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by

DAVIES A.F. OMOJOLA, B.Sc. (Lond.), Grad.I.M.A.

Department of Mathematics,
Imperial College of Science and Technology,
South Kensington,
London, S.W.7.

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DEDICATION

To my children

and

To the memory of my parents without whom this thesis would never have been written.

PREFACE

The work presented in this thesis was carried out in the Department of Mathematics, Imperial College of Science and Technology, South-Kensington, London, S.W.7 between October, 1965 and June, 1968 under the supervision of Dr. S. Hochberg, B.Sc., Ph.D., A.R.C.S.

The work described here is divided into four parts. The first part deals with the new formulation of the integro-differential equations for light nuclei with particular reference to deuteron, triton and the alpha-particles. Part two deals with the scattering of neutrons by alpha-particles. Part three deals with the variational calculation of the binding energy of alpha-particles using the principal S- and D-states wave functions of the alpha-particles. The effect of the hard core is also investigated. Part four deals with the numerical analysis and computation.

It is a pleasure for me to express deep gratitude to my supervisor, Dr. S. Hochberg, for suggesting the problems and for his constant encouragement and valuable guidance throughout this work. Our stimulating discussions and his suggestions have a great value to me.

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Last but not least my wife, 'Bolanle, and my children, Olanike and Olaniyi, for the patience they have had with me and my work during a period of time when I have not been able to take such an active part in the family life as I usually do. Thanks are also due to Miss Margaret Hudgell, B.A., for undertaking the difficult task of typing this thesis at short notice from what must have been an almost illegible script.

D.A.F. OMOJOLA.

ABSTRACT

(i) A new formulation of the elastic neutron-Helium ($n\text{-}He^4$) scattering using the most general form of the nuclear interaction which includes the Central, Non-Central Exchange, Linear Spin-Orbit, Tensor and Quadratic Spin-Orbit Forces is given.

(ii) The resonating group method of J.A. Wheeler (1937) is employed to construct the five-body wave functions and from the Schrödinger's equation a set of simultaneous integro-differential equations is derived.

(iii) The Hamada and Johnston's potentials used are expressed in Gaussian form permitting analytical integrations and leading to great economy of computing time. There are repulsive cores in all states. These potentials are used to calculate the binding energy of the alpha-particles (Chapter IX). It is shown that by using a repulsive core of suitable radius the excessive binding obtained with two body central potentials may be reduced to reasonable values.

(iv) An extension of the $n\text{-}He^4$ scattering formulation to include the D-state of the alpha wave function is discussed.

(v) The resulting integro-differential equations are then solved by the method of finite differences.

Programmes for computing the Direct and Indirect (Kernels) Terms and for the solutions of the equations written in Algol language were prepared for the University of London Atlas Computer. The equations are solved at different incident neutron energies.

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INTRODUCTION

The work of Hamada (1960, 1961), Hamada and Johnston (1962), Signell and Marshak (1957, 1958) and Gammel and Thaler (1957) has confirmed that nuclear forces consist of Central, Non-Central Exchange, Linear Spin-Orbit, Tensor and the Quadratic Spin-Orbit Forces. The theoretical work relating to Nucleon-Nucleon (hereafter referred to as N-N) Forces to the properties of nuclei is very tedious even for light nuclei and prohibitive for medium and heavy nuclei.

Also in the method of the resonating groups (J.A. Wheeler, 1937) many types of direct and indirect terms or potentials and kernels respectively occur in the integro-differential equations describing a scattering or binding energy problem. This arises already with central forces. When other type of forces are included many additional terms appear and further spin, isospin and orbital operator matrix elements have to be evaluated.

S. Hochberg (1967) proposed two modifications in calculations based on the method of the resonating groups which reduce the algebraic and numerical work, while maintaining the accuracy. Moreover, the symmetry of the kernels is automatically ensured. The results for the neutron-deuteron (n-d) in terms of phase-shifts and cross-sections have been published recently by Hochberg, Omojola and Sribhibhadh (1968). Work on elastic neutron-triton (n-T) scattering problems is almost complete.

The alpha nucleus which is strongly bound will now be considered in detail and we report the numerical results of neutron-alpha (n-He^4) scattering problems in terms of

phase-shifts in this thesis.

PART I

INTEGