$

$$\times \int d\underline{R}\, d\Omega(\theta,\phi)\, \phi_D(R)\, V^{T\,(II)}(\underline{r}_{12})\, Y^{*\ell'}_{m'}(\theta,\phi)$$

$$\times \langle X^{S'}_{M-m'}(1,\overline{23}) | S_{23}(\underline{R}^2)\, S_{12}(\underline{r}^2_{12}) | X^S_{M-m}(1,\overline{23})\rangle\, \phi_s(R)\, Y^{\ell}_{m}(\theta,\phi)\, f^S_{J\ell M}(r)$$

$$\ldots \qquad \text{(IX.5.1)}$$

Without going into further details in the analysis, equation (IX.5.1) is finally given in the doublet ($s=\frac{1}{2}$)and quartet ($s=3/2$) states by the following expressions:

$$ {}^{t}D_{J\ell' M(D-s)}(r) = \sum_{\ell} {}^{t(1)}B_3(r)\; f^{\frac{1}{2}}_{J\ell M}(r)\; \delta(\ell',\ell) \qquad \ldots \quad (IX.5.2) $$

and

$$ {}^{t}D_{J\ell' M(D-s)}(r) = \sum_{\ell} {}^{t(2)}B_3(r)\; f^{3/2}_{J\ell M}(r)\; \delta(\ell',\ell) \qquad \ldots \quad (IX.5.3) $$

where

$$ {}^{t(1)}B_3(r) = \frac{4\,M}{3\hbar^2} \sum_{i,j,k=1}^{2} A'_i\, A_j\, {}^{t(1)}U_k\, (\pi/\lambda''_{ijk})^{3/2} $$

$$ \times\, \mathrm{Exp}\Big(-\,{}^{t(1)}\mu_k \Big(1- \frac{{}^{t(1)}\mu_k}{4\,\lambda''_{ijk}}\Big) r^2\Big) \Big[-\frac{15}{4\,\lambda''^2_{ijk}} + 10\, \frac{\gamma''_{ijk}}{\lambda''_{ijk}} (1-\tfrac{1}{2}\,\gamma''_{ijk}) r^2 $$

$$ -\, 4\, \gamma''^2_{ijk}\, (1-\tfrac{1}{2}\,\gamma''_{ijk})^2\, r^4 \Big] \qquad \ldots \quad (IX.5.4) $$

and

$$ {}^{t(2)}B_3(r) = \frac{4\,M}{3\hbar^2} \sum_{i,j,k=1}^{2} A'_i\, A_j\, {}^{t(2)}U_k\, (\pi/\lambda''_{ijk})^{3/2} $$

$$ \times\, \mathrm{Exp}\Big(-\,{}^{t(2)}\mu_k \Big(1 - \frac{{}^{t(2)}\mu_k}{4\,\lambda''_{ijk}}\Big) r^2\Big) \Big[A(\ell' 3/2\,;\,\ell 3/2) $$

$$ \times \Big\{ \gamma''^2_{ijk}\, (1 - \tfrac{1}{2}\,\gamma''^2_{ijk})\, r^4 - \frac{7}{4}\, \frac{\gamma''_{ijk}}{\lambda''_{ijk}}\, (1 - \tfrac{1}{2}\,\gamma''_{ijk})\, r^2 \Big\} $$

$$ +\, 2\, \gamma''^2_{ijk}\, (1 - \tfrac{1}{2}\,\gamma''_{ijk})^2\, r^4 - \frac{5\,r^2}{\lambda''_{ijk}}\, \gamma''_{ijk}\, (1 - \tfrac{1}{2}\,\gamma''_{ijk}) $$

$$ +\, \frac{15}{8\,\lambda''^2_{ijk}} \Big] \qquad \ldots \quad (IX.5.5) $$

(IX.6.) THE TENSOR EXCHANGE TERM

The exchange term of the tensor force ${}^{t}E_{J\ell' M(D-s)}(r)$ is given in both cases by:

$$ {}^{t}E^{S'}_{J\ell' M(D-s)}(r) = -(4/3)^4 \frac{M}{\hbar^2} \sum_{\ell', S} \sum_{m', m} C_{\ell' S'}(J\ M; m'\ M-m') $$

$$ \times C_{\ell S}(J\ M; m\ M-m) \int_0^\infty dr'\ (rr')\ f^{S}_{J\ell M}(r') \int d\Omega'(\theta', \phi') \int d\Omega(\theta, \phi) $$

$$ \times \overset{*}{Y}{}^{\ell'}_{m'}(\theta, \phi) \langle X^{S'}_{M,m'}(1, \overline{23}) |\ \phi_D(u)\ {}^{t}V^{(II)}(t)\ S_{23}(u^2)\ S_{12}(t^2) | X^{S}_{M-m}(2, \overline{13}) \rangle $$

$$ \times \phi_s(V)\ Y^{\ell}_{m}(\theta', \phi') \qquad \ldots \quad (IX.6.1) $$

Following the same procedure as in the (s-D) case, we finally obtain from equation (IX.6.1) the following expressions

$$ {}^{t}E_{J\ell' M(D-s)}(r) = \sum_{\ell} \int_0^\infty dr\ (rr')\ {}^{t}e_3^{(1)}(r', r)\ f^{\frac{1}{2}}_{J\ell M}(r') $$

$$ \times \Big\{ \Big[(4r^4 - 34 r^2 r'^2 + 16 r'^4) + \frac{(16 r'^2 - 3r^2)}{C''_{kij}} + \frac{22}{C''^2_{kij}} \Big] $$

$$ \times I_{\ell'+\frac{1}{2}}(C''_{kij}\ rr')\ \delta(\ell', \ell) + \Big[(16 r'^3 r - 3 r^3 r' + 44 \frac{rr'}{C''_{kij}} $$

$$ I'_{\ell'+\frac{1}{2}}(C''_{kij}\ rr') + 22 r^2 r'^2\ I''_{\ell'+\frac{1}{2}}(C''_{kij}\ rr') \Big]\ \delta(\ell', \ell) $$

$$ + \sum_{L} F_1(\ell\ell'; \tfrac{1}{2} L) \Big[(2r'^2 - r^2 + 1)\ I_{+\frac{1}{2}}(C''_{kij}\ rr') - rr'\ I'_{+\frac{1}{2}} $$

$$ \times (C''_{kij}\ rr') \Big] \Big\} \qquad \ldots \quad (IX.6.2) $$

and in the doublet state

$$ {}^{t}E_{J\ell' M(D-s)}(r) = \sum_{\ell} \int_{0}^{\infty} dr'(rr')\ {}^{t\,(2)}e_3(r,r')\ f^{3/2}_{J\ell M}(r') \Big\{ \Big[\Big[(8r'^4 $$

$$ - 2 r^4 - 17 r^2 r'^2) - \frac{2}{C''_{kij}} (8 r'^2 - 4 r^2 - 11)(2\ell' - 1) \Big] $$

$$ \times I_{\ell'+\frac{1}{2}}(C''_{kij}\ rr') + A(\ell' 3/2\ ;\ \ell 3/2) \Big[\Big\{ \Big[22 r'^2 + 11 r^2 $$

$$ - \frac{(2\ell' - 1)}{C''_{kij}} \Big] I_{\ell'+\frac{1}{2}}(C''_{kij}\ rr') - \Big\{ \Big[11 r'^2 - 10 r^2 - \frac{(2\ell - 1)}{2\, C''_{kij}} \Big\} $$

$$ \times I_{\ell+\frac{1}{2}}(C''_{kij}\ rr') + \sum_{L} FF(\ell\ \ell;L) \Big\{ \Big[r^2 - 2 r'^2 - 9 rr' + \frac{19}{2C''_{kij}} $$

$$ \times (2 L+1) \Big] \Big\} I_{L+\frac{1}{2}}(C''_{kij}\ rr') \Big] + A(\ell' 3/2\ ;\ \ell 3/2) \Big[rr'\ I_{\ell+3/2}(C''_{kij} rr') $$

$$ - 2 rr'\ I_{\ell'+3/2}(C''_{kij}\ rr') + 19 rr' \sum_{L} FF(\ell' \ell\ ;\ L) $$

$$ \times I_{L+3/2}(C''_{kij}\ rr') \Big] - (8 r'^2 - 4 r^2 - 11)(rr')\ I_{\ell'+3/2}(C''_{kij}\ rr') $$

$$ + \frac{12}{7} \sum_{L} F_5(\ell' \ell\ ;3/2L) \Big[(2r' - r^2)\ I_{L+\frac{1}{2}}(C''_{kij}\ rr') - \frac{1}{2C''_{kij}} $$

$$ \times (2L - 1)\ I_{L+\frac{1}{2}}(C''_{kij}\ rr') - rr'\ I_{L+3/2}(C''_{kij}\ rr') \Big] \Big\} \quad \ldots \quad (IX.6.3) $$

where

$$ {}^{t\,(1)}e_3(r',r) = (4/3)^4 (2/3)^4 \frac{2\pi M}{\hbar^2} \sum_{i,j,k=1}^{2} A'_i\ A_j\ {}^{t\,(3)}U_k $$

$$ \times (2\pi / C''_{kij}\ rr')^{\frac{1}{2}} \mathrm{Exp}(- a''_{jik}\ r'^2 - b''_{jik}\ r^2) \quad \ldots \quad (IX.6.4) $$

and

$$ {}^{t\,(2)}e_3(r',r) = -\,(4/3)^4\,(2/3)^4\,\frac{2\pi M}{\hbar^2}\sum_{i,j,k=1}^{2} A_i'\,A_j\,{}^{t\,(4)}U_k $$

$$ \times\ \mathrm{Exp}(-\,a''_{jik}\,r'^2 - b''_{jik}\,r^2) \qquad \ldots \quad (\mathrm{IX}.6.5) $$

and $F_5(\ell'\ell\ ;\ 3/2\ L)$ was given in (VIII.3.b.4)

(IX.7.) THE SPIN-ORBIT DIRECT TERM

This term is given by the following expression

$$ {}^{s.o}D^{S'}_{J\ell'M(D-s)}(r) = \frac{4Mr}{3\hbar^2}\sum_{\ell,S}\ \sum_{m',m} C_{\ell'S'}(J\ M;m'\ M-m')\ C_{\ell S}(J\ M;m\ M-m) $$

$$ \times \int_0^\infty dR\,R^2\int d\Omega_R(\Theta_R,\phi_R)\int d\Omega(\Theta,\phi)\langle X^{S'}_{M-m'}(1,\overline{23})|\,\phi_D(R)\ {}^{s.o\,(II)}V(\underline{r}_{12})\ Y^{\ell'}_{m'}(\Theta,\phi) $$

$$ \times\ \frac{1}{4}\,(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\ S_{23}(\underline{R}^2)\ |X^S_{M-m}(1,\overline{23})\rangle\ \phi_s(R)\ Y^{\ell}_{m}(\Theta,\Phi)\ \frac{1}{r}\ f^S_{J\ell M}(r) $$

$$ \ldots \quad (\mathrm{IX}.7.1) $$

Since the spin-orbit operator $\frac{1}{4}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\ S_{23}(R^2)$ is a Hermitian as has been indicated before it follows that the result for this operator will be exactly the same as that obtained in (VI.4.5). Hence, the direct spin-orbit interaction term in the doublet state is given by

$$ {}^{s.o}D_{J\ell'M(D-s)}(r) = \sum_{\ell}\ {}^{s.o}B_3(r)\ A_{J\ell}\ f^{\frac{1}{2}}_{J\ell M}(r)\ \delta(\ell',\ell) \ \ldots \quad (\mathrm{IX}.7.1) $$

and in the quartet state, by:

$$ {}^{s.o}_{J\ell' M(D-s)}D(r) = \sum_{\ell} \Big[{}^{s.o\,2}B_3(r)\, A_{J\ell}\, \delta(\ell',\ell) + {}^{s.o\,3}B_3(r)\, A(\ell' 3/2;\ell 3/2) $$

$$ + {}^{s.o}B_3(r)\, E_1(\ell' 3/2 \,;\, \ell 3/2) \Big] f^{3/2}_{J\ell M}(r) \qquad \ldots \quad (IX.7.2) $$

where

$$ {}^{s.o\,1}B_3(r) = \frac{4\,M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i'\, A_j\, {}^{s.o\,(1)}U_k\, \lambda''^{-5/2}_{ijk}\, \gamma''_{ijk} $$

$$ \times \Big[{}^{s.o\,(1)}\mu_k\, (1 - \tfrac{1}{2}\, \gamma''_{ijk})\, r^2 - \tfrac{5}{2} \Big] \mathrm{Exp}(-({}^{s.o\,(1)}\mu_k - \lambda''_{ijk}\, \gamma''_{ijk}) r^2) $$

$$ \ldots \quad (IX.7.3) $$

$$ {}^{s.o\,2}B_3(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i'\, A_j\, {}^{s.o\,(2)}U_k\, (\pi / \lambda''_{ijk})^{3/2} $$

$$ \times \Big[\frac{7}{8}\, \frac{\gamma''_{ijk}}{\lambda''_{ijk}} - \frac{1}{2}\, (1 - \tfrac{1}{2}\, \gamma''_{ijk})^2 r^2 \Big] \mathrm{Exp}(- {}^{s.o\,(2)}\mu_k\, (1 - \frac{{}^{s.o\,(2)}\mu_k}{4\, \lambda''_{ijk}}) r^2) $$

$$ \ldots \quad (IX.7.4) $$

$$ {}^{s.o\,3}B_3(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i'\, A_j\, {}^{s.o\,(2)}U_k\, (\alpha_i' + \alpha_j)\, \frac{\gamma''_{ijk}}{\lambda''_{ijk}}\, (\pi / \lambda''_{ijk})^{3/2} $$

$$ \times\, \mathrm{Exp}(- {}^{s.o\,(2)}\mu_k\, (1 - \frac{{}^{s.o\,(2)}\mu_k}{4\, \lambda''_{ijk}}) r^2) \qquad \ldots \quad (IX.7.5) $$

and

$$ {}^{s.o\,4}B_3(r) = \frac{M r^2}{\hbar^2} \sum_{i,j,k=1}^{2} A_i'\, A_j\, {}^{s.o\,(2)}U_k\, \gamma''^{2}_{ijk}\, (1 - \tfrac{1}{2}\, \gamma''_{ijk}) $$

$$ \times\, (\pi / \lambda''_{ijk})^{3/2}\, \mathrm{Exp}(- {}^{s.o\,(2)}\mu_k\, (1 - \frac{{}^{s.o\,(2)}\mu_k}{4\, \lambda''_{ijk}}) r^2) \qquad \ldots \quad (IX.7.6) $$

and $E_1(\ell' 3/2;\ell 3/2)$ was given in (VI.4.8.5)

CHAPTER X

THE COMPLETE INTEGRODIFFERENTIAL EQUATIONS FOR THE (P-d)-SCATTERING

The resulting terms obtained in the previous chapters are now collected, regrouped and finally put into a form suitable for numerical computation.

(X.1.) THE DOUBLET STATE

The integrodifferential equations describing the scattering of nucleons by deuterons are written in the form of single equations for $\ell', \ell = |J-\frac{1}{2}|$ and $J+\frac{1}{2}$ for $J \geq \frac{1}{2}$.

$$D^2_{\ell'} F_{\ell}(r) + \sum_{\ell} \Big[U_{\ell'\ell}(r) F_{\ell}(r) + {}^{Q}P_{\ell'\ell}(r) F_{\ell}(r) + {}^{Q}V_{\ell'\ell}(r) \times \frac{d}{dr} F_{\ell}(r) + {}^{Q}X_{\ell'\ell}(r) \frac{d^2}{dr^2} F_{\ell}(r) + \int_0^{\infty} dr' \, Q_{\ell'\ell}(r,r') F_{\ell}(r') \Big] = 0 \qquad \text{... (X.1.1)}$$

where

$$D^2_{\ell'} = \frac{d^2}{dr^2} - \frac{\ell'(\ell'+1)}{r^2} + K^2 \qquad \text{... (X.1.2)}$$

and

$$K^2 = \frac{4M}{3\hbar^2} E_p \qquad \text{... (X.1.3)}$$

and where

$$U_{\ell'\ell}(r) = {}^{c}U_{\ell'\ell}(r) + {}^{coul}U_{\ell'\ell}(r) + {}^{s.o}U_{\ell'\ell}(r) + {}^{Q}U_{\ell'\ell}(r) + {}^{s.o\,\prime}U_{\ell'\ell}(r)$$

$$+ {}^{t}U'_{\ell\ell}(r) + {}^{s.o}U''_{\ell\ell}(r) + {}^{t}U''_{\ell\ell}(r) \qquad \ldots \quad (X.1.4)$$

$$^{Q}P_{\ell\ell}(r) = \frac{4M}{3\hbar^2}\left[\frac{4}{3}\,{}^{Q(1)}P_{\ell\ell}(r) - 3\,{}^{Q(2)}P_{\ell\ell}(r)\right]\left[\ell(\ell+1)\right] \qquad \ldots \quad (X.1.5)$$

$$^{Q}V_{\ell\ell}(r) = \frac{4M}{3\hbar^2}\left[\frac{4}{3}\,{}^{Q(1)}V_{\ell\ell}(r) - 3\,{}^{Q(2)}V_{\ell\ell}(r)\right] \qquad \ldots \quad (X.1.6)$$

and

$$^{Q}X_{\ell\ell}(r) = \frac{4M}{3\hbar^2\lambda_{ijk}}\left[\frac{3}{4}\,{}^{Q(1)}X_{\ell\ell}(r) - \frac{27}{16}\,{}^{Q(2)}X_{\ell\ell}(r)\right] \qquad \ldots \quad (X.1.7)$$

and

$$Q_{\ell\ell}(r,r') = {}^{c}K_{\ell\ell}(r;r') + {}^{coul}K_{\ell\ell}(r,r') + {}^{s.o}K_{\ell\ell}(r,r') + {}^{Q}K_{\ell\ell}(r,r')$$

$$+ {}^{s.o}K'_{\ell\ell}(r,r') + {}^{t}K'_{\ell\ell}(r,r') + {}^{s.o}K''_{\ell\ell}(r,r') + {}^{t}K''_{\ell\ell}(r,r')$$

$$+ W_{\ell\ell}(r,r') + T_{\ell\ell}(r,r') \qquad \ldots \quad (X.1.8)$$

The symbols attached represent the contribution from various interactions. The prime and the double prime denote the (s-D) and (D-s) interactions respectively. Thus,

$$^{c}U_{\ell\ell}(r) = -\frac{4M}{3\hbar^2}\sum_{i,j,k=1}^{2} A_i A_j\, {}^{c(1)}U_k\, (\pi/\lambda_{ijk})^{3/2}\, \mathrm{Exp}(-\mu_k^{Q(1)}(1-\gamma_{ijk}/2)r^2) \qquad \ldots \quad (X.1.9)$$

$$^{coul}U_{\ell\ell}(r) = -\frac{8Me^2\pi}{3\hbar^2 r}\sum_{i,j=1}^{2} A_i A_j\,(\pi/(\alpha_i+\alpha_j))^{1/2} \qquad \ldots \quad (X.1.10)$$

$$ {}^{s.o}U_{\ell'\ell}(r) = -\frac{M}{\hbar^2}\sum_{i,j,k=1}^{2} A_i\, A_j\, {}^{s.o\,(1)}U_k\, A_{J\ell}\,(\pi/\lambda_{ijk})^{3/2} $$

$$ \times\,(1-\gamma_{ijk}/2)\,\mathrm{Exp}(-{}^{s.o\,(1)}\mu_k\,(1-{}^{s.o\,(1)}\mu_k/4\,\lambda_{ijk})r^2) \quad \ldots \quad (X.1.11) $$

$$ {}^{Q}U_{\ell'\ell}(r) = \frac{4\,M}{\hbar^2}\left[\frac{4}{3}\,{}^{Q\,(1)}U_{\ell'\ell}(r) - 3\,{}^{Q\,(2)}U_{\ell'\ell}(r)\right] \quad \ldots \quad (X.1.12) $$

where

$$ {}^{Q\,(II)}U_{\ell'\ell}(r) = \sum_{i,j,k=1}^{2} A_i\, A_j'\, {}^{Q\,(II)}U_k\,(\pi/\lambda_{ijk})^{3/2}\left[\frac{3}{2}\,\phi_{ij}+\delta_{ij}(1-3\,\gamma_{ijk}/4)\right. $$

$$ \left. +\,4\alpha_j r^2\,\eta_{ijk}\right]\mathrm{Exp}(-{}^{Q\,(II)}\mu_k\,(1-{}^{Q\,(II)}\mu_k/4\,\lambda_{ijk})r^2) $$

$$ (II=1,2) \quad \ldots \quad (X.1.13) $$

$$ {}^{s.o}U'_{\ell'\ell}(r) = -\frac{M}{4\hbar^2}\sum_{i,j,k=1}^{2} A_i\, A_j'\, {}^{s.o\,(1)}U_k\,(\pi/\lambda_{ijk})^{3/2} $$

$$ \times\,(\gamma'_{ijk}/\lambda'_{ijk})\left[{}^{s.o\,(1)}\mu_k\,(1-\gamma'_{ijk}/2)r^2-5/2\right] $$

$$ \times\,\mathrm{Exp}(-{}^{s.o\,(1)}\mu_k\,(1-{}^{s.o\,(1)}\mu_k/4\,\lambda_{ijk})r^2) \quad \ldots \quad (X.1.14) $$

$$ {}^{t}U'_{\ell'\ell}(r) = -\frac{4\,M}{3\hbar^2}\sum_{i,j,k=1}^{2} A_i\, A_j'\, {}^{t\,(1)}U_k\,(\pi/\lambda'_{ijk})^{3/2} $$

$$ \times\left[-4\,\gamma'^{2}_{ijk}\,(1-\gamma'_{ijk}/2)^2\, r^4+(10\gamma'_{ijk}/\lambda'_{ijk})\,(1-\gamma'_{ijk}/2)r^2\right. $$

$$ \left.-\,15/4\,\lambda'^{2}_{ijk}\right]\mathrm{Exp}(-{}^{t\,(1)}\mu_k\,(1-{}^{t\,(1)}\mu_k/4\,\lambda'_{ijk})r^2) \quad \ldots \quad (X.1.15) $$

$$ {}^{s.o}U''_{\ell'\ell}(r) = -\frac{M}{4\hbar^2}\sum_{i,j,k=1}^{2} A_i'\, A_j\, {}^{s.o\,(1)}U_k\,(\pi/\lambda''_{ijk})^{3/2} $$

$$\times\ (\gamma''_{jik} / \lambda''_{jik}) \left[\overset{s.o\ (1)}{\mu_k} (1 - \gamma''_{jik}/2) r^2 - 5/2 \right]$$

$$\times\ \mathrm{Exp}(- \overset{s.o\ (1)}{\mu_k} (1 - \overset{s.o\ (1)}{\mu_k} / 4\ \lambda''_{jik}) r^2) \qquad \ldots \quad (X.1.16)$$

$$\overset{t}{U''}_{\ell'\ell}(r) = - \frac{4\ M}{3\hbar^2} \sum_{i,j,k=1}^{2} A'_i\ A_j\ \overset{t\ (1)}{U_k} (\pi / \lambda''_{jik})^{3/2} \left[-4\ \gamma''^2_{ijk} \right.$$

$$\times\ (1 - \gamma''_{jik}/2)^2\ r^4 + (10\ \gamma''_{jik} / \lambda''_{jik})(1 - \gamma''_{jik}/2) r^2$$

$$\left. - 15/4\ \lambda''_{jik} \right] \mathrm{Exp}(- \overset{t\ (1)}{\mu_k} (1 - \overset{t\ (1)}{\mu_k} / 4\ \lambda''_{jik}) r^2) \qquad \ldots \quad (X.1.17)$$

$$\overset{Q\ (II)}{P}_{\ell'\ell}(r) = \sum_{i,j,k=1}^{2} A_i\ A_j\ \overset{Q\ (II)}{U_k} (\pi / \lambda_{ijk})^{3/2}\ \psi_{ijk}$$

$$\times\ \mathrm{Exp}(- \overset{Q\ (II)}{\mu_k} (1 - \overset{Q\ (II)}{\mu_k} / 4\ \lambda_{ijk})\ r^2)$$

$$(II=1,2) \qquad \ldots \quad (X.1.18)$$

and

$$\overset{Q\ (II)}{V}_{\ell'\ell}(r) = \sum_{i,j,k=1}^{2} A_i\ A_j\ \overset{Q\ (II)}{U_k} (\pi / \lambda_{ijk})^{3/2} \left[\frac{3}{2}\ r(1 + \gamma_{ijk} - 3/4\ \gamma^2_{ijk}) \right.$$

$$\left. - 3\alpha_j / \lambda_{ijk} \right] \mathrm{Exp}(- \overset{Q\ (II)}{\mu_k} (1 - \overset{Q\ (II)}{\mu_k} / 4\ \lambda_{ijk}) r^2)$$

$$(II=1,2) \qquad \ldots \quad (X.1.19)$$

and $\overset{Q\ (II)}{X}_{\ell\ell}(r) = \overset{Q\ (II)}{B}_{L_{12}}(r)$ where $\overset{Q\ (II)}{B}_{L_{12}}(r)$ was given in (III.5.12).

$$\overset{c}{K}_{\ell'\ell}(r,r') = (4/3)^4\ \frac{2\ M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i\ A_j\ \overset{c\ (3)}{U_k} (2\pi / C_{ijk} rr')^{\frac{1}{2}}$$

$$\times\ I_{\ell+\frac{1}{2}}(C_{ijk}\ rr')\ \mathrm{Exp}(- a_{ijk}\ r^2 - b_{ijk}\ r'^2) \qquad \ldots \quad (X.1.20)$$

$$ {}^{coul}K'_{\ell\ell}(r,r') = +\,(4/3)^4 \frac{3\pi\, Me^2 rr'}{\hbar^2} \sum_{i,j=1}^{2} A_i\, A_j $$

$$ \times\ \mathrm{Exp}(-\,e_{ij}\, r^2 - f_{ij}\, r'^2) \int_{-1}^{+1} d\eta\, P_\ell(\eta)\,(r^2 + r'^2 - 2\,\underline{r}\cdot\underline{r}')^{-\frac{1}{2}} $$

$$ \times\ \mathrm{Exp}(\,b_{ij}\,\underline{r}\cdot\underline{r}') \qquad \ldots \quad (X.1.21) $$

$$ {}^{s.o}K'_{\ell\ell}(r,r') = (4/3)^4 \frac{16\pi M\, rr'}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i\, A_j\, {}^{s.o\,(3)}U_k $$

$$ \times \left[\,(\alpha_i + \alpha_j)\,/\,C_{ijk}\right] (2\pi/\,C_{ijk}\, rr')^{\frac{1}{2}}\, A_{J\ell}\, I_{\ell+\frac{1}{2}}(C_{ijk}\, rr') $$

$$ \times\ \mathrm{Exp}(-\,a_{ijk}\, r^2 - b_{ijk}\, r'^2) \qquad \ldots \quad (X.1.22) $$

$$ {}^{Q}K'_{\ell\ell}(r,r') = -\,{}^{Q}E'_{J\ell\,M(s-s)}(r) \qquad \ldots \quad (X.1.23) $$

where ${}^{Q}E'_{J\ell\,M(s-s)}(r)$ was given in (V.5.30)

$$ {}^{s.o}K'_{\ell\ell}(r,r') = -\,{}^{s.o}E'_{J\ell\,M(s-D)}(r) \qquad \ldots \quad (X.1.24) $$

${}^{s.o}E'_{J\ell\,M(s-D)}(r)$ was given in (VIII.4.10)

$$ {}^{t}K'_{\ell\ell}(r,r') = -\,{}^{t}E'_{J\ell\,M(s-D)}(r) \qquad \ldots \quad (X.1.25) $$

where ${}^{t}E'_{J\ell\,M(s-D)}(r)$ was given (VIII.3.a.3)

$$ {}^{s.o}K''_{\ell\ell}(r',r) = {}^{s.o}K'_{\ell\ell}(r \rightarrow r',\ r' \rightarrow r\ ,\ i \longleftrightarrow j) \ldots \quad (X.1.26) $$

and

$$ {}^{t}K''_{\ell\ell'}(r',r) = {}^{t}K'_{\ell\ell'}(r \rightarrow r',\ r' \rightarrow r\ ,\ i \longleftrightarrow j). \quad \ldots \quad (X.1.27)$$

we have also

$$ W_{\ell\ell'}(r,r') = W_{J\ell\ell' M(s-s)}(r) + W_{J\ell\ell' M(s-D)}(r) \quad \ldots \quad (X.1.28)$$

$$ T_{\ell\ell'}(r,r') = T_{J\ell\ell' M(s-s)}(r) + T_{J\ell\ell' M(s-D)}(r) \quad \ldots \quad (X.1.29)$$

where $W_{J\ell\ell' M(s-s)}(r)$ ane $W_{J\ell\ell' M(s-D)}(r)$ were given in (IV.1.5)

and (VII.1.2) respectively.

and $T_{J\ell\ell' M(s-s)}(r)$ and $T_{J\ell\ell' M(s-D)}(r)$ were given in (IV.2.19) and

(VII.2.5) respectively.

(X.2.) THE QUARTET STATE

The integral equations in the quartet state have the following form:

$$D^2_{\ell'} F_{\ell}(r) + \sum_{\ell} \Big[U_{\ell'\ell}(r) + {}^{Q}P_{\ell'\ell}(r)\, F_{\ell}(r) + {}^{Q}V_{\ell'\ell}(r) \frac{d}{dr} F_{\ell}(r)$$

$$+ X_{\ell'\ell}(r) \frac{d^2}{dr^2} F_{\ell}(r) + \int_0^{\infty} dr' \Big\{ K_{\ell'\ell}(r,r') + W_{\ell'\ell}(r,r')$$

$$+ T_{\ell'\ell}(r,r') \Big\} F_{\ell}(r') \Big] = 0 \qquad \ldots \text{(X.2.1)}$$

There are two coupled equations for $\ell', \ell = |J-3/2|, \ldots, J+\frac{3}{2}$ with $J \geq 3/2$, and another two independent equations for $\ell' = \ell = 1,2$ but with $J = \frac{1}{2}$.

The operator $D^2_{\ell'}$ was given in (X.1.2) and the functions $U_{\ell'\ell}(r)$, ${}^{Q}p_{\ell'\ell}(r)$, ${}^{Q}V_{\ell'\ell}(r)$ and ${}^{Q}X_{\ell'\ell}(r)$ as well as the kernels $K_{\ell'\ell}(r,r')$, $W_{\ell'\ell}(r,r')$ and $T_{\ell'\ell}(r,r')$ are all given below. Thus,

$$U_{\ell'\ell}(r) = {}^{c}U_{\ell'\ell}(r) + {}^{coul}U_{\ell'\ell}(r) + {}^{s.o}U_{\ell'\ell}(r) + {}^{t}U_{\ell'\ell}(r) + {}^{Q}U_{\ell'\ell}(r)$$

$$+ {}^{c}U'_{\ell'\ell}(r) + {}^{c}U''_{\ell'\ell}(r) + {}^{coul}U'_{\ell'\ell}(r) + {}^{coul}U''_{\ell'\ell}(r) + {}^{s.o}U'_{\ell'\ell}(r) + {}^{s.o}U''_{\ell'\ell}(r)$$

$$+ {}^{t}U'_{\ell'\ell}(r) + {}^{t}U''_{\ell'\ell}(r) \qquad \ldots \text{(X.2.2)}$$

$${}^{Q}P_{\ell'\ell}(r) = -\ell(\ell+1) \Big[{}^{Q}P^{(1)}_{\underline{L}_{12}}(r) + {}^{Q}P^{(1)}_{\underline{M}_{12}}(r) \Big] \qquad \ldots \text{(X.2.3)}$$

$${}^{Q}V_{\ell'\ell}(r) = - {}^{Q}V^{(1)}_{\underline{L}_{12}}(r) - {}^{Q}V^{(1)}_{\underline{M}_{12}}(r) \qquad \ldots \text{(X.2.4)}$$

$$^{Q}X_{\ell'\ell}(r) = {}^{Q}X^{(1)}_{\underline{L}_{12}}(r) - H_1(\ell, L)\; {}^{Q}X^{(1)}_{\underline{M}_{12}}(r) \qquad \ldots \quad (X.2.5)$$

where ${}^{Q}X^{(1)}_{\underline{L}_{12}}(r) = (9/16\lambda_{ijk})\, {}^{Q}B^{(II)}_{\underline{L}_{12}}(r)$; ${}^{Q}X^{(1)}_{\underline{M}_{12}}(r) = {}^{Q}B^{(1)}_{\underline{M}_{12}}(r)$

and ${}^{Q}B^{(1)}_{\underline{L}_{12}}(r)$ and ${}^{Q}B^{(1)}_{\underline{M}_{12}}(r)$ are given in (III.5.12) and (III.5.16) respectively.

$$K_{\ell'\ell}(r,r') = {}^{c}K_{\ell'\ell}(r,r') + {}^{coul}K_{\ell'\ell}(r,r') + {}^{s.o}K_{\ell'\ell}(r,r')\; {}^{t}K_{\ell'\ell}(r,r')$$

$$ {}^{Q}K_{\ell'\ell}(r,r') + {}^{s.o}K'_{\ell'\ell}(r,r') + {}^{s.o}K''_{\ell'\ell}(r,r') + {}^{t}K'_{\ell'\ell}(r,r')$$

$$+ {}^{t}K''_{\ell'\ell}(r,r') \qquad \ldots \quad (X.2.6)$$

$$W_{\ell'\ell}(r,r') = W^{(1)}_{\ell'\ell}(r) \quad + W^{(2)}_{\ell'\ell}(r) \qquad \ldots \quad (X.2.7)$$

and

$$T_{\ell'\ell}(r,r') = T^{(1)}_{\ell'\ell}(r) \quad + T^{(2)}_{\ell'\ell}(r) \qquad \ldots \quad (X.2.8)$$

Thus,

$$ {}^{c}U_{\ell'\ell}(r) = -\frac{4\,M}{3\hbar^2}\sum_{i,j,k=1}^{2} A_i\, A_j\; {}^{c}U^{(2)}_{K}\,(\pi/\lambda_{ijk})^{3/2}$$

$$\times\, \mathrm{Exp}(-\,{}^{c}\mu^{(2)}_{k}\,(1-\,{}^{c}\mu^{(2)}_{k}\,/\,4\,\lambda_{ijk})r^2) \qquad \ldots \quad (X.2.9)$$

$$ {}^{coul}U_{\ell'\ell}(r) = -\frac{8\,M\,e^2\pi}{3\,\hbar^2\,r}\sum_{i,j=1}^{2} A_i\, A_j\,(\pi/(\alpha_i+\alpha_j))^{1/2}$$

$$\ldots \quad (X.2.10)$$

$$ {}^{t}U_{\ell'\ell}(r) = -\frac{4Mr^2}{3\,\hbar^2}\sum_{i,j,k=1}^{2} A_i\, A_j\; {}^{t}U^{(2)}_{k}\,(\pi/\lambda_{ijk})^{3/2}\,(1-\gamma_{ijk}/2)^2$$

$$\times\, A(\ell' 3/2\; ;\; \ell 3/2)\; \mathrm{Exp}(-\,{}^{t}\mu^{(2)}_{k}\,(1-\,{}^{t}\mu^{(2)}_{k}\,/4\,\lambda_{ijk})\,r^2)$$

$$\ldots \quad (X.2.11)$$

$$ {}^{s.o}U_{\ell'\ell}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i A_j \, {}^{s.o}U_k^{(2)} \, (\pi/\lambda_{ijk})^{3/2} \, (1-\gamma_{ijk}/2) $$

$$ \times A_{J\ell} \, \delta(\ell',\ell) \, \mathrm{Exp}(- {}^{s.o}\mu_k^{(2)} (1- {}^{s.o}\mu_k^{(2)} / 4 \lambda_{ijk}) r^2) $$

... (X.2.12)

$$ {}^{Q}U_{\ell'\ell}(r) = {}^{Q}U^{(1)}_{\underline{L}_{12}}(r) - {}^{Q}U^{(1)}_{\underline{M}_{12}}(r) \qquad \ldots \quad (X.2.13) $$

where

$$ {}^{Q}U^{(1)}_{\underline{L}_{12}}(r) = \frac{4M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i \, A_j \, {}^{Q}U_k^{(1)} \, (\pi/\lambda_{ijk})^{3/2} $$

$$ \times \left[\frac{3}{2} \phi_{ij} + \delta_{ij} (1 - (3/4)\gamma_{ijk}) + 4\alpha_j \, r^2 \, \eta_{ijk} \right] $$

$$ \times \mathrm{Exp}(- {}^{Q}\mu_k^{(1)} (1 - {}^{Q}\mu_k^{(1)} / 4 \lambda_{ijk}) r^2) \qquad \ldots \quad (X.2.14) $$

and

$$ {}^{Q}U^{(1)}_{\underline{M}_{12}}(r) = {}^{Q}B^{(4)}_{\underline{M}_{12}}(r) \qquad \ldots \quad (X.2.15) $$

where ${}^{Q}B^{(4)}_{\underline{M}_{12}}(r)$ was given in (III.5.19).

$$ {}^{c}U'_{\ell'\ell}(r) = - \frac{4M}{3\hbar^2} \, A(\ell' 3/2 \, ; \, \ell 3/2) \sum_{i,j,k=1}^{2} A_i \, A'_j \, {}^{c}U_k^{(2)} \, \gamma'^2_{ijk} $$

$$ \times (\pi/\lambda'_{ijk})^{3/2} \, \mathrm{Exp}(- {}^{c}\mu_k^{(2)} (1 - {}^{c}u_k^{(2)} / 4 \lambda'_{ijk}) r^2) $$

... (X.2.16)

$$ {}^{coul\ 1}U_{\ell'\ell}(r) = - \frac{M e^2}{4 \hbar^2 r^3} \, A(\ell' 3/2; \ell 3/2) \sum_{i,j=1} A_i A'_j \, (1/\alpha_i + \alpha'_j)^2 $$

$$ \times (\pi/(\alpha_i + \alpha'_j))^{3/2} \qquad \ldots \quad (X.2.17) $$

$$ {}^{t}U'_{\ell'\ell}(r) = -\frac{4M}{3\hbar^2}\sum_{i,j,k=1}^{2} A_i A'_j \; {}^{t}U_k^{(2)} (\pi/\lambda_{ijk})^{3/2} $$

$$ \times \Big\{ A(\ell 3/2\; ; \ell 3/2) \Big[\gamma'^{2}_{ijk} (1 - \gamma^{2}_{ijk}/2) r^4 - \frac{7}{4} (\gamma'_{ijk}/\lambda'_{ijk}) $$

$$ \times (1 - \gamma'_{ijk}/2) r^2 \Big] + 2\, \gamma'^{2}_{ijk} (1 - \tfrac{1}{2}\gamma'_{ijk})^2 r^4 - (5\, r^2/\lambda'_{ijk}) $$

$$ \times \gamma'_{ijk} (1 - \gamma'_{ijk}/2) + (15/8\, \lambda'^{2}_{ijk}) \Big\} \mathrm{Exp}(- {}^{t}\mu_k^{(2)} $$

$$ \times (1 - {}^{t}\mu_k^{(2)}/4\lambda'_{ijk}) r^2) \qquad \ldots \quad (X.2.18) $$

$$ {}^{s.o}U'_{\ell'\ell}(r) = -\frac{M}{\hbar^2}\sum_{i,j,k=1}^{2} A_i A'_j \; {}^{s.o}U_k^{(2)} (\pi/\lambda'_{ijk})^{3/2} $$

$$ \times \Big\{ \Big[(7\gamma'_{ijk}/8\lambda'_{ijk}) + \tfrac{1}{2}(1 - \gamma'_{ijk}/2)\, \gamma'^{2}_{ijk} r^2 \Big] A_{J\ell}\, \delta(\ell',\ell) $$

$$ + (\gamma'_{ijk}/\lambda'_{ijk}) (\alpha_i + \alpha'_j) A(\ell' 3/2\; ; \ell 3/2) + \gamma'^{2}_{ijk} r^2 $$

$$ \times (1 - \gamma'_{ijk}/2)\, E_1(\ell' 3/2\; ; \ell 3/2) \Big\} \mathrm{Exp}(- {}^{s.o}\mu_k^{(2)} $$

$$ \times (1 - {}^{s.o}\mu_k^{(2)}/4\lambda'_{ijk}) r^2) \qquad \ldots \quad (X.2.19) $$

The (D-s)-terms can be obtained by the interchange of i and j respectively. i.e. the (D-s) term of the central interaction

$$ {}^{c}U''_{\ell'\ell}(r) = -\frac{4M}{3\hbar^2} A(\ell' 3/2\ ;\ \ell 3/2) \sum_{i,j,k=1}^{2} A_i\ A_j\ {}^{c}U_k^{(2)}\ \gamma''^{2}_{ijk} $$

$$ \times\ (\pi/\lambda''_{ijk})^{3/2}\ \mathrm{Exp}(-\ {}^{c}\mu_k^{(2)}\ (1-\ {}^{c}\mu_k^{(2)}/4\lambda''_{ijk})r^2) \quad \ldots \quad (X.2.20) $$

we also have

$$ {}^{Q}P^{(1)}_{\underline{L}_{12}}(r) = \frac{4M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i\ A_j\ {}^{Q}U_k^{(1)}\ \psi_{ijk}\ (\pi/\lambda_{ijk})^{3/2}\ \cdot $$

$$ \times\ \mathrm{Exp}(-\ {}^{Q}\mu_k^{(1)}\ (1-\ {}^{Q}\mu_k^{(1)}/4\lambda_{ijk})r^2) \quad \ldots \quad (X.2.21) $$

$$ {}^{Q}P^{(1)}_{\underline{M}_{12}}(r) = \frac{M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i\ A_j\ {}^{Q}U_k^{(1)}\ (\pi/\lambda_{ijk})^{3/2} \left[2-5r\ {}^{Q}\mu_k^{(1)}/4\lambda_{ijk}\right] $$

$$ \times\ \mathrm{Exp}(-\ {}^{Q}\mu_k^{(1)}\ (1-\ {}^{Q}\mu_k^{(1)}/4\lambda_{ijk})r^2) \quad \ldots \quad (X.2.22) $$

$$ {}^{Q}V^{(1)}_{\underline{L}_{12}}(r) = \frac{4M}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i\ A_j\ {}^{Q}U_k^{(1)}\ (\pi/\lambda_{ijk})^{3/2} \left[\frac{3}{2}(1+\gamma_{ijk}\right. $$

$$ \left. -\ \frac{3}{4}\gamma^2_{ijk})r^2 - 3\alpha_j\ r/\lambda_{ijk}\right]\ \mathrm{Exp}(-\ {}^{Q}\mu_k^{(1)}(1-\ {}^{Q}\mu_k^{(1)}/4\lambda_{ijk})r^2) $$

$$ \ldots \quad (X.2.23) $$

and

$$ {}^{Q}V^{(1)}_{\underline{M}_{12}}(r) = {}^{Q}B^{(2)}_{\underline{M}_{12}}(r) \quad \ldots \quad (X.2.24) $$

where ${}^{Q}B^{(2)}_{\underline{M}_{12}}(r)$ was given in (III.5.17)

$$ {}^{c}K_{\ell'\ell}(r,r') = (4/3)^4\ \frac{2\pi M}{\hbar^2} \sum_{i,j,k=1}^{2} A_i\ A_j\ {}^{Q}U_k^{(4)}\ (2\pi/C_{ijk}\ rr')^{\frac{1}{2}} $$

$$\times I_{\ell+\frac{1}{2}}(C_{ijk}\, rr')\, \mathrm{Exp}(-\, a_{ijk}\, r^2 - b_{ijk}\, r'^2) \qquad \ldots \quad (X.2.25)$$

$${}^{coul}K_{\ell'\ell}(r,r') = (4/3)^4 \frac{3\pi M e^2 rr'}{\hbar^2} \sum_{i,j,=1}^{2} A_i\, A_j\, \mathrm{Exp}(-\, e_{ij} r^2 - f_{ij} r'^2)$$

$$\times \int_{-1}^{+1} d\eta\, P_\ell(\eta)\, (r^2 + r'^2 - 2\underline{r}\cdot\underline{r}')^{-\frac{1}{2}}\, \mathrm{Exp}(b_{ij}\, \underline{r}\cdot\underline{r}') \ldots \quad (X.2.26)$$

$${}^{t}K_{\ell'\ell}(r,r') = (4/3)^4 \frac{8\pi M}{9\hbar^2} \sum_{i,j,k=1}^{2} A_i\, A_j\, {}^{t}U_k^{(4)}\, (2\pi/C_{ijk}\, rr')^{\frac{1}{2}}$$

$$\times \mathrm{Exp}(-\, a_{ijk}\, r^2 - b_{ijk}\, r'^2)\, A(\ell' 3/2\, ;\, \ell 3/2) \Big[r^2\, I_{\ell+\frac{1}{2}}(C_{ijk}\, rr')$$

$$+ r'^2\, I_{\ell'+\frac{1}{2}}(C_{ijk}\, rr') - rr' \sum_{L} FF(\ell' \ell, L)\, I_{L+\frac{1}{2}}(C_{ijk}\, rr') \Big]$$

$$\ldots \quad (X.2.27)$$

$${}^{s.o}K_{\ell'\ell}(r,r') = (4/3)^4 \frac{16\pi M\, rr'}{3\hbar^2} \sum_{i,j,k=1}^{2} A_i\, A_j\, {}^{s.o}U_k^{(4)}$$

$$\times (2\pi/\, C_{ijk}\, rr')^{\frac{1}{2}} \Big[(\alpha_i + \alpha_j)\, /C_{ijk} \Big]\, A_{J\ell}\, I_{\ell+\frac{1}{2}}(C_{ijk}\, rr')$$

$$\times \mathrm{Exp}(-\, {}^{s.o}\mu_k^{(4)}\, (1 - {}^{s.o}\mu_k^{(4)}\, /4\lambda_{ijk}) r^2) \qquad \ldots \quad (X.2.28)$$

$${}^{Q}K_{\ell'\ell}(r,r') = {}^{Q}E_{J\ell' M(s-s)}(r) \qquad \ldots \quad (X.2.29)$$

where ${}^{Q}E_{J\ell' M(s-s)}(r)$ was given in (V.5.31).

$${}^{c}K'_{\ell'\ell}(r,r') = (4/3)^4 \frac{8\pi M}{9\hbar^2} \sum_{i,j,k=1}^{2} A_i\, A_j\, {}^{c}U_k^{(4)}\, (2\pi/C'_{ijk}\, rr')^{\frac{1}{2}}$$

$$\times A(\ell' 3/2\ ;\ \ell 3/2) \Big[4r^2 \, I_{\ell+\frac{1}{2}}(C'_{ijk}\, rr') + r'^2 \, I_{\ell'+\frac{1}{2}}(C'_{ijk}\, rr')$$

$$+ 2\, rr' \sum_L FF(\ell'\ell\ ;\ L)\, I_{L+\frac{1}{2}}(C'_{ijk}\, rr') \Big] \, Exp(-\mu_k^{c\,(4)} (1-\mu_k^{c\,(4)}/4\lambda'_{ijk}) r^2)$$

$$\ldots \quad (X.2.30)$$

$${}^{coul}K'_{\ell'\ell}(r,r') = -\,{}^{coul}E_{J\ell' M(s-D)}(r) \qquad \ldots \quad (X.2.31)$$

where ${}^{coul}E_{J\ell' M(s-D)}(r)$ was given in (VIII.2.5)

$${}^{t}K'_{\ell'\ell}(r,r') = -\,{}^{t}E_{J\ell' M(s-D)}(r) \qquad \ldots \quad (X.2.32)$$

where ${}^{t}E_{J\ell' M(s-D)}(r)$ was given in (VIII.3.b.2)

$${}^{s.o}K'_{\ell'\ell}(r,r') = -\,{}^{s.o}E_{J\ell' M(s-D)}(r) \qquad \ldots \quad (X.2.33)$$

where ${}^{s.o}E_{J\ell' M(s-D)}(r)$ was given in (VIII.4.15)

$$W^{(1)}_{\ell'\ell}(r,r') = -\,W_{J\ell' M(s-s)}(r) \qquad \ldots \quad (X.2.34)$$

$$W^{(2)}_{\ell'\ell}(r,r') = -\,W_{J\ell' M(s-D)}(r) \qquad \ldots \quad (X.2.35)$$

also where $W_{J\ell' M(s-s)}(r)$ and $W_{J\ell' M(s-D)}(r)$ were given in (IV.1.5) and (VIII.1.2) respectively.

$$T^{(1)}_{\ell'\ell}(r,r') = -\,T_{J\ell' M(s-s)}(r) \qquad \ldots \quad (X.2.36)$$

$$T^{(2)}_{\ell'\ell}(r,r') = -\,T_{J\ell' M(s-D)}(r) \qquad \ldots \quad (X.2.37)$$

where $T_{J\ell' M(s-s)}(r)$ and $T_{J\ell' M(s-D)}(r)$ were given in (IV.2.19) and (VII.2.5) respectively.

Similarly, the (D-s) terms can be obtained by interchanging the variables ℓ', ℓ and i , j as well as the r and r' consecutively. e.g.

$$
\begin{aligned}
{}^{c''}K_{\ell'\ell}(r,r') &= (4/3)^4 \, \frac{8\pi M}{9\hbar^2} \sum_{i,j,k=1}^{2} A'_i \, A_j \, {}^{c}U_k^{(4)} \, (2\pi/C''_{ijk})^{\frac{1}{2}} \\
&\times A(\ell 3/2 \; ; \; \ell' 3/2) \Big[\, r^2 \, I_{\ell+\frac{1}{2}}(C''_{ijk}\, rr') + 4\, r'^2 \, I_{\ell'+\frac{1}{2}}(C''_{ijk}\, rr') \\
&+ 2\, rr' \sum_{L} F(\ell\, \ell' ; L) \, I_{L+\frac{1}{2}}(C''_{ijk}\, rr') \Big] \\
&\times \mathrm{Exp}\big(- {}^{c}\mu_k^{(4)} (1 - {}^{c}\mu_k^{(4)} / 4\, \lambda''_{ijk}) r^2 \big) \qquad \ldots \quad (X.2.38)
\end{aligned}
$$

PART (3)

NUMERICAL ANALYSIS AND COMPUTATION

CHAPTER XI

NUMERICAL METHODS

The numerical work was done on the CDC 6600 and 503 machines, at Chelsea College Computer Centre, Pulton Place, London, S.W.6.

The main purpose of this calculation is to obtain phase-shifts, differential and total cross-sections. In solving the integro-differential equations given in (X.1.1) and (X.2.1), one converts these equations into an equivalent set of algebraic equations and these are then solved by matrix inversion.

The equations required to be solved numerically for p(d,d)p, elastic scattering have the following form:

$$\frac{d^2}{dr^2} F_{\ell}(r) + \sum_{\ell} \Big[Z_{\ell'\ell}(r)\, F_{\ell}(r) + {}^{Q}V_{\ell'\ell}(r) \frac{d}{dr} F_{\ell}(r) + {}^{Q}X_{\ell'\ell}(r) \times \frac{d^2}{dr^2} F_{\ell}(r) + \int_0^{\infty} dr'\, Q_{\ell'\ell}(r,r')\, F_{\ell}(r') \Big] = 0 \qquad \text{... (XI.1)}$$

where

$$Z_{\ell'\ell}(r) = \Big[k^2 - \frac{\ell(\ell+1)}{r^2} \Big] \delta(\ell',\ell) + {}^{Q}P_{\ell'\ell}(r) + U_{\ell'\ell}(r) \qquad \text{... (XI.2)}$$

$$Q_{\ell'\ell}(r,r') = K_{\ell'\ell}(r,r') + W_{\ell'\ell}(r,r') + T_{\ell'\ell}(r,r') \qquad \text{... (XI.3)}$$

and

$$F_{\ell}(r) = f^{S}_{J\ell M}(r)$$

The functions $Z_{\ell'\ell}(r)$, $V_{\ell'\ell}(r)$ and $X_{\ell'\ell}(r)$ converge fairly rapidly as the variables r and r' become large.

In carrying out the computation, we noted that the kernels as well as the matrix solution of the coupled equations consumed most of the time required to solve the problem, and they in fact constitute a major part of the whole computation. For this reason, the basic internal functions (i.e. s- and D- state functions), as well as the potential function, are all chosen to have a Gaussian shapes.

This enables the angular integration part to be carried out analytically in terms of the modified spherical Bessel functions of the type $I_n(X) = (-1)^{-n} J_n(iX)$. Equation(XI.I.1) can now be solved, with the following conditions imposed upon $F_\ell(r)$. That is $F_\ell(0) = 0$ and $F_\ell(h) = 1$, where h is the interval of integration. Again, the kernels in(XII.1)converge rapidly, and this enables us to replace the infinite limit in the integral by a convenient finite limit R', and the range of integration can be split up into a number of pivotal points r'_0, r'_1, r'_2, ...- , R' at small interval h (Robertson, 1955).

Thus,

$$\int_0^\infty Q_{\ell'\ell}(r,r')\, F_\ell(r')\, dr' = \int_0^{R'} Q_{\ell'\ell}(r,r')\, F_\ell(r')\, dr' \quad \ldots \text{(XI.4)}$$

At $r = r_n$, the integral can be expanded as a sum

$$\int_0^{R'} Q_{\ell'\ell}(r,r')\, F_\ell(r')\, dr' = \sum_{p=0}^{q} T_p\, Q_{\ell'\ell}(r_q, r'_p)\, F_\ell(r'_p) \quad \ldots \text{(XI.5)}$$

where the coefficients T_p are the numerical factors of the integration formula.

Choosing the same pivotal points in the range of r, we can replace the first and second derivatives in the integro-differential equations by their finite-difference approximation (Fox and Goodwin, 1949).

$$h^2 \frac{d^2}{dr^2} F_\ell(r) = \left(\delta^2 - \frac{1}{12} \delta^4 + \frac{1}{90} \delta^6 + \dots \right) F_\ell(r) \quad \dots \quad (XI.6)$$

and

$$h \frac{d}{dr} F_\ell(r) = \mu\left(\delta - \frac{1}{6} \delta^3 + \frac{1}{30} \delta^5 - \frac{1}{140} \delta^7 + \dots \right) F_\ell(r) \quad \dots \quad (XI.7)$$

where δ, and μ have their usual definitions (Buckingham, 1962).

Using (XI.5), (XI.6) and (XI.7), we can write equation (XI.1) as follows:

$$\sum_{\ell} \Big[\left(\delta(\ell', \ell) + X_{\ell'\ell}(r) \right) \left(\delta^2 - \frac{1}{12} \delta^4 + \frac{1}{90} \delta^6 + \dots \right) F_\ell(r)$$
$$+ h^2 Z_{\ell'\ell}(r) F_\ell(r) + h V_{\ell'\ell}(r) \mu\left(\delta - \frac{1}{6} \delta^3 + \frac{1}{30} \delta^5 + \dots \right) F_\ell(r)$$
$$+ h^2 \sum_{p=0}^{q} T_p Q_{\ell'\ell}(r_q, r'_p) \Big] = 0 \quad \dots \quad (XI.8)$$

Taking r = th, for all points of tabulation, we use the following relations (Comrie, 1942):

$$\mu F_\ell(r) = \frac{1}{2} \left[F_\ell(r+1) - F_\ell(r-1) \right] \quad \dots \quad (XI.9)$$

$$\delta^2 F_\ell(r) = \left[F_\ell(r+1) - 2 F_\ell(r) + F_\ell(r-1) \right] \quad \dots \quad (XI.10)$$

$$\mu \delta^3 F_\ell(r) = \frac{1}{2} \left[F_\ell(r+2) - 2 F_\ell(r+1) + 2 F_\ell(r-1) - F_\ell(r-2) \right] \qquad \ldots \text{(XI.11)}$$

and

$$\delta^4 F_\ell(r) = \left[F_\ell(r+2) - 4 F_\ell(r+1) + 6 F_\ell(r) - 4 F_\ell(r-1) + F_\ell(r-2) \right] \qquad \ldots \text{(XI.12)}$$

Now putting $F_\ell(th) = F_t$,

$$M^t_{\ell'\ell} = \delta(\ell',\ell) + X_{\ell'\ell}(th) \quad \text{and}$$

$$a^{t\,p}_{\ell'\ell} = T_p \; Q_{\ell'\ell}(th,ph)$$

Equation (XI.8) can then be written as:

$$M^t_{\ell'\ell} \left(-\frac{1}{12} F^{t-2}_\ell + \frac{3}{4} F^{t-1}_\ell - \frac{5}{2} F^t_\ell + \frac{4}{3} F^{t+1}_\ell - \frac{1}{12} F^{t+2}_\ell\right)$$

$$+ h V^t_{\ell'\ell} \left(\frac{1}{12} F^{t-2}_\ell - \frac{2}{3} F^{t-1}_\ell + \frac{2}{3} F^{t+1}_\ell - \frac{1}{12} F^{t+2}_\ell\right)$$

$$+ h^2 Z^t_{\ell'\ell} F^t_\ell + h^2 \sum_{p=0}^{q} a^{t\,p}_{\ell'\ell} F^p_\ell = 0 \qquad \ldots \text{(XI.13)}$$

Using the three point difference formulae, equation (XI.13) reduces to the following form:

$$\sum_\ell \Big[M^t_{\ell'\ell} \left(F^{t+1}_\ell - 2 F^t_\ell + F^{t-1}_\ell \right) + \frac{h}{2} V^t_{\ell'\ell} \left(F^{t+1}_\ell - F^{t-1}_\ell\right)$$

$$+ h^2 Z^t_{\ell'\ell} F^t_\ell + h^2 \sum_{p=0}^{q} a^{t\,p}_{\ell'\ell} F^p_\ell \Big] = \sum_\ell E^t_{\ell'\ell} F^t_\ell \qquad \ldots \text{(XI.14)}$$

where

$$E^{t}_{\ell' \ell} \; F^{t}_{\ell} = M^{t}_{\ell' \ell} \left(\frac{1}{12} \delta^{4} - \frac{1}{90} \delta^{6} + \ldots \right) F^{t}_{\ell} + h \, V^{t}_{\ell' \ell}$$

$$\times \mu \left(\frac{1}{6} \delta^{3} - \frac{1}{30} \delta^{6} + \ldots \right) F^{t}_{\ell} \quad (t=1,2,3,..,n-1) \quad \ldots \quad (XI.15)$$

putting

$$\lambda^{S}_{\ell' \ell} = M^{S}_{\ell' \ell} + \frac{h}{2} V^{S}_{\ell' \ell} \quad \ldots \quad (XI.16)$$

$$\mu^{S}_{\ell' \ell} = M^{S}_{\ell' \ell} - \frac{h}{2} V^{S}_{\ell' \ell} \quad \ldots \quad (XI.17)$$

and

$$\nu^{S}_{\ell' \ell} = h^{2} Z^{S}_{\ell' \ell} - 2 M^{S}_{\ell' \ell} \quad \ldots \quad (XI.18)$$

and using the boundary conditions imposed upon $F_{\ell}(r)$ [i.e. $F_{\ell}(0) = 0$, $F_{\ell}(1) = 1$], enables us to write equation (X.14) in the following form:

$$\sum_{n=1}^{2} H^{ij}_{n'n} F^{j+1}_{n} = \sum_{n} \left(B^{il}_{n'n} + E^{i}_{n'n} \right) \quad (n'=1,2) \quad \ldots \quad (XI.19)$$

where

$$H^{ij}_{n'n} = \left[\delta(i+1,j+1) \lambda^{i-1}_{n'n} + \delta(i,j+1) \lambda^{j+1}_{n'n} + \delta(i-1,j+1) \mu^{j+2} \right] \quad \ldots \quad (XI.20)$$

and

$$B^{il}_{n'n} = - \left[h^{2} A^{il}_{n'n} + \delta(i+1,1) \lambda^{0}_{n'n} - \delta(i,1) \nu^{1}_{n'n} \right.$$

$$-\delta(i - 1,1)\, \mu^{2}_{n'n} \Big] \qquad \ldots \quad (XI.21)$$

Further more, equation (XI.19) can be written more concisely in a matrix form as:

$$H\, F = B + C \qquad \ldots \quad (XI.22)$$

Where H is a square matrix of order i(j-1) x (j-1)i for the coupled equations, and F,B and C are vectors or single column matrices of order i(j-1). The vector C represents the overall truncation error which is usually taken into account if higher terms other than the third are considered. Again, the solution of equation (XI.22) will be defined only if one of $f^{,S}$ is prescribed.

For convenience this is normally f_1 or f_n, bearing in mind the f_o nust be zero. If f_1 is chosen and C is neglected then equation (XI.22) can finally be written as

$$H\, F = b \qquad \ldots \quad (XI.23)$$

CHAPTER XII

THE PHASE-SHIFTS ANALYSIS AND CROSS-SECTIONS

(XII.1.) THE PHASE-SHIFTS ANALYSIS

The introduction of the non-central forces in the nuclear interactions cause the states to couple with different values of ℓ. The phase-shifts of the scattered waves split into components, depending on the values of ℓ,J and P, the parity. Below we give a listing of the radial wave functions and the phase-shifts in both $S=\frac{1}{2}$ and $S=3/2$ corresponding to the substates of (J,p), with $J=\frac{1}{2}$ and $J=3/2$.

The parity of the states is defined by

$$P = (-1)^{J+\ell-\frac{1}{2}} \qquad \text{... (XII.1.1)}$$

State	ℓ , S	J , P	Wave function	Phase-shifts
Doublet	0 , $\frac{1}{2}$	$\frac{1}{2}$, +	${}^{2}f_{0}^{+}$	${}^{2}\delta_{0}^{+}$
	1 , $\frac{1}{2}$	$\frac{1}{2}$, -	${}^{2}f_{1}^{-}$	${}^{2}\delta_{1}^{-}$
	1 , $\frac{1}{2}$	$\frac{3}{2}$, +	${}^{2}f_{1}^{+}$	${}^{2}\delta_{1}^{+}$
	2 , $\frac{1}{2}$	$\frac{3}{2}$, -	${}^{2}f_{2}^{-}$	${}^{2}\delta_{2}^{-}$
Quartet	1 , $\frac{3}{2}$	$\frac{1}{2}$, -	${}^{4}f_{1}^{-}$	${}^{4}\delta_{1}^{-}$
	2 , $\frac{3}{2}$	$\frac{1}{2}$, +	${}^{4}f_{2}^{+}$	${}^{4}\delta_{2}^{+}$
	0 , $\frac{3}{2}$	$\frac{3}{2}$, -	${}^{4}f_{0}^{-}$	${}^{4}\delta_{0}^{-}$
	2 , $\frac{3}{2}$	$\frac{3}{2}$, -	${}^{4}f_{2}^{-}$	${}^{4}\delta_{2}^{-}$
	1 , $\frac{3}{2}$	$\frac{3}{2}$, +	${}^{4}f_{1}^{+}$	${}^{4}\delta_{1}^{+}$
	3 , $\frac{3}{2}$	$\frac{3}{2}$, +	${}^{4}f_{3}^{+}$	${}^{4}\delta_{3}^{+}$

The inclusion of the coulomb interaction causes the direct and exchange terms to converge slowly, and the radial function $f_\ell(r)$ which is a solution to the integral equations, is given by the following asymptotic expression:

$$f_\ell(r) = k_\ell \Big[\cos \delta_\ell \sin(kr - \frac{\pi}{2}\ell - \text{Ln}(2kr) + \sigma_\ell) + \sin \delta_\ell$$

$$\times \cos(k r - \frac{\pi}{2}\ell - \text{Ln}(2kr) + \sigma_\ell)\Big] \qquad \text{.... (XII.1.2)}$$

Which at two neighbouring points r_1 and r_2 can be written as:

$$\mathrm{Tan}\,\delta_\ell = -\frac{f_\ell(r_2)\sin A - f_\ell(r_1)\sin B}{f_\ell(r_2)\cos A - f_\ell(r_1)\cos B} \qquad \ldots \text{(XII.1.3)}$$

where

$$A = kr_1 - \frac{\pi}{2}\ell - \mathrm{Ln}(2kr_1) + \sigma_\ell \text{ and } B = kr_2 - \frac{\pi}{2}\ell - \mathrm{Ln}(2kr_2) + \sigma_\ell$$

and where k_ℓ is a constant amplitude and σ_ℓ is the coulomb phase-shift, defined by

$$\sigma_\ell = \arg\Gamma(1 + \ell + i\gamma) \qquad \ldots \text{(XII.1.4)}$$

where

$$\gamma = \frac{2\,M\,e^2}{3\,\hbar^2 k} \qquad \ldots \text{(XII.1.5)}$$

and

$$k^2 = \frac{4\,M}{3\hbar^2}\,E_p \qquad \ldots \text{(XII.1.6)}$$

σ_ℓ can also be expressed in terms of the following expansion

$$\sigma_\ell = \gamma\,E(\ell) + \sum_{n=0}\left(\frac{\gamma}{1+\gamma+n} - \arctan\frac{\gamma}{1+\ell+n}\right) \ldots \text{(XII.1.7)}$$

where $E(\ell)$ is the Euler's constant

$$E(\ell) = \lim_{\ell\to\infty}\left[\left(1 + \tfrac{1}{2} + \tfrac{1}{3} + \ldots + \frac{1}{\ell}\right) - \mathrm{Ln}(\ell)\right]$$

$$= 0.5772156649 \qquad \ldots \text{(XII.1.8)}$$

The $\sigma_{\ell+1}$ is easily obtained by using the recurrence relation

$$\sigma_{\ell+1} = \sigma_\ell + \arctan(\gamma/1+\ell) \qquad \ldots \text{(XII.1.9)}$$

(XII.2.) THE DIFFERENTIAL AND TOTAL CROSS-SECTION

The total differential cross-section for the elastic (p-d) scattering is given by

$$\sigma(\theta) = \sigma_c(\theta) + \sigma_I(\theta) + \sigma_N(\theta) \qquad \ldots \text{(XII.2.1)}$$

where $\sigma_c(\theta)$ is the coulomb cross-section given by

$$\sigma_c(\theta) = (\gamma/2k)^2 \operatorname{cosec}^4 (\theta/2) \qquad \ldots \text{(XII.2.2)}$$

and

$$\sigma_I(\theta) = \sum_S \sum_{L_1,L_2} \sum_{J,p,j} \frac{\gamma}{6k^2} \operatorname{cosec}^2(\theta/2)\,(i)^{L_1-L_2}$$

$$\times \sin(W + {}^J\delta_j^p + \sigma_{L_1} + \sigma_{L_2} - 2\sigma_o)\,\hat{L}_1\hat{L}_2 \sin {}^J\delta_j^P\, {}^J D^P_{L_1,S}(j)$$

$$\times {}^J D^p_{L_2,S}(j) \sum_M C_{L_1 S}(J\ M;\ OM)\, C_{L_2 S}(J\ M;\ OM)\, p_{L_2}(\mu)$$

$$(\mu = \cos\theta) \qquad \ldots \text{(XII.2.3)}$$

where $W = 2\gamma\, \mathrm{LN}(\sin \frac{\theta}{2})$, $\hat{L}_1 = (2L_1 + 1)^{\frac{1}{2}}$, and $\hat{L}_2 = (2L_2 + 1)^{\frac{1}{2}}$.

Further simplification of the above expression leads to

$$\sigma_I(\theta) = \frac{\gamma}{3k^2} \operatorname{cosec}^2(\frac{\theta}{2}) \Big[\sin(W + {}^2\delta_o^+) \sin {}^2\delta_o^+ + 2\sin(W + {}^4\delta_o^-)$$

$$\times \sin {}^4\delta_o^- + \Big\{ \Big[\sin(W + {}^2\delta_1^- + 2\sigma_1 - 2\sigma_o) \sin {}^2\delta_1^- + 2\sin(W + {}^2\delta_1^+$$

$$+ 2\sigma_1 - 2\sigma_o) \sin {}^2\delta_1^+ + \sin(W + {}^4\delta_1^- + 2\sigma_1 - 2\sigma_o) \sin {}^2\delta_1^-$$

$$+ 2\sin(W + {}^4\delta_1^+ + 2\sigma_1 - 2\sigma_o) \sin {}^4\delta_1^+ \Big] p_1(\mu) + \Big\{ \Big[2\sin(W + {}^2\delta_2^-$$

$$+ 2\sigma_2 - 2\sigma_o)\sin{}^{2}\delta_o^{-} + \sin(W + {}^{4}\delta_2^{+} + 2\sigma_2 - 2\sigma_o)\sin{}^{4}\delta_2^{+}$$

$$+ 2\sin(W + {}^{4}\delta_2^{-} + 2\sigma_2 - 2\sigma_o)\sin{}^{4}\delta_2^{-}\Big\}P_2(\mu) + 2\sin(W + {}^{4}\delta_3^{+}$$

$$+ 2\sigma_3 - 2\sigma_o)\sin{}^{4}\delta_3^{+}P_3(\mu)\Big] \qquad \ldots (XII.2.4)$$

and where

$$\sigma_N(\theta) = (1/6K)\sum_{S,\ell} A_\ell(S)\,P_\ell(\mu) \qquad \ldots (XII.2.5)$$

where

$$A_\ell(S) = (-1)^{S-\frac{1}{2}} \sum_{J_1,P_1}\sum_{J_2,P_2}\sum_{i,j} \sin{}^{J_1}\delta_i^{P_1}\,\sin{}^{J_2}\delta_j^{P_2}$$

$$\times\cos({}^{J_1}\delta_i^{P_1} - {}^{J_2}\delta_j^{P_2})\Big[T(i\,J_1\,P_1\,;\,j\,J_2\,P_2)\Big]^2 \qquad \ldots (XII.2.6)$$

and

$$T(i\,J_1\,P_1\,;\,j\,J_2\,P_2) = \sum_{\ell_1,\ell_2} X(\ell_1 J_1\,;\,\ell_2 J_2\,;\,S\ell)\;{}^{J_1}D^{P_1}_{\ell_1,S}(i)$$

$$\times\;{}^{J_1}D^{P_2}_{\ell_2 S}(j) \qquad \ldots (XII.2.7)$$

After performing all the sums, the nuclear differential cross-section may be brought into the following form:

$$\sigma_N = 1/3k^2\Big\{\Big[\sin^2{}^{2}\delta_1^{-} + \sin^2{}^{2}\delta_o^{+} + \sin^2{}^{4}\delta_1^{-} + \sin^2{}^{4}\delta_2^{+}$$

$$+ 2\sin^2{}^{2}\delta_1^{+} + 2\sin{}^{4}\delta_2^{-} + 2\sin^2{}^{2}\delta_2^{-} + 2\sin^2{}^{4}\delta_o^{-} + 2\sin^2{}^{4}\delta_1^{+}$$

$$+ 2\sin^2{}^{4}\delta_3^{+}\Big]P_o(\mu) + \Big[4\sin{}^{2}\delta_1^{-}\sin{}^{2}\delta_2^{-}\cos({}^{2}\delta_1^{-} - {}^{2}\delta_2^{-})$$

$$+ 2\sin{}^{4}\delta_o^{-}\sin{}^{4}\delta_1^{-}\cos({}^{4}\delta_o^{-} - {}^{4}\delta_1^{-}) + 2\sin{}^{4}\delta_1^{-}\sin{}^{4}\delta_2^{-}$$

$$\times \cos({}^4\delta_1^- - {}^4\delta_2^-) + 4 \sin {}^2\delta_0^+ \sin {}^2\delta_1^+ \cos({}^2\delta_0^+ - {}^2\delta_1^+) + 0.4$$

$$\times \sin {}^4\delta_1^+ \sin {}^4\delta_2^+ \cos({}^4\delta_1^+ - {}^4\delta_2^+) + 3.6 \sin {}^4\delta_2^+ \sin {}^4\delta_3^+$$

$$\times \cos({}^4\delta_2^+ - {}^4\delta_3^+) \Big] p_1(\mu) + \Big[2 \sin^2 {}^2\delta_1^+ + 1.28 \sin^2 {}^4\delta_1^+ + 1.44$$

$$\times \sin {}^4\delta_1^+ \sin {}^4\delta_3^+ \cos({}^4\delta_1^+ - {}^4\delta_3^+) + 2 \sin^2 {}^2\delta_2^- + 1.28 \sin^2 {}^4\delta_3^+$$

$$+ 4 \sin {}^4\delta_0^- \sin {}^4\delta_2^- \cos({}^4\delta_0^- - {}^4\delta_2^-) \Big] p_2(\mu) \Big\} \quad \ldots \text{(XII.2.8)}$$

Therefore, the total cross-section for (p-d) scattering is given by

$$\sigma_t = 2\pi \int_0^{\pi} \sigma(\theta) \sin\theta d\theta \quad \ldots \text{(XII.2.9)}$$

Phase-shifts due to coulomb and nuclear interactions are calculated from the expressions(XII.1.3)and(XI I.1.7) and their values are given in tables (I) to (VI).

TABLE (I) THE COULOMB PHASE-SHIFTS (IN RADIANS)

E_{Lab}(MEV)	σ_0	σ_1	σ_2	σ_3
2.775	-0.04487422	0.03271227	0.07156398	0.09747237
4.50	-0.03523888	0.03573521	0.05625062	0.07659773
6.30	-0.02978229	0.02176847	0.04756098	0.06475811
7.50	-0.02729592	0.01995782	0.04359789	0.05935956
11.175	-0.02228703	0.01630507	0.03560830	0.04847801
17.25	-0.01799839	0.01317291	0.02876235	0.03915578
22.50	-0.01575931	0.01153619	0.02518649	0.03428700
30.00	-0.01364796	0.00999211	0.02181379	0.02969512

The phases are given in radians between the range

$$-\frac{\pi}{2} \leq \sigma \leq \frac{\pi}{2}$$

TABLE (II) THE ${}^{2}\delta_{0}^{+}$ PHASES (IN RADIANS)

E_{Lab}(MEV)	Ours	PA*	BHM+	VBx
2.775	-0.33722	-0.36		
2.53				-0.3313
3.00				-0.3748
4.20			-0.98	
4.50	-0.56336	-0.79		
5.00				-0.8478
6.30	-1.42208	-1.24		
7.40			-1.28	
7.50	-1.53859	-1.26		
7.85				-0.9656
11.175	-1.36314	-1.31		
11.50			-1.55	-1.321
17.25	0.76874	0.90		

The above phases are given in radians between the range

$$-\frac{\pi}{2} \leq \delta \leq \frac{\pi}{2}$$

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* PA- Pramanik, A., 1971.

+ BHM- Buckingham, Hubbard, and Massey, 1952.

x VB- Van Oers and Brockman, 1967.

TABLE(III) THE PHASES ${}^{2}\delta^{-}_{1}$, ${}^{2}\delta^{+}_{1}$ and ${}^{2}\delta^{-}_{2}$ (IN RADIANS)

$E_{c.m}$ (MEV)	${}^{2}\delta^{-}_{1}$		${}^{2}\delta^{+}_{1}$		${}^{2}\delta^{-}_{1}$	
	Ours	PA	Ours	PA	Ours	PA
1.85	-0.20759	0.254	-1.1483		-0.40123	
3.00	1.45848	-0.325	-0.9391	-0.67	-0.95834	-0.54
4.20	-1.54700	-0.540	-1.5532		-1.33310	
5.00	0.73656	-1.45	0.14495	-0.88	-1.4091	-0.92
7.45	0.487234	-1.60	1.51611		-0.95051	
7.50				1.59		-1.36
11.50	1.065266		0.20817	-1.55	-1.32445	

The above phases are given in radians between

$$-\frac{\pi}{2} \leq \delta \leq \frac{\pi}{2}$$

TABLE (IV) THE PHASES $^{4}\delta_{o}^{-}$ (IN RADIANS)

$E_{c.m}$(MEV)	E_{Lab}(MEV)	ours	PA	BHM	VB
2.80	4.20			-1.15	
3.00	4.50	-0.19883	-1.351		
	5.00				-.1335
4.20	6.30	-0.62074			
	7.40			-1.54	
5.00	7.50	1.42868	-1.54		

The above phases are given in radians between

$$-\frac{\pi}{2} \leq \delta \leq \frac{\pi}{2}$$

TABLE (V) THE PHASES ${}^{4}\delta_{1}^{-}$ AND ${}^{4}\delta_{2}^{+}$ (IN RADIANS)

$E_{c.m.}$ (MEV)	${}^{4}\delta_{1}^{-}$		${}^{4}\delta_{2}^{+}$	
	Ours	PA	Ours	PA
1.85	1.03106	-1,259	-0.77735	-0.131
3.00	-0.27090	-0.355	-1.10885	1.255
4.20	1.06516	0.436	-1.35656	1.456
5.00	-1.34473	0.259	-1.53621	1.250

TABLE (VI) THE PHASES ${}^{4}\delta_{1}^{+}$, ${}^{4}\delta_{2}^{-}$ AND (IN RADIANS)

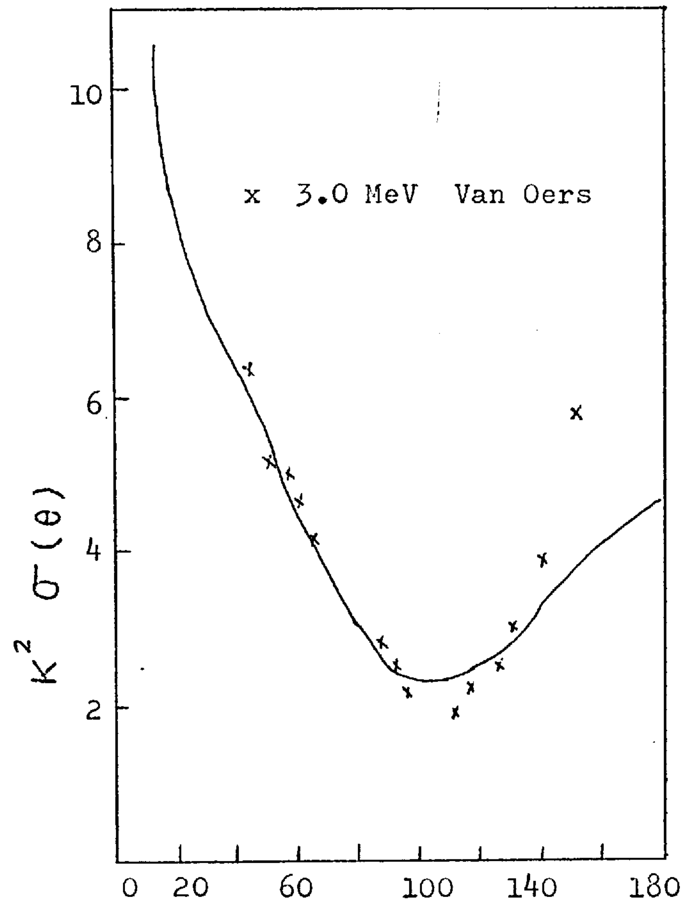
E(MEV) c.m	${}^{4}\delta_{1}^{+}$		${}^{4}\delta_{2}^{-}$		${}^{4}\delta_{3}^{+}$	
	Ours	PA	Ours	PA	Ours	PA
3.00	0.92031	0.426	0.07978	-1.015	0.67963	-0.635
4.20	-1.18357		-1.35029		-0.27545	
5.00	1.399449	-0.376	-1.45213	1.163	-0.30735	-0.521

The above phase-shifts are then used to calculate differential and total cross-section at different incident proton anergy.

TABLE (VII) TOTAL CROSS-SECTIONS

E(Mev)	Q_C(Barns)		Q_N(Barns)		Q_I(Barns)		Q(Barns)	
	Ours	PA	Ours	PA	Ours	PA	Ours	PA
3.00	0.40428	0.2041	5.72207	3.1919	12.8612	10.983	18.9876	14.379
4.20	0.20626		6.95547		17.3186		24.4803	
5.00	0.14554	0.0734	5.85176	2.5491	11.6119	8.5159	17.6092	11.138

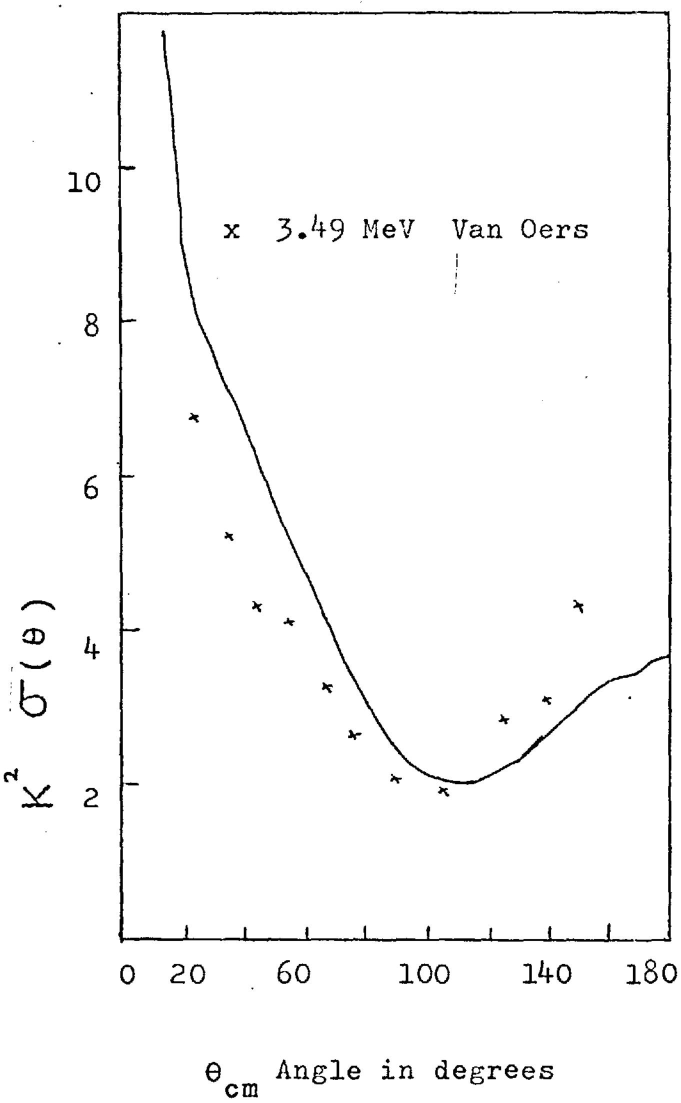
Fig. (1)



θ_{cm} Angle in degrees

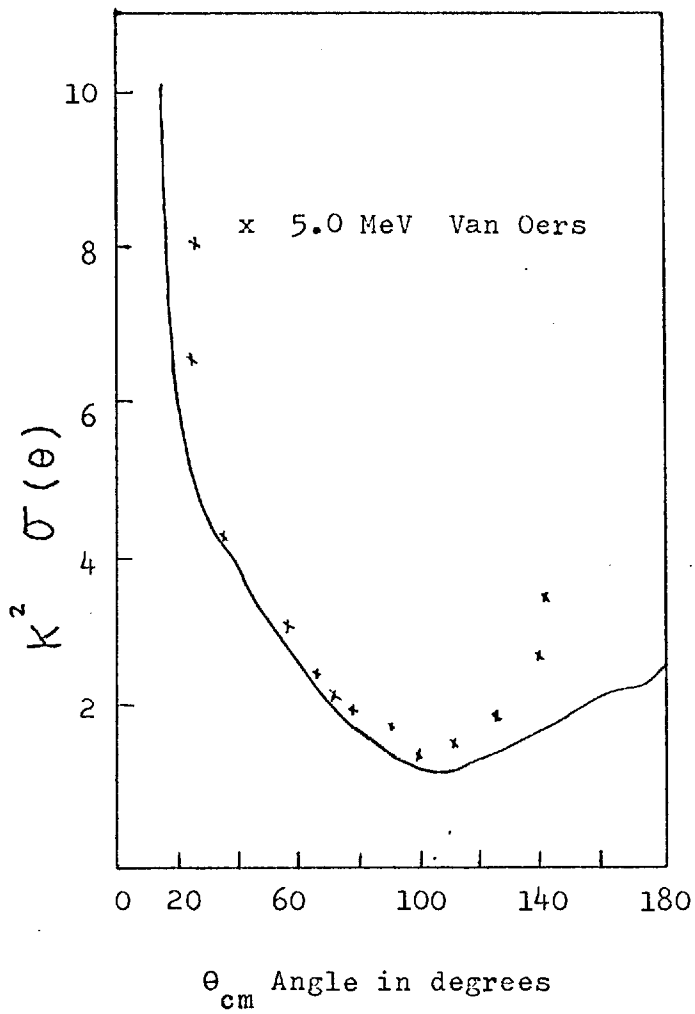
Angular distributions for proton-deuteron scattering at 3.0 MeV.

Fig. (2)



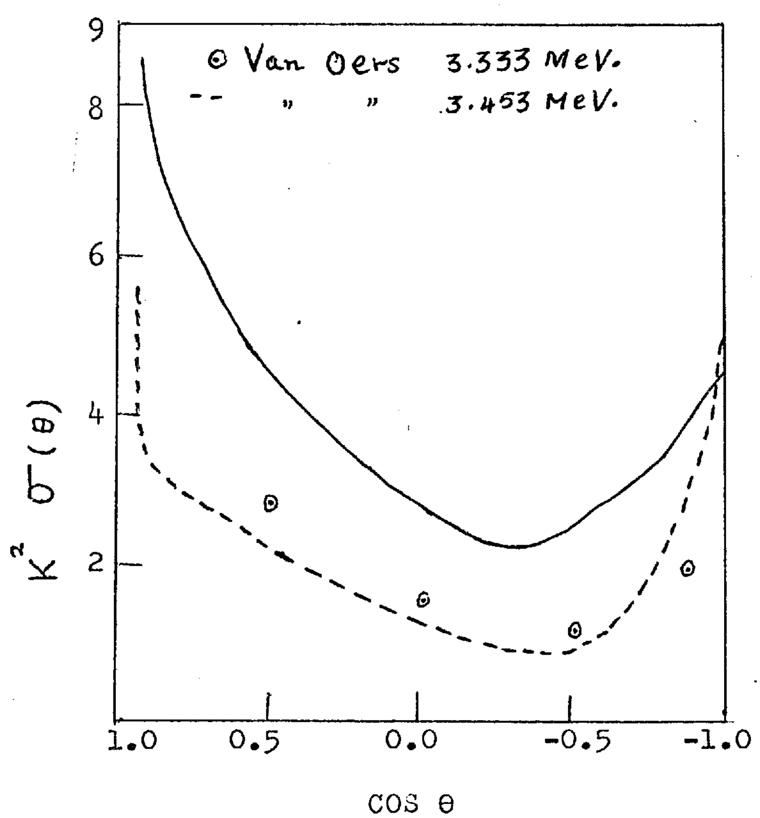
Angular distributions for proton-deuteron scattering at 4.20 MeV.

Fig. (3)



Angular distributions for proton-deuteron scattering at 5.0 MeV.

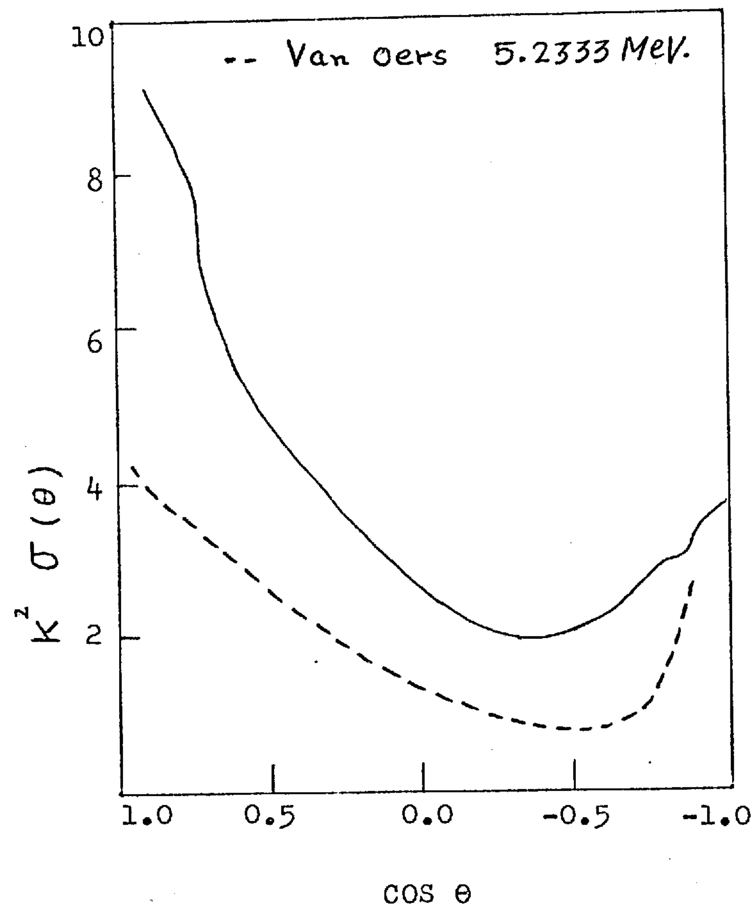
Fig. (4)



Angular distributions for proton-deuteron

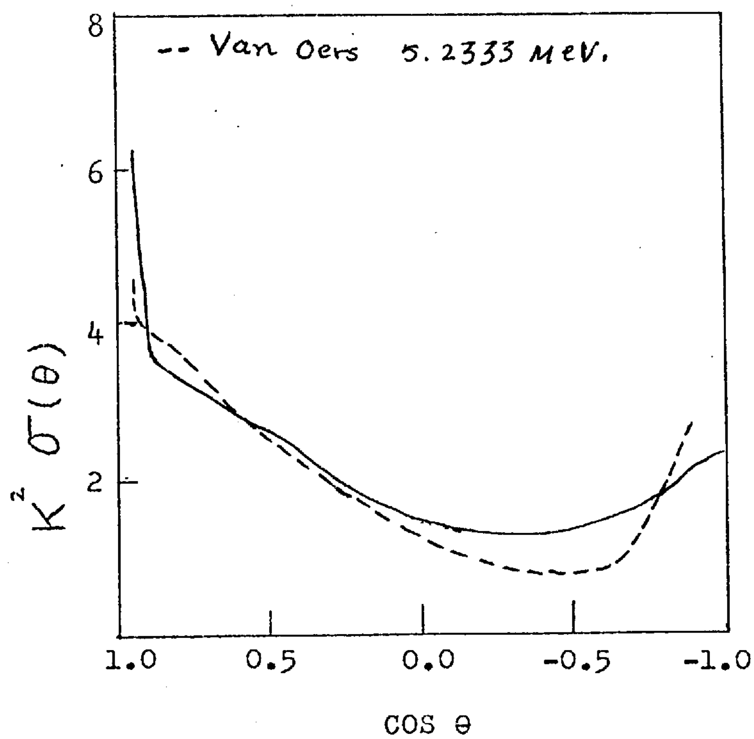
scattering at 3.0 MeV.

Fig. (5)



Angular distributions for proton-deuteron scattering at 4.20 MeV.

Fig. (6)



Angular distributions for proton-deuteron

scattering at 5.0 MeV.

SUPPLEMENTRY I

DIFFERENTIAL CROSS-SECTIONS AND FITTINGS

Equation (1) in P. 145, is now used to interpolate differential cross-sections at different energies. We write

$$K^2 \sigma(k,\mu) = h(k)\ g(k,\mu) \qquad (\mu = \cos\theta) \quad \ldots(1)$$

k is a wave number defined in (II.1.6), and h(k) and g(k,μ) have the following forms:

$$h(k) = \sum_{i=0}^{2} a_i\ k^i \qquad \ldots(2)$$

and

$$g(k,\mu) = 1 + \sum_{j=1}^{5} b_j(k)\ \mu^j \qquad \ldots(3)$$

where

$$b_j(k) = \sum_{m=0}^{2} b_{jm}\ k^{2m} \qquad \ldots(4)$$

and where a_i, $b_j(k)$ and b_{jm} are constants, and their values are given in the following tables:

Table (I)

i	a_i
0	-29.014861
1	163.65516
2	-211.33153

Table (II)

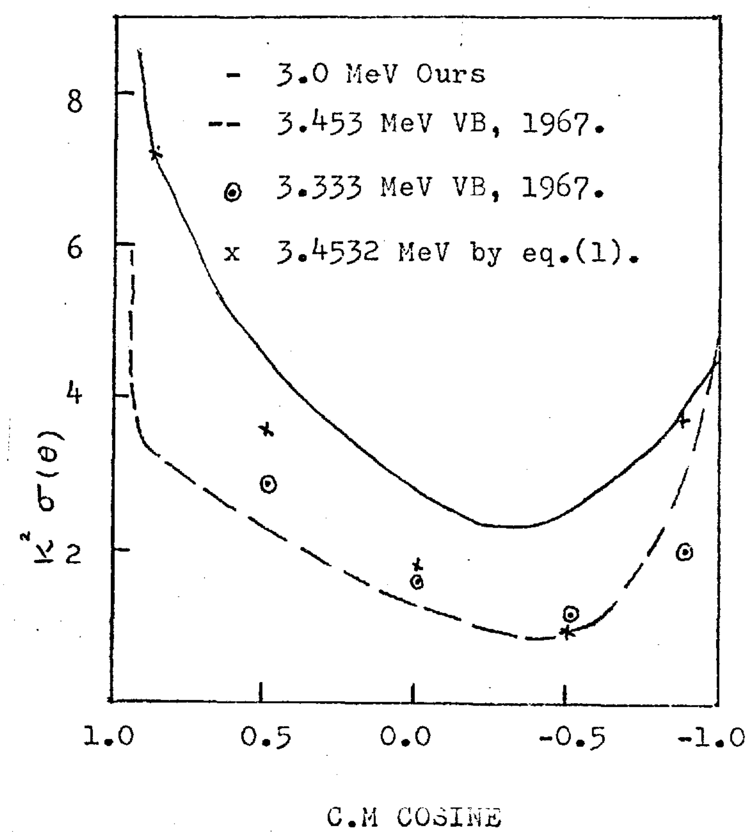
$E_{c.m}$ (MeV)	b_1	b_2	b_3	b_4	b_5
3.00	1.0019075	1.7106778	-.54493191	-.00141043	0.82820520
4.20	1.4431798	1.8566060	-4.1700294	0.31963656	5.8571198
5.00	0.83056814	1.4504653	-0.26939026	0.02889075	0.26456704

Table (III)

j \ m	b_{j0}	b_{j1}	b_{j2}
1	-7.2422896	138.25989	-547.51329
2	-2.6186347	74.1924	-303.9638
3	58.267231	-977.48556	3814.3700
4	-4.7791575	78.917120	-304.77981
5	-82.187412	1381.3872	-5401.0060

Graphs of the calculated differential cross-sections as well as those obtained by interpolation are compared with Van Oers and Brockman, 1967; Seagrave, 1970; and the experimental ones, and are all given below:

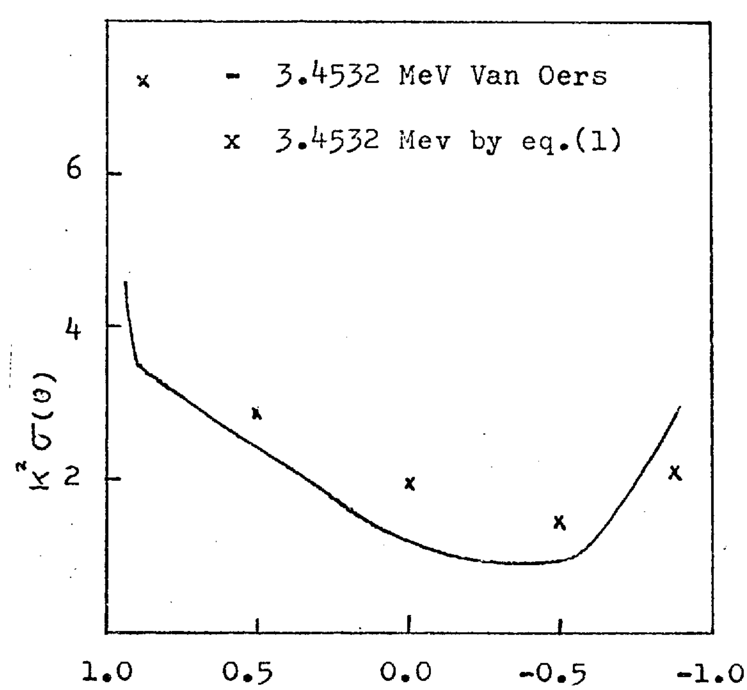
Supp. Fig.(1)



Differential cross-sections for

proton-deuteron scattering

Supp. Fig.(2)



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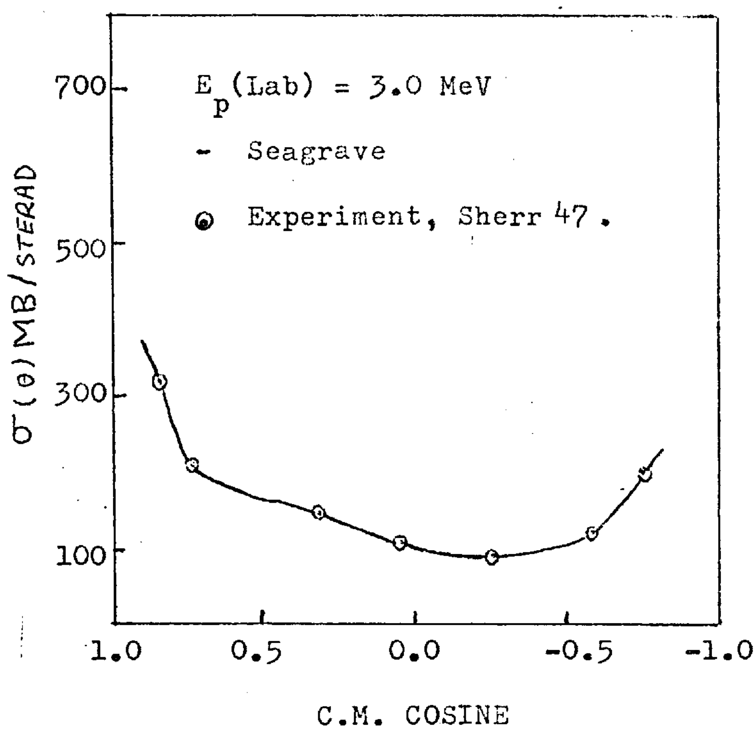
Differential cross-sections for

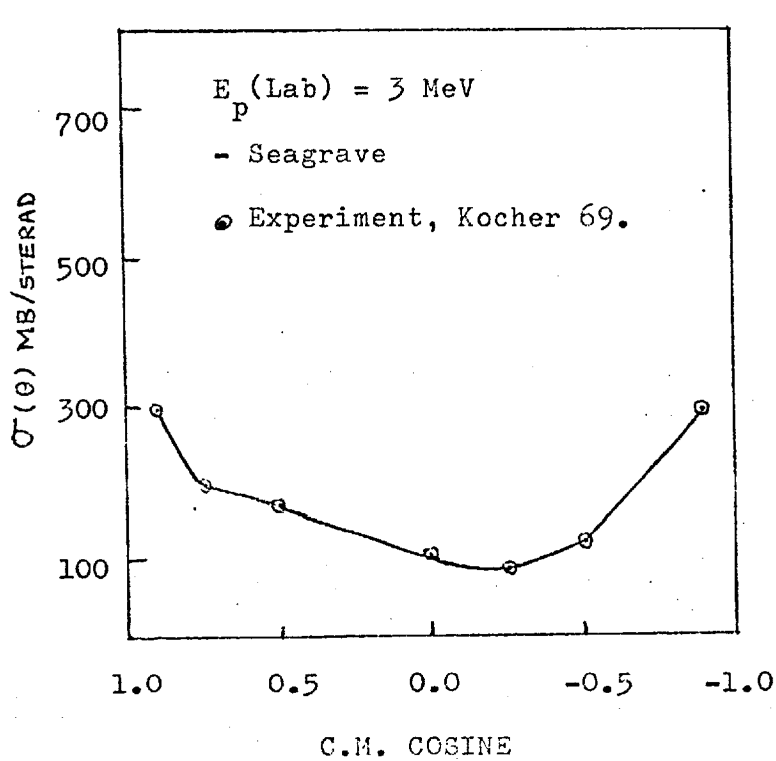
proton-deuteron scattering

Supp. Fig.(3)



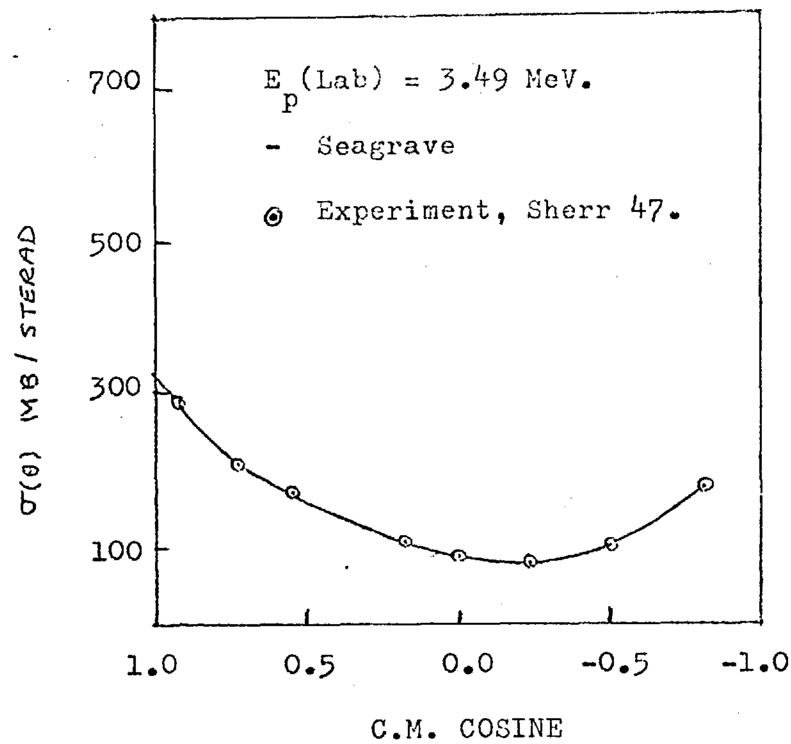
R. Sherr, Phys. Rev. 72 (1947), 662

Supp. Fig.(4)



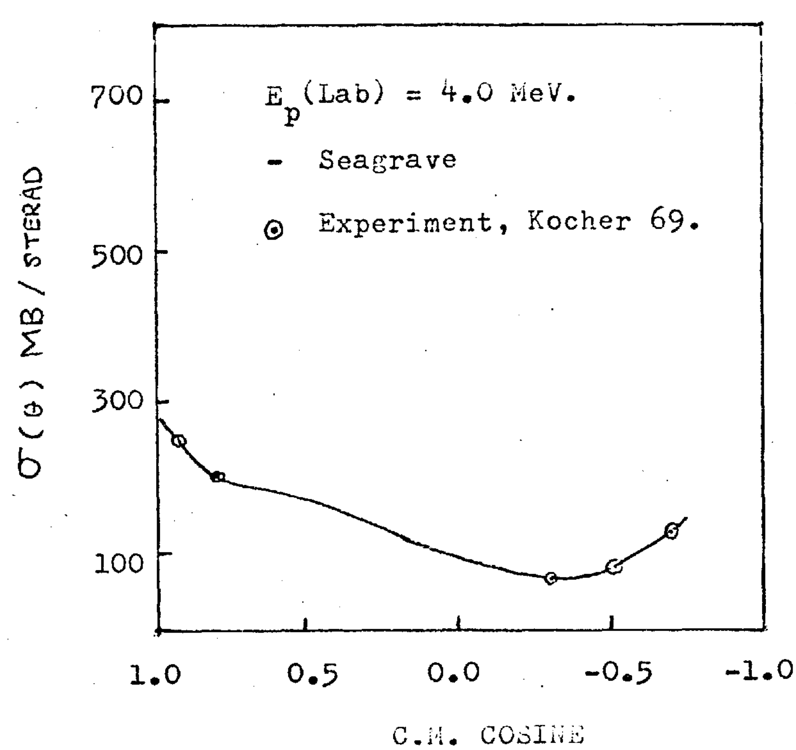
D.C. Kocher, Wisc. 69, Nucl. Phys. (In Press).

Supp. Fig.(5)



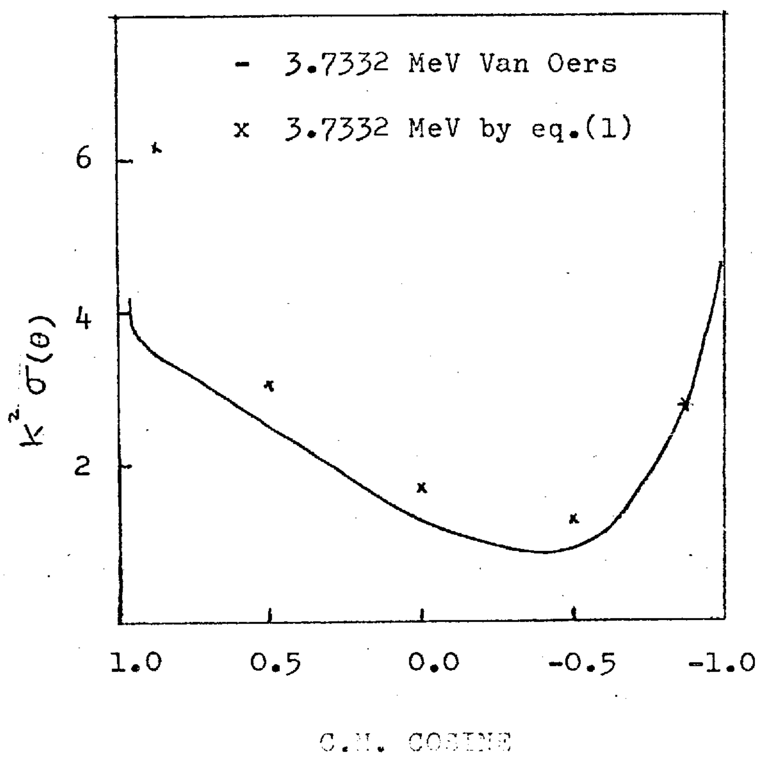
R. Sherr, Lasl Phys. Rev. 72 (1947), 662.

Supp. Fig.(6)



D.C. Kocher, Wisc. 69, Nucl. Phys. (In Press)

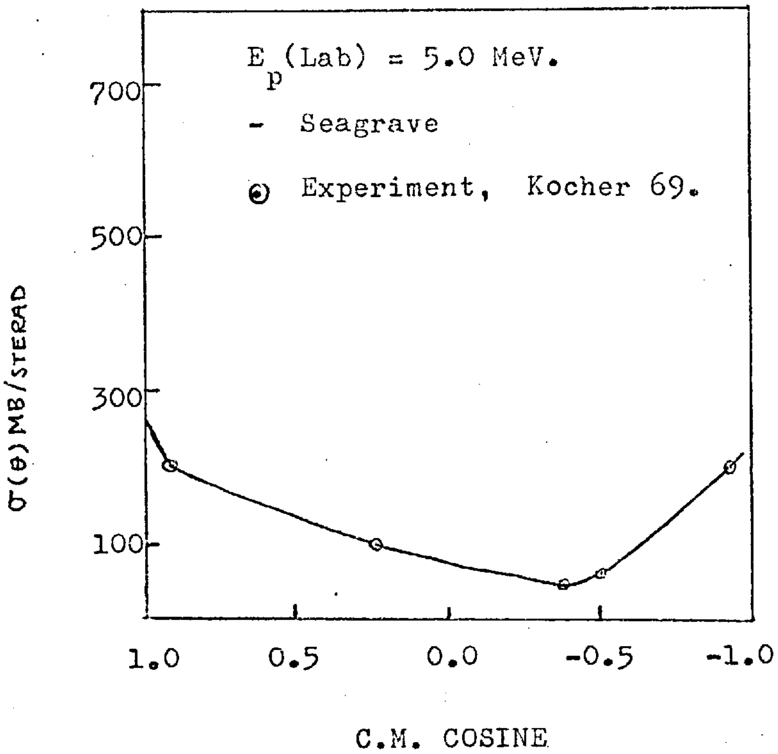
Supp. Fig.(7)



Differential cross-sections for

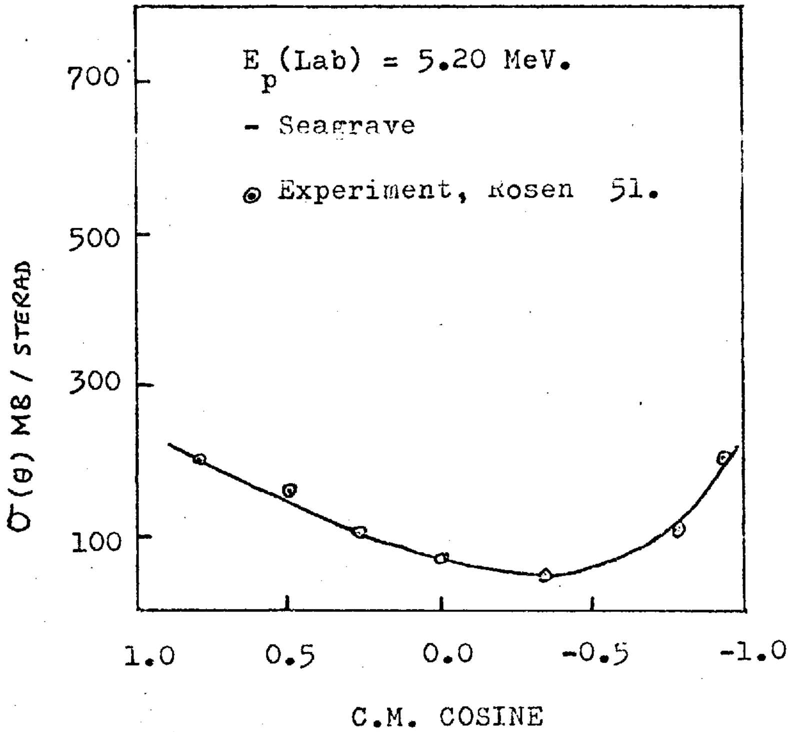
proton-deuteron scattering

Supp. Fig.(8)



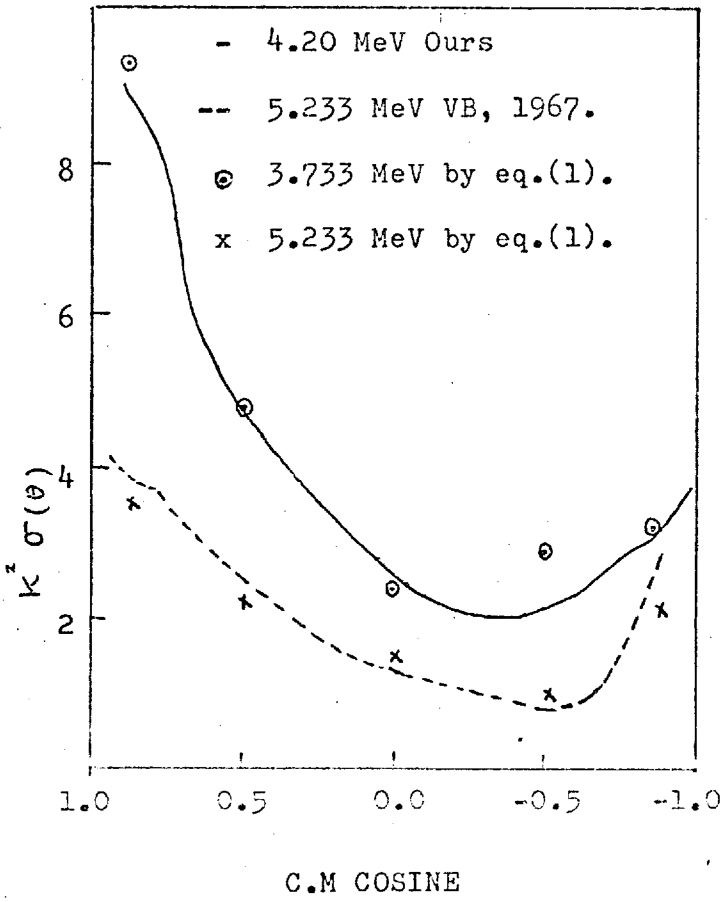
D.C. Kocher, Wisc. 69, Nucl. Phys.(In Press)

Supp. Fig.(9)



L. Rosen, Lasl 51, Phys. Rev. 82 (1951), 777.

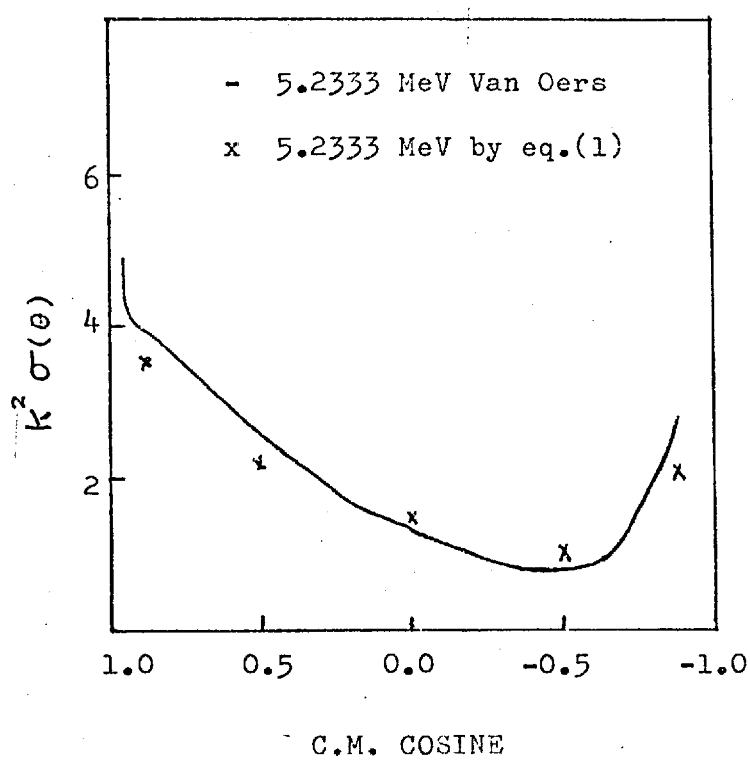
Supp. Fig. (10)



Differential cross-sections for

proton-deuteron scattering

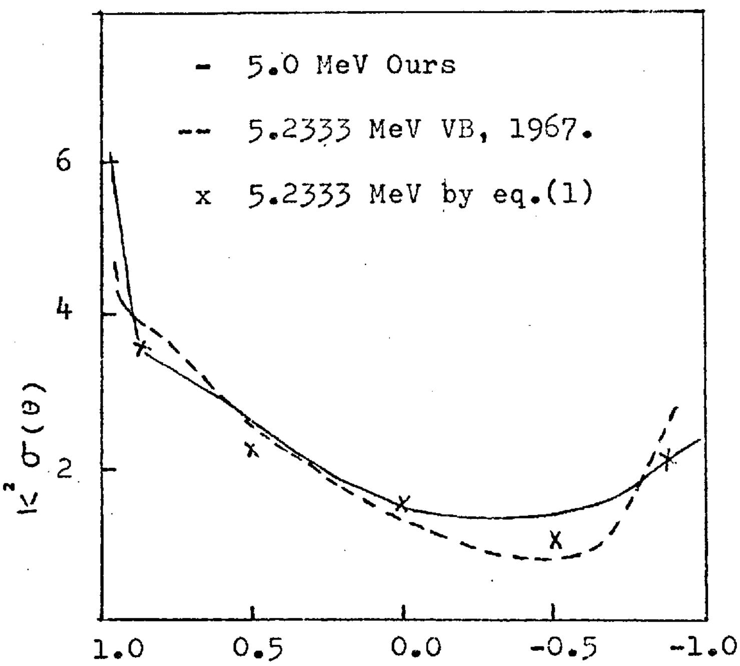
Supp. Fig.(11)



Differential cross-sections for

proton-deuteron scattering

Supp. Fig.(12)

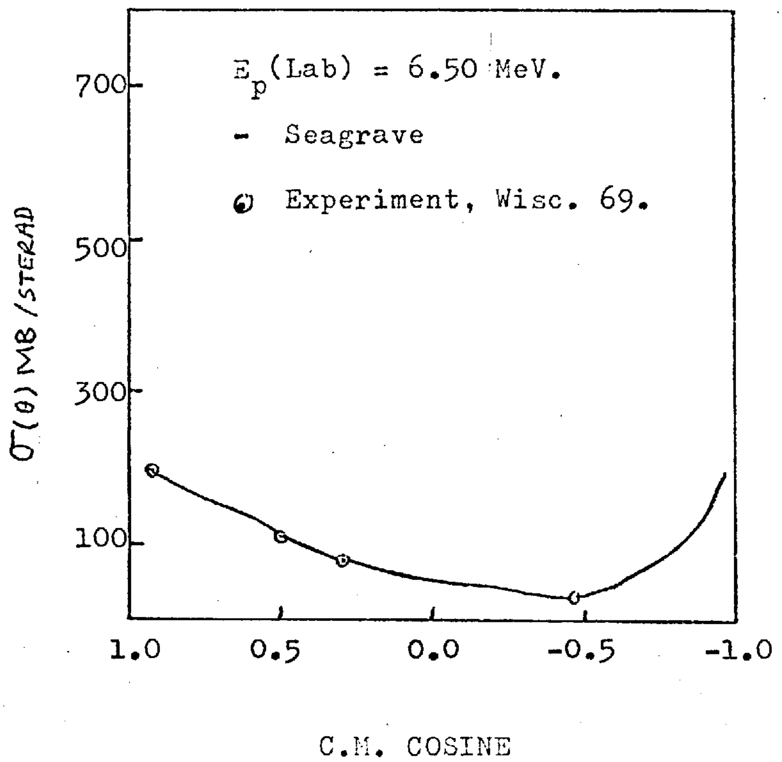


C.M COSINE

Differential cross-sections for

proton-deuteron scattering

Supp. Fig.(13)



A.S. Wilson, Rice 69, Nucl. Phys.(In Press)

CONCLUSION

Programs to solve uncoupled and coupled simultaneous linear equations for the radial functions $f^{S}_{J\ell M}(r)$, were prepared by the author and the calculation was performed on a CDC 6600 machine, through a 200 terminal located at Chelsea College Computer Centre, to obtain phase-shifts differential and total cross-sections for both the doublet ($S=\frac{1}{2}$) and quartet ($S=3/2$) states. Using (XI.1.8) and (XI.1.11), phase shifts for (P-d) elastic scattering in the energy range (2.775-17.23 MeV) were calculated and their values are given in tables (I) to (VI).

In the present calculation, our phase shifts split into components depending on the values of the total angular momentum J, the orbital angular momentum ℓ, and the parity P.

In these tables a comparison was made with several authors (Buckingham and Massey, 1952; Christian and Gammel, 1953; and Van Oers and Brockman, 1967).

A direct comparison was made only with the phases ${}^{2}\delta_{0}$ calculated by the above authors and Pramanik (1971) and this gives a close agreement.

Similar comparison with the P- and D- phases obtained by Buckingham and Massey 1952; and Christian and Gammel, 1953 was not possible, because their phase shifts do not split and also the potential they used does not include all known forces (i.e. tensor, spin-orbit and quadratic spin-orbit forces).

In fact, Christian and Gammel used in their calculation the scattering lenghts as a guide line in finding the S-state phase shifts. They also used the Born approximation to find phase shifts for partial waves with $\ell \geq 1$.

The only direct comparison made was with Pramanik(1971), and our phase shifts sometimes disagree with his.

The values of the phase shifts which were directly obtained from the solution of the integrodifferential equations are then used to obtain the differential and total cross-sections for $\theta = 5^{\circ}$ (5°) 180°, from an expression given by Blatt and Biedenharn (1952), and the results are displayed and compared with others as shown in Fig. (1) to (6).

Our data for the differential cross-sections $\sigma(K,\theta)$ are also used to fit the following expression

$$\sigma(K,\theta) = h(K) \sum_{j=0}^{5} b_j(K) P_j (\cos \theta) \qquad \ldots \quad (1)$$

where

$$h(K) = \sum_{i=0}^{2} a_i K^i$$

K is a wave number defined in (II.1.6), and $P_j(\cos \theta)$ is the Legendre polynomial and a_i and b_j are constants.

A similar fitting procedure was also adopted with the experimental differential cross-section data (Seagraves, 1970, Van Oers and Brockman, 1967). Our graphs in general fairly well agree with the experimental points, apart from the fact that the minima in our graphs are not deep enough and show a small increasing displacement towards higher scattering angles with increasing energies.

A possible explanation to this may be the following:

(i) Our calculation of the differential cross-sections is based on the expression given by Blatt and Biedenharn (1952), in which the differential cross-sections are directly dependent on the channel spin S, the total angular momentum J, the orbital angular momentum ℓ, and the parityP.

(ii) In calculating the differential and total cross-sections we used the values of the split phase-shifts obtained from the direct solution of the integrodifferential equations.

(iii)The contribution of the partial waves with $\ell > 3$, were neglected in our calculation. However, from the analysis carried out using expression (1), it is found that a small contribution of one or more odd harmonics could do two things (a) increase the differential cross-sections for $90^{\circ} < \theta \leq 180^{\circ}$ and (b) shift the minimum value of $\sigma(\theta)$ slightly to the left. Therefore the inclusion of higher phase-shifts are certainly necessary to give the required contribution (Christian and Gammel, 1953), in the backward scattering and produce minima as shown in the experiment . Further calculations to settle this are required and may be undertaken in due course.

THE BINDING ENERGY OF ^{3}HE

Using the resonating group method and the Hamada-Johnston potential (1962), the binding energy of ^{3}He was calculated and found to be + 6.032353 MeV.

This result is within the experimental value +7.718 $\pm$ 0.17 MeV considering the relativistic correction and possibly the effect of three-body forces. Many calculations for the binding energy of the three-nucleon systems have been carried out using different kinds of potentials and techniques.

To my knowledge no reliable estimate of the relativistic correction exist so far, though general considerations suggest that these corrections could contribute anything between 10 and 20% to the triton binding energy. Gupta, Bhakar and Mitra (1965) calculated the binding energy of the ^{3}H and estimated the relativistic correction to be of order of + 0.5 MeV.

Several variational calculations using realistic potentials of the Hamada and Johnston (HJ) and Reid soft-core (RSC,1968), are due to Hennel and Delves (1972), Humberston and Hennel (1970) and Delves and Blatt (1969). Hennel and Delves obtained values of +6.5 $\pm$ 0.2 MeV (HJ) and + 7.95 $\pm$ 0.5 MeV (RSC) for the triton, and Humberston and Hennel whose resutls and conclusion are similar of those of Delves and Blatt, obtained a value of + 6.7 MeV (HJ) for ^{3}H. In fact Humberston and Hennel in their calculation introduced a correction to the Hamada-Johnston potential for the hard-core radius r_o, and the pion mass μ, and claim that a change in the triton binding energy from + 6.3 MeV to + 8.48 MeV requires a change in both r_o and μ (i.e. $\delta r_o \simeq -0.104$ fm and $\delta\mu \simeq -10$ MeV).

However, these corrections of the Hamada and Johnston potential may affect the phase-shifts, polarizations and cross-sections of the N-N system which would require a change in the other force parameters for agreement with experiment.

Therefore their figure of +8.48 MeV for the binding energy of ^3H is uncertain. The Faddeev formulism (1963) has only recently been applied to the problem of three-nucleon systems (Lee 1969; Sibbel 1971; and Harper, Kim, and Tubis 1972). However, it appears from these calculations that all potentials used (including the one developed by the Yale group), underbind the three-nucleon systems.

Also, it seems that the Hamada and Johnston analysis which is based on a Schroedinger wave equation requires a relativistic correction, or better still the Lippmann-Schwinger equations , so as to bring the binding anergy of the three-nucleon systems close to the experimental value whilst retaining the fit to theN-N data. One has to remember that the Hamada-Johnston potential is claimed to be valid for N-N phenomena for energies 0-300 MeV and therefore relativistic effects cannot be ignored.

Further calculations to settle this are required.

APPENDICES AND REFERENCES

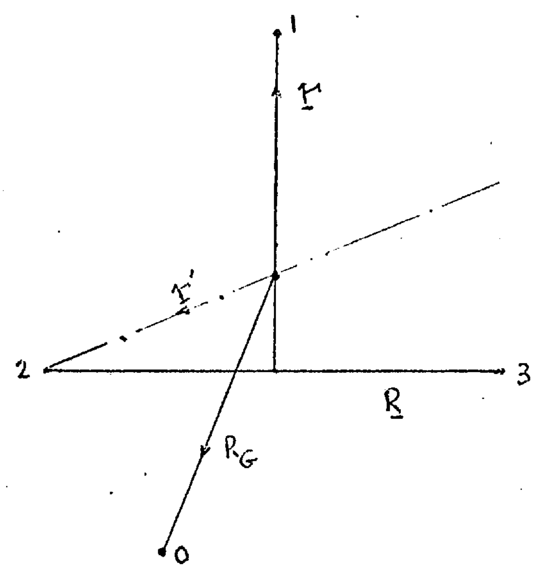
APPENDIX I

CO-ORDINATES AND TRANSFORMATIONS

In this system we refer to the incident proton as particle 1, the other proton and neutron in the deuteron are labelled as particles 2 and 3, together with position vectors $\underline{r}_1$, $\underline{r}_2$ and $\underline{r}_3$ from the origin O .

We define $\underline{r}$ as the co-ordinate of particle 1 relative to the centre of mass (C.M) of the other two, and $\underline{r}'$ as the co-ordinate of particle 2 relative to the C.M. of the other two.

CHOICE OF CO-ORDINATES



$$R_G = \frac{1}{3}(\underline{r}_1 + \underline{r}_2 + \underline{r}_3)$$

$$\underline{r}_1 = R_G + \frac{2}{3}\underline{r}$$

$$\underline{r}_2 = R_G + \frac{1}{2}\underline{R} - \frac{1}{2}\underline{r}$$

$$\underline{r}_3 = R_G - \frac{1}{2}\underline{R} - \frac{1}{3}\underline{r}$$

$$\underline{r} = \underline{r}_1 - \frac{1}{2}(\underline{r}_2 + \underline{r}_3)$$

$$\underline{r}' = \underline{r}_2 - \frac{1}{2}(\underline{r}_1 + \underline{r}_3)$$

The interparticle distances $\underline{r}_{12}$, $\underline{r}_{23}$ and $\underline{r}_{13}$ are defined in the direct interaction by

$$\underline{r}_{12} = \underline{r} - \frac{1}{2}\underline{R}$$

$$\underline{r}_{23} = \underline{r}_2 - \underline{r}_3 = \underline{R}$$

$$\underline{r}_{13} = \underline{r} + \frac{1}{2}\underline{R}$$

and in the indirect interaction by

$$\underline{t} = \frac{2}{3}(\underline{r} - \underline{r}')$$

$$\underline{u} = \frac{2}{3}(\underline{r} + 2\underline{r}')$$

$$\underline{V} = \frac{2}{3}(2\,\underline{r} + \underline{r}')$$

Again, if $\underline{p}_1$ and $\underline{p}_2$ are the momentum vectors of the particles 1 and 2, referred to a fixed origin then

$$i\,\underline{p}_1 = \frac{\partial}{\partial \underline{r}_1} = \frac{\partial}{\partial \underline{r}}$$

$$i\,\underline{p}_2 = \frac{\partial}{\partial \underline{r}_2} = -\frac{1}{2}\frac{\partial}{\partial \underline{r}} + \frac{\partial}{\partial \underline{R}}$$

$\underline{p}_1$ and $\underline{p}_2$ can also be expressed in terms of other co-ordinates (namely the indirect case), as

$$i\,\underline{p}_1 = \frac{\partial}{\partial \underline{r}} - \frac{1}{2}\frac{\partial}{\partial \underline{r}'}$$

$$i\,\underline{p}_2 = \frac{\partial}{\partial \underline{r}'} - \frac{1}{2}\frac{\partial}{\partial \underline{r}}$$

from which we get

$$i\,\underline{L}_{12} = (\underline{r} - \underline{r}')\wedge\left(\frac{\partial}{\partial \underline{r}} - \frac{\partial}{\partial \underline{r}'}\right)$$

The transformation used for the volume integration is

$$d\,\underline{r}_{23} = (4/3)^3\, d\,\underline{r}'$$

and

$$d\,\underline{r}' = r'^2\, d\,r'\, d\,\Omega'$$

where Ω' is the solid angle of $\underline{r}'$.

APPENDIX II

SPIN FUNCTIONS

As we have stated in appendix I, the particles forming the Helium-three are being labled 1,2 for protons and 3 for the neutron.

If α_i and β_i are the spin functions for the nucleon i, then we can write the three-body spin wave functions $|X^{S}_{m_S}\rangle$ as follows:

(II.1.) IN THE DOUBLET STATE $(S = \frac{1}{2}\ ;\ m_S = \pm \frac{1}{2})$

$$|X^{\frac{1}{2}}_{\frac{1}{2}}(1,\overline{23})\rangle = \frac{1}{6}(\alpha_1 \alpha_2 \beta_3 + \alpha_1 \beta_2 \alpha_3 - 2\beta_1 \alpha_2 \alpha_3) \quad \ldots \quad (II.1.1)$$

and

$$|X^{\frac{1}{2}}_{-\frac{1}{2}}(1,\overline{23})\rangle = \frac{1}{6}(\beta_1 \beta_2 \alpha_3 + \beta_1 \alpha_2 \beta_3 - 2\alpha_1 \beta_2 \beta_3) \quad \ldots \quad (II.1.2)$$

The above spin functions are symmetrical in 2 and 3.

Other anti-symmetrical spin functions are being used in order to simplify, the spin products

$$|X^{\frac{1}{2}}_{\frac{1}{2}}(1,\widetilde{23})\rangle = \frac{1}{\sqrt{2}}\alpha_1(\alpha_2 \beta_3 - \alpha_3 \beta_2). \quad \ldots \quad (II.1.3)$$

and

$$|X^{\frac{1}{2}}_{-\frac{1}{2}}(1,\widetilde{23})\rangle = \frac{1}{\sqrt{2}}\beta_1(\alpha_2 \beta_3 - \alpha_3 \beta_2). \quad \ldots \quad (II.1.4)$$

These spin functions have the following properties:

$$< \chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})| \ \sigma_i \ |\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})> = 0 \text{ (If } i = 2 \text{ or } 3\text{)} \qquad \ldots \quad (II.1.5)$$

and

$$f\ (\underline{\sigma}_2\ ,\ \underline{\sigma}_3)(\underline{\sigma}_2 + \underline{\sigma}_3)\ |\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})> = 0 \qquad \ldots \quad (II.1.6)$$

for any function f.

The following transformations were made use of, and enable us to perform the spin summation

$$|\chi^{\frac{1}{2}}_{m_S}(1,\overline{23})> = \frac{1}{3}\ \underline{\sigma}_1 \cdot \underline{\sigma}_2\ |\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})>, \qquad \ldots \quad (II.1.7)$$

and

$$|\chi^{\frac{1}{2}}_{m_S}(2,\overline{13})> = \frac{1}{2\sqrt{3}}\ (3 - \underline{\sigma}_1 \cdot \underline{\sigma}_2)\ |\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})>. \qquad \ldots \quad (II.1.8)$$

as an example, we consider

$< \chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})|(\underline{\sigma}_1 + \underline{\sigma}_2).\ \underline{L}\,|\chi^{\frac{1}{2}}_{m_S}(2,\overline{13})$ which by making use of (II.1.7) and (II.1.8) becomes

$$<\chi^{\frac{1}{2}}_{m_S}(1,\overline{23})|\,(\underline{\sigma}_1 + \underline{\sigma}_2)\ \cdot\ \underline{L}\,|\chi^{\frac{1}{2}}_{m_S}(2,\overline{13})>$$

$$= \frac{1}{6}<\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})|\Big[\ (\underline{\sigma}_1 \cdot \underline{\sigma}_2)(\underline{\sigma}_1 + \underline{\sigma}_2).\ \underline{L}\ (3 - \underline{\sigma}_1 \cdot \underline{\sigma}_2)\ \Big]|\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})>$$

$$= \frac{1}{3}<\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})|\,(\underline{\sigma}_1 \cdot \underline{L})\,|\chi^{\frac{1}{2}}_{m_S}(1,\widetilde{23})>$$

<u>(II.2.) IN THE QUARTET STATE</u> ($S=3/2$; $m_S = 3/2\ ,\ \frac{1}{2}\ ,\ -\frac{1}{2}\ ,\ -3/2$)

The spin functions in this case are symmetrical in 1,2 and 3. Thus,

$$\left| X^{3/2}_{3/2}(1,23)\right\rangle = \alpha_1 \alpha_2 \alpha_3$$

$$\left| X^{3/2}_{1/2}(1,23)\right\rangle = \frac{1}{\sqrt{3}} (\alpha_1 \alpha_2 \beta_3 + \alpha_1 \beta_2 \alpha_3 + \beta_1 \alpha_2 \alpha_3)$$

$$\left| X^{3/2}_{1/2}(1,23)\right\rangle = \frac{1}{\sqrt{3}} (\beta_1 \alpha_2 \beta_3 + \beta_1 \beta_2 \alpha_3 + \alpha_1 \beta_2 \beta_3)$$

$$\left| X^{3/2}_{3/2}(1,23)\right\rangle = \beta_1 \beta_2 \beta_3 \ .$$

APPENDIX III

(III.1.) THE ADJUSTMENT OF THE DEUTERON RADIAL WAVE FUNCTIONS

The s- and D- radial wave functions of the deuteron defined in (I.2.3) and (I.2.4) are interpolated from the data given by Hamada and Johnston (1962). The spline procedure [Christian H. Reinsch, in the Numerische Mathematik 10 (1967), 177] was used, and the values of the constants A and α are then found by Prony method (CCST 376).

TABLE (VIII)

i	A_i	A'_i	α_i	α'_i
1	0.64461574	0.24129498	0.40872076	0.34243311
2	-0.83921827	-0.47087868	2.39298669	4.00785669

A and α are in units of 10^{26} cm^{-2}

(III.2.) THE NUCLEAR INTERACTION POTENTIALS

The potential functions of the nuclear interaction was defined in various chapters as:

$$V(r_{12}) = \sum_{k=1}^{2} U_k^{(II)} \operatorname{Exp}(- \mu_k^{(II)} r_{12}^2) \qquad \ldots \quad (III.2.1)$$

except in the tensor force, in which case it was given by:

$$V(r_{12}) = r_{12}^2 \sum_{k=1}^{2} U_k^{(II)} \operatorname{Exp}(- \mu_k^{(II)} r_{12}^2) \qquad \ldots \quad (III.2.2)$$

The numerical values of $U_k^{(II)}$ and $\mu_k^{(II)}$ are given in table (IX)

TABLE (IX)

	II	$U_1^{(II)}$	$\mu_1^{(II)}$	$U_2^{(II)}$	$\mu_2^{(II)}$
Central	1	-57.301321	0.77821032	-228.3421632	3.10052341
	2	-148.9876342	1.03567201	-1237.4638791	2.9763682
	3	-18.89990532	1.15361054	-47.189002	2.3008962
	4	-10.5324821	0.353112362	2432.0562353	3.789620256
spin-orbit	1	9.21005671	0.83701562	37.5467239	3.80245621
	2	-210.3564210	1.50678932	-189.67458932	5.09156783
Tensor	1	-76.10093256	0.83562410	-2465.0326790	2.70367201
	2	15.3201935	0.7409356	239.86203521	2.88043101
Quadratic spin-orbit	1	38.011136791	1.20009683	596.94365201	4.39767302
	2	7.1025934	0.9853672	-62.40003421	3.7357872
	3	11.3567892	2.3401935	-2200.9898701	8.99587035
	4	-135.111346	3.0612872	-4649.03251	5.28359001

$U_k^{(II)}$ are given in MeV,

and $\mu_k^{(II)}$ are in units of 10^{26} cm^{-2}

APPENDIX IV

COLLECTION OF PARAMETERS

All parameters used in the direct and exchange interaction calculations are now collected and defined as follows:

(IV.1.) THE (s-s) INTERACTIONS

$$\lambda_{ijk} = \alpha_i + \alpha_j + \mu_k / 4$$

$$\gamma_{ijk} = \mu_k / 2\lambda_{ijk}$$

$$e_{ij} = \frac{4}{9}(\alpha_i + 4\alpha_j)$$

$$f_{ij} = \frac{4}{9}(4\alpha_i + \alpha_j)$$

$$W_{ij} = (8/9)^2 (\alpha_i^2 + 8\alpha_i\alpha_j + 4\alpha_j^2)$$

$$\Psi_{ij} = (8/9)^2 (4\alpha_i^2 + \alpha_j^2 + 8\alpha_i\alpha_j)$$

$$\phi_{ij} = (8/9)^2 (4\alpha_i^2 + 4\alpha_j^2 + 20\alpha_i\alpha_j)$$

$$a_{ijk} = \frac{4}{9}(\alpha_i + 4\alpha_j + \mu_k)$$

$$b_{ijk} = \frac{4}{9}(4\alpha_i + \alpha_j + \mu_k)$$

$$C_{ijk} = \frac{4}{9}(2\mu_k - 4\alpha_i - 4\alpha_j)$$

$${}_1a_{ij} = \frac{8}{9}(4\alpha_i + \alpha_j)$$

$${}_1b_{ij} = -\frac{16}{9}(\alpha_i + \alpha_j)$$

$${}_2a_{ij} = \frac{8}{9}(\alpha_i + 4\alpha_j)$$

$${}_1d_{ij} = \frac{8}{9}(\alpha_i^2 + 5\alpha_j^2)$$

$${}_2d_{ij} = \frac{8}{9}(4\alpha_i^2 + \alpha_j^2)$$

$${}_3d_{ij} = \frac{32}{9}(\alpha_i^2 + \alpha_j^2)$$

$${}_1g_{ij} = \frac{32}{9}(\alpha_i^2 + 2\alpha_i \alpha_j)$$

$${}_1\zeta_{ijk} = {}_1b_{ij} + \frac{4}{9}\mu_k$$

$${}_2\zeta_{ijk} = \frac{8}{9}({}_1b_{ij} + 4\mu_k)$$

$${}_3\zeta_{ijk} = \frac{8}{27}(4\alpha_i + 4\alpha_j + \mu_k)$$

$${}_4\zeta_{ijk} = \frac{32}{27}(2\alpha_i + 2\alpha_j + \mu_k)$$

$$\Psi_{ijk} = \frac{9}{4}(1 - \gamma_{ijk}/2)^2 + (9/16\, r^2 \lambda_{ijk})$$

$$\phi_{ijk} = 1 + \alpha_j / \lambda_{ijk}$$

$$\delta_{ijk} = \frac{3}{2}\gamma_{ijk}(1 - \frac{8}{3}\alpha_j r^2)$$

(IV.2.) THE (s-D) INTERACTION

$$\lambda'_{ijk} = \alpha_i + \alpha_j' + \mu_k / 4$$

$$\gamma'_{ijk} = \mu_K / 2\lambda'_{ijk}$$

$$e'_{ij} = \frac{4}{9}(\alpha_i + 4\alpha_j')$$

$$f'_{ij} = \frac{4}{9}\,(4\alpha_i + \alpha_j')$$

$$W'_{ij} = (8/9)^2\,(\alpha_i^2 + 8\alpha_i\alpha_j' + 4\alpha_j'^2)$$

$$\psi'_{ij} = (8/9)^2\,(4\alpha_i^2 + \alpha_j'^2 + 8\alpha_i\alpha_j')$$

$$\phi'_{ij} = (8/9)^2\,(4\alpha_i^2 + 4\alpha_j'^2 + 20\alpha_i\alpha_j')$$

$$a'_{ijk} = \frac{4}{9}\,(\alpha_i + 4\alpha_j' + \mu_k)$$

$$b'_{ijk} = \frac{4}{9}\,(4\alpha_i + \alpha_j' + \mu_k)$$

$$c'_{ijk} = \frac{4}{9}\,(2\mu_k - 4\alpha_i - 4\alpha_j')$$

$${}_1b'_{ij} = -\frac{16}{9}\,(\alpha_i + \alpha_j')$$

(IV.3.) THE (D-s) INTERACTION

$$\lambda''_{jik} = \alpha_j + \alpha_i' + \mu_k/4$$

$$\gamma''_{jik} = \mu_k/2\,\lambda''_{jik}$$

$$e''_{ij} = \frac{4}{9}\,(\alpha_j + 4\alpha_i')$$

$$f''_{ji} = \frac{4}{9}\,(4\alpha_j + \alpha_i')$$

$$W''_{ji} = (8/9)^2\,(\alpha_j^2 + 8\alpha_j\alpha_i' + 4\alpha_i'^2)$$

$$\psi''_{ji} = (8/9)^2\,(4\alpha_j^2 + \alpha_i'^2 + 8\alpha_j\alpha_i')$$

$$\phi''_{ji} = (8/9)^2\,(4\alpha_j^2 + 4\alpha_i'^2 + 20\alpha_j\alpha_i')$$

$$a''_{jik} = \frac{4}{9}(\alpha_j + 4\alpha'_i + \mu_k)$$

$$b''_{jik} = \frac{4}{9}(4\alpha_j + \alpha'_i + \mu_k)$$

$$c''_{jik} = \frac{4}{9}(2\mu_k - 4\alpha_j - 4\alpha'_i)$$

$$_1b''_{ji} = -\frac{16}{9}(\alpha_j + \alpha'_i)$$

APPENDIX V

In extending the analysis of both the direct and interaction terms, the following formulae are used

$$K \int \mathrm{Exp}\left[-\lambda(\underline{R} - r\,\underline{r})^2\right] d\underline{R} = 1$$

$$K \int \underline{R}\,\mathrm{Exp}\left[-\lambda(\underline{R} - r\,\underline{r})^2\right] d\underline{R} = \gamma\,\underline{r}$$

$$K \int R^2\,\mathrm{Exp}\left[-\lambda(R - r\,\underline{r})^2\right] d\underline{R} = \frac{3}{2\lambda} + \gamma^2 r^2$$

$$\int_0^\infty R^{2n}\,\mathrm{Exp}(-\lambda R^2)\,dR = (1.3\ldots(2n-1)/(2)^{n+1}\lambda^n)(\pi/\lambda)^{\frac{1}{2}}$$

$$(\mathrm{Re}\,\lambda > 0\ ;\ n = 0,1,2\ldots)$$

$$\int_0^\infty R^{n+1} J_n(\mu r R)\,\mathrm{Exp}(-\lambda R^2)\,dR = ((\mu r)^n/(2\lambda)^{n+1})\,\mathrm{Exp}(-\mu^2 r^2/4\lambda)$$

$$(\mathrm{Re}\,\lambda > 0\ ,\ \mathrm{Re}\,n > -1)$$

$$\int_{-1}^{+1} \mathrm{Exp}(b\,\underline{r}.\underline{r}')\,p_n(\eta)\,d\eta = (2\pi/b\,rr')^{\frac{1}{2}}\,I_{n+\frac{1}{2}}(b\,rr')$$

where

$$K = (\lambda/\pi)^{3/2}$$

and $I_{n+\frac{1}{2}}(X)$ is the modified spherical Bessel function of the first kind of order $(n+\frac{1}{2})$, and is related to $\mathcal{J}_{n+\frac{1}{2}}(X)$ by the following relation

$$\mathcal{J}_{n+\frac{1}{2}}(X) = (-1)^n(\pi X/2)^{\frac{1}{2}}\,I_{n+\frac{1}{2}}(X)$$

The recurrence relations between the functions are (Bateman 1953, Vol. II and Whittaker and Watson, 1952)

$$\mathcal{J}_{n+\frac{1}{2}}(X) = \frac{X}{(2n+1)} \left[\mathcal{J}_{n+3/2}(X) - \mathcal{J}_{n-\frac{1}{2}}(X) \right]$$

and

$$\mathcal{J}'_{n+\frac{1}{2}}(X) = \frac{(n+1)}{X} \mathcal{J}_{n+\frac{1}{2}}(X) - \mathcal{J}_{n+3/2}(X)$$

from which one obtains

$$\mathcal{J}''_{n+\frac{1}{2}}(X) = \left[\frac{n(n+1)}{X^2} + 1 \right] \mathcal{J}_{n+\frac{1}{2}}(X)$$

the $\mathcal{J}'_{n+\frac{1}{2}}(X)$ and $\mathcal{J}''_{n+\frac{1}{2}}(X)$ denote the first and second derivatives w.r. to X.

The Bessel functions $I_{n+\frac{1}{2}}(X)$ can be calculated by using the power series or the asymptotic form (Bateman, 1953).

$$I_{n+\frac{1}{2}}(X) = (-1)^n \frac{X^2}{2^n} \sum_{n=0} \left((m+n)! \;/m! \left[(2m+n)+1 \right]! \right) \text{ for } X < \infty$$

and

$$I_{n+\frac{1}{2}}(X) = \frac{(-1)^n}{2} \left\{ e^X \left[\sum_{m=0}^{m-1} (-1)^m \frac{(n+\frac{1}{2},m)}{(2X)^m} + O(|X|^{-m}) \right] \right.$$

$$\left. + (-1)^{n+1} e^{-X} \left[\sum_{m=0}^{m-1} (-1)^m \frac{(n+\frac{1}{2},m)}{(2X)^m} + O(|X|^{-m}) \right] \right\} \text{ for } X > \infty$$

where

$$(n + \tfrac{1}{2}, m) = \frac{\Gamma(n + m + 1)}{\Gamma(n - m + 1)m!}$$

REFERENCES

1. Abraham, G.; Cohen, I.; and Roberts, A.S.; Proc. Phy. Soc. London 68A (1955), 265.

2. Abramowitz, M.; and Segun, I.A., Handbook of Mathematical functions (Dover publiction, Inc., New York, Seventh ed. 1968).

3. Adair, R.L; Okazaki, A.; and Walt, M.; Phy. Rev. 89 (1953), 1165.

4. Allred, J.C.; Armstrong, A. H; Bondelid, R.O.; and Rosen, L.; Phy. Rev.; 88 (1952), 433.

5. Bateman, H.; 1953, Higher transcendental functions, Vol. II, McGraw-Hill, London.

6. Bahetti, O.P.; and Fuda, M.G., Phys. Rev., 7C (1973), 1845.

7. Bhaker, B.S., Nucl. Phys., 46 (1963), 572.

8. Bencze, Gy.; and Doleschall, P., Phy. lett., 44B (1973), 235.

9. Blatt, J.N.; and Weisskop, V.F.; Theoretical Nuclear Physics (1952), John Wiley and Sons, New York.

10. Blatt, J.M.; Derrick, G.H.; and Lyness, J.N.; Phy. Rev. Lett. 8 (1962), 323.

11 Blatt, J.M.; Delves, L.M., Phys. Rev. Letters, 12 (1964), 544.

12. Blatt, J.M.; and Derrick, G., Nucl. Phy. 8 (1958),602.

13. Blatt, J.M.; and Biedenharn, L.C., Rev. Mod. Phy. 24 (1952), 257.

14. Brolley, JR, J.E.; Putnam, T.M.; Rosen, L.; and Stewart, L., Phys. Rev. 117 (1960), 1307.

15. Buckingham, R.A.;; 1957, Numerical Methods, Sir Isaac Pitman and Sons Ltd., London.

16. Buckingham, R.A.; 1962, Rview paper in the proceedings of the summer school in Oxford (1961), on numerical solutions of ordinary and partial differential equations, Oxford, Pergamon. Press.

17. Burke, P.G., 1960, Review paper in the proceedings of the London conference (1959), on Nuclear forces and the Few-Nucleon Problem, London, pergamon press.

18. Bruinsma, J.; and Van Wageningen, R., Phy. lett., 44B (1973), 221.

19. Bransden, B.H.; and Robertson, H.H.; Proc. Phy. Soc., London 72A (1958), 770.

20. Bransden, B.H.; Robertson, H.H.; and Swan,P; Proc., 69A (1956), 877.

21. Bransden, B.H.; Smith, K.; and Tate, G., Proc. Roy. Soc. 247A (1958), 73.

22. Brady, T.J.; Phy. Lett. 45B (1973), 4.

23. Brueckner, K.A., and Gammel, J.L., Phys. Rev. 109 (1958), 1023.

24. Bhatt, S.C.; and Levinger, J.S.; Phy. Lett. 40B (1972),67.

25. Buckingham, R.A.; Hubbard, S.J.; and Massey, H.S.W., Proc. Roy. Soc. 211A (1952), 183.

26. Buckingham, R.A.; and Massey, H.S.W., Proc. Roy. Soc. 179A (1941), 123.

27. Burke, P.G.; and Robertson, H.H., Proc. Rhys. Soc. 70A (1957), 777.

28. Brayshow, D.D.; Phys. Rev. 7C (1973), 1731.

29. Cahill, T.A.; and Greenwood, J., Phys. Rev. 40(1971),1499.

30. Caldwell, D.O.; and Richardson, J.R., Rev., 98 (1955), 28.

31. Christian, R.S.; and Gammel, J.L., Phys. Rev. 91 (1953), 199.

32. Condon, E.U.; and Shortley, G.H., Theory of atomic spectra, Cambridge University press, 1935.

33. Clapp, R.E. Phys. Rev. 76 (1949), 873.

34. Derrick, G.H., and Blatt, J.M., Nucl. Phys., 17(1960),67.

35. De Brode, A.H., and Massey, H.S.W., Proc. Phys. Soc. 68A (1955), 769.

36. Delves, L.M.; and Phillips, A.C., Rev. of Mod. Phys. 41 (1969), 497.

37. Delves, L.M., Blatt, J.M., Pask, C., and Davies, B., Phys., lett. 26B (1969), 472.

38. Edmonds, A.R., Angular Momenta in Quantum Mechanics, 1957, Princeton University press.

39. Elwyn, A.J.; Lane, R.D.; and Lanysdorf, JR., A.m Phy. Rev. 128 (1962), 779.

40. Fox. L., and Goodwin, E.T., Proc. Camb. Phil. Soc., 45 (1949), 373.

41. Gammel, J.L., and Thaler. R.M., Phy. Rev. 107 (1957), 291.

42. Gajewski, T., Nucl. Phy., 41 (1963), 323.

43. Gammel, J.L., and Thaler, R.M., Phys. Rev. 109(1958), 20141.

44. Gammel, J.L.; Christian, R.S.; and Thaler, R.M., Phys. Rev. 105 (1957), 311.

45. Gerjuoy, E., and Schwinger, J., Phys. Rev. 61(1942),138.

46. Hamada, T., Prog. Theor. Phys. 21 (1959), 769.

47. Hamada, T., Prog. Theor. Phys. 24 (1960), 1033.

48. Hamada, T., Prog. Theor. Phys. 25 (1961), 247.

49. Hamada, T., and Johnston, I.D., Nucl. Phys.34(1962),382.

50. Hochberg, S., 1953, Thesis, London University(unpublished).

51. Hochberg, S.; Massey, H.S.W; and Underhill, L.H., Proc. Phy. Soc. London 67A (1954), 957.

52. Hochberg, S.; Massey, H.S.W.; Robertson, H.; and Underhill, L.H., Proc. Phy. Soc. London 68A(1955),746.

53. Hochberg, S.; Omojola, P.A.F.; and Sribhibadh, S., 1968, (unpublished).

54. Hodgson, P. E., Phil. Mag. 7 (1958), 25.

55. Horie, H.; Tamura, T., and Yashida, S., Prog. Theor. Phys., 8 (1952), 341.

56. Hoshizaki, N.; and Machida, S., Prog. Theor. Phys. 24 (1960), 1325.

57. Hu, T.M. and Hsu, K.N. Proc. Roy. Soc. London, 204A (1951), 476.

58. Haby, R.; Proc. Phys. Soc. 67A (1954), 1103.

59. Jahn, H.A.; and Hope, J.; Phys. Rev. 93 (1954), 318.

60. Kikuta, T.; Morita, M.; and Yamada, M., Prog. Theor. Phys. 15 (1956), 222.

61. Mckellar, B.H.H., Rajaraman, R., Phys. Rev. Lett., 21 (1968), 450.

62. McMillan, M.; and Best, M., Nucl. Phys. 105A (1867),649.

63. Mott, N.F.; and Massey, H.S.W., the Theory of atomic collisions, 1949, Sec. ed. Oxford Clarendon press.

64. Newman, D.J., 1959, Thesis, London. (unpublished).

65. Okubo, S.; and Marshak, R.E., Annal. Phys., 4(1958),166.

66. Omojola, D.A.F., Thesis, University of London 1968.

67. Ord-Smith, R.J., Phy. Rev. 94 (1954), 1227.

68. Pask, C., Phys. lett., 33B (1970), 325.

69. Pease, R.L. and Feshbach, H. Phys. Rev. 88(1952),971.

70. Pieper, S.C., Nucl. Phys. 193A (1972), 519.

71. Racah, G., Phys. Rev., 62 (1942), 438.

72. Racah, G., phys. Rev., 63 (1943), 367.

73. Reid, R.V., Ann. Phys. (N.Y.) 50 (1968), 411.

74. Rose, M.E., Elementary theory of angular momentum (John Wiley and Sons, Inc., New York, 1957).

75. Robertson, H.H., Proc., Caub., Phil., Soc., 52(1956),538.

76. Rosen, L., Phys., Rev., 82 (1951), 777.

77. Shiff, L.I., Phys., Rev., 133B (1964), 802.

78. Seagrave, J.S., in the proceeding of the first international conferences on three-body problims in nuclear and particle physics, edited by McKee, J.S.C.; and Rolph, P.M., North Holland publishing Co., Amasterdam-London. 1970.

79. Sherr, R.; Blair, J.M.; Kratz, H.R.; Bailey, C.L.; and Taschek, R.F., Phys., Rev., 72 (1947), 662.

80. Signell, P.S.; and Marshak, R.E., Phys., Rev., 106(1957), 832.

81. Signell, P.S.; and Marshak, R.E., Phys., Rev., 109 (1958), 1229.

82. Sugie, A.; Hodgson, P.E.; and Robertson H.H., Proc., Phys., Soc., London 70A (1957), 1.

83. Sribhibhadh, S., 1966, Ph.S. thesis London University.

84. Tang, Y.C.; Schmid, E.W.; and Herndon, R.C., Nucl., Phys., 65 (1965), 203.

85. Thomas, L.H., Phys. Rev. 47 (1935), 903.

86. Van Oers, W.T.H., Brockman, K.W., Nucl. Phys. 92A(1967), 561.

87. Watson, G.N., 1944, the theory of Bessel functions, Cambridge University press.

88. Wheeler, J.A., Phys., Rev., 52 (1937), 1083, 1107.

89. Wheeler, J.A.; and Barschall, H.H., Phys., Rev., 58 (1940), 682.

90. Whittaker, E.T., and Watson, G.N., 1952, Modern Analysis, Cambridge University press.

91. Pramanik, M.H.A., 1971, thesis London University.

92. Lee, S.P.Y., 1969, thesis London University.

93. Sibbel, R., 1971, thesis London University.

94. Gupta, V.K., Bhakar, B.S., and Mitra, A.N., Rhys. Rev. lett. 15 (1965), 974.

95. Jackson, A.D., and Tjon, J.A., phys. lett. 32B (1970), 9.

96. Loisean, B.A., and Nogame, Y., Nucl. Phys. B2(1967), 470.

97. Pask, C., Phys. lett., 25B (1967), 78.

98. Brayshaw, D.D., Phys. Rev. 7C (1972) 6.

99. Harper, E.P.; Kim, Y.E.; and Tubes, A., Phys. Rev. lett. 28 (1972), 1533.

100. Humberston, J.W., and Hunnel, M.A., Phys. lett. 31B (1970), 423.

101. Delves, L.M., Blatt, J.M., Pask, C., and Davies, B. Phys. lett. 28B (1969), 472.

102. Hunnel, M.A., and Delves, L.M., Phy. lett., 40B (1972),20.

SUPPLEMENTARY II

COMPUTER PROGRAMMING OF THE PROBLEM

Below we give the general structure of all programmes constrected by the author to calculate the problem of scattering of protons by deuterons and the binding energy of ^{3}He.

(1) INTERPOLATION AND FITTING

The preliminary step in the calculation is to find the values of all constants of the potential and wave functions. This was done by interpolating them from the data given by Hamada and Johnston (1962).

An outline of the programme for the interpolation and fitting is given in (table A).

(2) EVALUATION OF THE DIRECT TERMS

There are three types of direct terms in the equations (XI.16,17,18) and are classified as $\lambda^{s}_{\ell'\ell}$, $\mu^{s}_{\ell'\ell}$ and $\nu^{s}_{\ell'\ell}$. In the actual computation, these functions are tabulated and used later as input data in the matrix solutions. Computer programme to evaluate these terms was written and prepared by the author, the general structure of which, we given in (table B).

It is to be noted that in carrying out the computation, one has to separate the programmes for the doublet and the quartet cases, because the data in these two cases are different.

(3) EVALUATION OF THE MATRIX EQUATIONS

There are two types of equations. In the doublet case, a programme was written to compute single equation of the form

$$\sum_{j=1}^{N} a_{ij} f_j = b_j \qquad (i = 1,2,\ldots,N \text{ and } \ell=0,1,2 \text{ with } J = \tfrac{1}{2}).$$

where f_j are the tabular values of the radial wave functions. Another programme in the quartet case was written to compute coupled equations. These coupled equations are not very different from the uncoupled equations. It involves doubling the number of rows and columns in the matrix to be enverted. Thus, if f_ℓ and g_ℓ are the coupled radial wave functions, we solve

$$\sum_{\ell=0}^{3} C^{ij}_{\ell'\ell} f^{j}_{\ell} + \sum_{\ell',0}^{3} e^{ij}_{\ell'\ell} g^{j}_{\ell} = \sum_{\ell} d^{j}_{\ell'\ell}$$

$$\sum_{\ell=0}^{3} C'^{ij}_{\ell'\ell} f^{j}_{\ell} + \sum_{\ell=0}^{3} e'^{ij}_{\ell'\ell} g^{j}_{\ell} = \sum_{\ell} d'^{j}_{\ell'\ell} \qquad (i,j=1,2,\ldots,N)$$

the above two equations couple and may be written in the following form

$$\sum_{\ell=0}^{3} H^{ij}_{\ell'\ell} F^{j}_{\ell} = \sum_{\ell} B^{j}_{\ell'\ell} \qquad (i,j=1,2,\ldots,2N)$$

The direct terms and the kernels are now used as part of the data in the matrix programme which is outlined in (table C).

(4) THE BINDING ENERGY OF ^3He

For the eigenvalue problem we solve

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - V(r) \right] f_\ell(r) - \int_0^\infty K(r,r')\, f_\ell(r')\, dr' = -E\, f_\ell(r)$$

In general we solve an equation of the form $A X = \lambda X$, where A is a matrix of nxn, and λ is the eigenvalues and X is the eigenvectors. A library procedure designed to solve this kind of problems was used, and the general structure of which we give in (table D).

(TABLE A) THE SPLINE INTERPOLATION AND EXPONENTIAL FIT

```
begin
      integer   m, nn;
      print     punch (3), ££L? No. of data points = ?;
      read      reader (3) nn;
      sameline; print  punch (3), ££L? No. of interpolation
      points = ?;
      read      reader (3), m;
begin
      integer   n,i,j,k;
      real      Z int, Z tol, fC, S, ff, ZZ, dZ, tol, Z start;
      comment   CBS: back store;
      array     y,Z,df,a,b,c,d [ 1:nn ] , f [ 0:(m-1) ] ;
      switch    Sp: = out ;
```

```
Library   spline;  Christian, H. R; Numerische Mathematik
     .
     .    10 (1967), 177.
     .
     .
          print  punch (3), ££L? z start = ?;
          read   reader (3), Z start;
          print  punch (3), ££L? delta - Z = ?;
          read   reader (3), d2;
          print  punch (3), ££L? spline tolerance = ?;
          read   reader (3), tol;
          for    i :=1  step  1  until nn do
             begin   read  Z [ i ]  , y [ i ] ;
             print  punch (4), sameline, digits (4), ££ S5?2=,
                       Z [ i ] , ££ S5 ? F= ?, scaled (g), y[ i ],
                       ££ ??; d f [ i ] = y [ i ]/ tol;
                  end   input;
 N:=1 ;    S:= 0.0 ;
 print     punch (4) , ££? S = ? , freepoint (4), S, ££L ??;
 spline (n,nn,Z,y,df,S,a,b,c,d);
 begin  comment CBS: back store;
      integer  array  check [ 0 : M ] ;
      for i : = 0 step 1 until  m do
      check [ i ] = 0 ;
      punch (4); sameline ;
      K: = 0 ;
      for  j : = 0  step  1  until  m do
      begin  real  h, Zh ;
        Zh : = Z start + j × d2;
```

```
ff : = (( d [ i ] * h + C [ i ] * h + A [ i ] ;
check [ j ] : = 1;
K : = K+1; if  K = m+1  then  goto  out;
if  j  = m  then   f [ j ] : = ff ;
end  i;
end  j ;
end  check ;
out :
begin
     integer   repeat, n, int ;
     switch SS: = again ;
     sameline ; punch (4) ; repeat : = 0;
     n : = m - 1;
     again:
     print  punch (3), ££ S5? Step = ?;
     read  reader (3) , int;
     begin
          integer  tab, i, j , k ;
          real  XX, yy, delta, Xo, Xn;
          comment  CBS :  back store;
          Array  a,b [ 1:2 ] , ff [ 0:((n+1) div int-1) ] ;
Procedure  prony 2 (y,X,ff, Xo, Xn, a , b , n , delta, tab);

   comment
          CCST library procedure NO. 376. evaluates the
          double exponential least square fit.
```

```
procedure   ortholin 2(a, b, n, m, eps, X, fail);

      comment
            CCST  library procedure No. 156. gives the
      least squares solution for a system of n linear
      equations in m unknowns. a is the nxm matrix of the
      system, b the constant vector on the r.h.s., eps
      the maximal relative rounding error, and X the
      solution vector.  S used if the iterative improvement
      is ineffective.
      .
      .
      .
  real   procedure   Scalarproduct (S, a, i, p, n);

    comment    this procedure porforms all inner products.
    .
    .
    .
 end   Scalarproduct;
  .
  .
  .
 end   of procedure ortholin 2;
  .
  .
  .
 end   prony 2;
  K : = - 1;
  for  i : = 0  step  int   until  n do
     begin
        K : = K + 1 ;
        ff [ k ] : = f [ i ] ;
           end ;
        Xo : = Z start;
       Xn : = Xo + d2 * int * (K-1);   tab : = 1;
```

```
prony 2(yy, XX, ff,Xn, a, b, K, delta, tab) ;
print  ££LS30 ?   exponential fit parameters £ L 2S 40 ?
       step size = ? , digits (2), int,
print  ££LS40 ? No. of points in fit = ? , digits (4),
       K + 1 , ££ Z ?? ;
print ££LS20 ? al : = ?, scaled (g), b[ 1 ] , ££S5 ? G
       Gammal = ? , a[ 1 ] , ££LS20 ? A2=?,  b[ 2 ] ,
       ££S5 ? Gamma 2 = ?, a[ 2 ] , ££L2??;
print  punch (3),  ££L ? repeat = ?; read reader (3), repeat;
       if  repeat = 1 then  goto again;
end    inner block ;
end    expon. fit;
end    outer block;
end    interpolation and expon. fit;
```

This programme was run on 503 Computer, if the user decides to run it on CDC 6600 or 7600 machines, then certain changes in the input-output have to be done.

(table b) THE DIRECT TERMS

The general structure of the programme in the doublet case ($S=\frac{1}{2}$) is not very different from that in the quartet case: This programme was run on CDC 6600 machine through the terminal 200 located at Chelsea College of Science and Technology, University of London.

```
'BEGIN'
      'INTEGER'  I, J1, I13, KL, NN, JJ,...;
      'REAL'  J, EP, H, AJL,... ;
      INPUT (60, '('5(N)')', J, EP, KL, NN, H);
```

```
OUTPUT (61,'('/,'('J= ')', N, 5B,'('EP = ')', N,5B,'('KL=')'
2ZD, 5B, '('NN=')', 2ZD, 5B, '('H=')',N')', J, EP, KL, NN,H);
'BEGIN'
  'REAL'  DLAMBDA, DMU, DNU;
  'ARRAY'  A, ALPHA, B, BETA, UC1, MUC1, ULS1, MULS1, UQ1,
           MUQ1, UQ3, MUQ3, UT1, NUT1(/ 1..2 /);
  'REAL'   'PROCEDURE' (I,J);
  'VALUE'  I,J;
  'INTEGER' I,J;
  'BEGIN'
      DELTA. ='IF' I=J  'THEN' 1 'ELSE' 0
      'END'  DELTA;
  'REAL'  'PROCEDURE' UU (I,H,L);
   'VALUE'  I,H,L;
   'INTEGER'  I,L;
   'REAL'  H;
   'BEGIN'
   .
   .
   .    USER  PROGRAMME
   .
   'END'  UU;
  'REAL'  'PROCEDURE' VV(IMHML);
    'VALUE' IMHML;
    'INTEGER' I,L;
    'REAL'  H;
    'BEGIN'
        .
        .
        .  USER PROGRAMME
        .
     'END'  VV;
  'REAL'   'PROCEDURE'  WW(I,H,L);
```

```
'VALUE'  I,H,L;
'INTEGER'  I,L;
'REAL'  H;
'BEGIN'
   .
   .  USER PROGRAMME
   .
 'END'  WW:
'REAL'  'PROCEDURE'  LAMBDA (I,H,LP,L);
'VALUE'  I,H,LP,L;
'INTEGER'  I,LP,L;
'REAL'  H;
'BEGIN'
LAMBDA. = DELTA(LP,L)+ WW(I,H,L) + 0.5 * H * VV(I,H,L);
'END'  LAMBDA;
'REAL'  'PROCEDURE'  MMU(I,H,LP,L);
'VALUE'  I,H,LP,L;
'INTEGER'  I,LP,L;
'REAL'  H;
'BEGIN'
   MMU. =  DELTA(LP,L) + WW(I,H,L)   0.5 * H * W(I,H,L);
   'END'  MMU;
   'REAL'  'PROCEDURE'  NU(I,H,LP,L,EP);
   'VALUE'  I,H,LP,L,EP;
   'INTEGER'  I,LP,L;
   'REAL'  H,EP;
   'BEGIN'
      NU. = (H' POWER' 2)*[ 4M/3ħ^2  * EP*(L *(L+1) / ((I * H)'
            POWER' 2)) * DELTA(LP,L) + UU(I,H,L) - 2.0
            *(DELTA(LP,L)+ WW(I,H,L) ] ;
```

```
'END'  NU;
'FOR'  JJ. = 1 'STEP'  1 'UNTIL'  2'DO'
'BEGIN'
INPUT (60,'('14(N)')', A(/JJ/), ALPHA(/JJ/),B(/JJ/),
       BETA(/JJ/), UC1(/JJ/), MUC1(/JJ/),...);
'END';
AJL. = (1.0/3.0) * (J * (J+1) - 0.75 - L * (L+1));
FOR I. = 1 'STEP' 1 'UNTIL' KL 'DO'
'BEGIN'
DLAMBDA. = LAMBDA(I,H,LP,L);
DMU. = MMU(I,H,LP,L);
DNU. =NU(I,H,LP,L,EP);
OUTPUT(61,'('//,'('DLAMBDA = )', N,5B, '('DMU=')', N, 5B,
       '('DNU=')', N')', DLAMBDA, DMU, DNU);
'END';
'END';
'END';
```

Other procedures may be required to calculate the angular coefficients. They can be included within this programme, or alternatively, can be done deparately.

Among these the following

'REAL' 'PROCEDURE' VCC(J1,J2,JM1, M2,M,FACTORIAL); to evaluate the 3-j symbol;

'REAL' 'PROCEDURE' SJS(J1,J2,J3,L1,L2,L3, FACTORIAL); to evaluate 6-j symbol;

'REAL' 'PROCEDURE' NJS(J11,J12,J13,J21,J22,J23,J13,J23, J33,FACTORIAL); to evaluate the 9-j symbol.

These procedures are available at Chelsea Computer Centre.

(TABLE C) THE MATRIX SOLUTION

The structure of the programme in the case of solving uncoupled equations is slightly differ from that in the coupled equation. In the latter, the kernels as well as the direct terms are here used as data.

THE UNCOUPLED MATRIX EQUATIONS

```
'BEGIN'
    'INTEGER' I,J1,II1,I13,JJ,MM,NN,KL,I12,M;
    'SWITCH'  SS.= U;
    'REAL'  J, EP, AJL;
     INPUT (60,'('5(N)')', J,MM,NN,EP,KL);
     OUTPUT (61,'('/,'('J=')', N,5B,'('MM= ')',2ZD,
     5B,'('NN=')', 2ZD, 5B,'('EP=')', N,5B,'('KL=')',N')',
     J,MM,NN,EP,KL);
     M = KL - 1 ;
     'BEGIN'
     'REAL' DEL, H;
     'INTEGER' LP,L,IM,JM,KM;
     INPUT(60,'('4(N)')', LP,L,H,DEL);
     OUTPUT(61,'('/,'('LP=')', 2ZD,5B, '('L=')', 2ZD,
           5B,'('H=')',N,5B,'('DEL= ')',N')',LP,L,H,DEL);
     'BEGIN'
     'ARRAY' A,AP, ALPHA, ALPHAP, UC2,...(/1..2/), ETA,
             W(/1..MM/), TT(/1..KL/), LAMBDA, MMU,
             NU(/1..KL/), HH(/1..M,1..KL/),  R(/1..M+1/),
             F(/1..M,1..M+1/);
     'REAL' 'PROCEDURE'  DELTA(I,J);
```

'REAL' 'PROCEDURE' LEGENDRE (N,X); available at Chelsea Computer Centre.

'REAL' 'PROCEDURE' T(Y); available at CCST Computer Centre.

'REAL' 'PROCEDURE' GAMMA(Z) available at CCST Comptuter Centre.

'REAL' 'PROCEDURE' SBESS 1(X,NMAX,SI) available at Chelsea Computer Centre, and is modified slightly, by the author to suit the problem.

```
'REAL' 'PROCEDURE' KERN(I,J1,H,L,MM,EP);
'VALUE'  I,J1,H,L,MM,EP:
'INTEGER' I,J1,L,MM;
'REAL'  H,EP;
'BEGIN'
    'INTEGER'  II,JJ,KK,NI,I1;
    'REAL' KEL, KTOT,...all-real. variables..;
    'ARRAY' SIC2,SILS2,SIQ2,SIQ4,...;(/0..NN/), U,V,T,LEGL,
            K coul(/1..MM/);
    'BEGIN'
        KEL. =0.0;
        'FOR. II. = 1 STEP  1  'UNTIL' 2  'DO'
        'FOR' JJ. = 1 'STEP'  1 'UNTIL' 2 'DO'
        'FOR' KK. = 1 'STEP' 1 'UNTIL' 2 DO
    'BEGIN'
            .
            .
            .
            .  USER PROGRAMME
            .
            .
     KEL. =  KEL + TT (/J1/) * KTOT ;
    'END' ;
     KERN . = KEL ;
    'END'   KERN ;
```

```
'PROCEDURE'  LLGAUSS(A,N,R, DELTA, U);
'COMMENT'  library procedure No. 262.
      This procedure solves a system of pinear equations
by eliminating and partial pivoting.  The parameters are:
N   The number of equations and the total matrix of the
    system including the R.H.S.
A   Is a matrix and has the dimensions A(/1..N,1..N+1/).
R   Upon exit the output parameter R contains the silution
    of the system.
U   The label U, must specify a jump to the main program if
    the codfficient matrix is ill-conditioned, which is
    expressed by the fact that the absolute value of the
    pivot element is less than the parameter delta;

'END'  LLGAUSS;
'FOR'  JJ. = / 'STEP' / 'UNTIL' 2 'DO'
'BEGIN'
      INPUT(60, '(all constants ')',) ;
'END' ;
AJL. = (1.0/3.0) * (J * (J+1) - o.75 - L * (L+1));
'FOR' II1. = / 'STEP' / 'UNTIL' MM 'DO'
'BEGIN'
INPUT (60, '('2(N)')', ETA(/II1/), W(/II1/));
OUTPUT(61,...);
'END' ;
'FOR' I 13. =1 'STEP' 1 'UNTIL' KL 'DO'
'BEGIN'
      INPUT (60. '('(N)')', TT(/I13/));
'END' ;
'FOR' I 12. = / 'STEP' / 'UNTIL' KL 'DO'
```

```
'END' ;
'END' ;
'END' ;
  U..
'END' ;
```

THE COUPLED MATRIX EQUATIONS

In this system of equations, the direct and the kernels as well as the total matrix H are all computed separately and used as input data.

```
'BEGIN'
      'INTEGER'  N ;
      'SWITCH' SS. = U ;
      'REAL'  DELTA ;
      INPUT (60, '('2(N)')', N, DELTA );
      'BEGIN'
            'INTEGER' I,J,K;
            'ARRAY'  R(/1..N+1/). A(/1..N,1..N+1/);
PROCEDURE   LLGAUSS(A,N,R, DELTA, U) ;
      .
      .
      .
 'END'   LLGAUSS ;
 'FOR'  J. = 1  'STEP' 1 'UNTIL' N 'DO'
 'BEGIN'
      OUTPUT (61, '('/,10B,'('J=')', 2ZD')',J);
 'FOR'  K. = 1 'STEP' 1 'UNTIL' N+1 'DO'
 'BEGIN'
     INPUT (60,'('(N)')', A(/J,K/));
 'END' ;
 'END' ;
```

```
LLGAUSS (A,N,R, DELTA, U);
'FOR' I. = 1 'STEP' 1 'UNTIL' N 'DO'
'BEGIN'
  OUTPUT (61, '('/, 10B, '('I=')', 27D, 10B, '('R=')' , 2B,N')',
  I,R(/I/));
'END' ;
'END' ;
U..
'END' ;
```

Our programs for the direct terms, the kernels, as well as those designed to solve the uncoupled and coupled matrix equations for (p-d)-scattering problem, are now used by H.Gaylani to solve scattering problem similar to ours but with the coulomb interaction switched off.

<u>(table D) THE BINDING ENERGY</u>

The direct terms and the kernels are separately computed. These are then used as an input data in the computation of the total matrix A. UCSF Library program was then used to find the eigenvalues with the matrix A input in the form of data.

It seems often true that while these may exist alternative ways of programming the problem, which make more and better use of peripheral facilities, the programmer may be compelled to adopt a less efficient apprach in terms of computer utilization, simply becouse the desired degree of efficiency may require more acess to the machine than is available (Sibbel 1971).

As it has been stated before, all our calculations performed on the CDC 6600 are input through a 200 terminal link, stationed either at Chelsea College of Science and Technology or at the Imperial College of Science and Technology. Inspite of that all, it should be noted that this does not alter the fundamental numerical and computational approach to the problem.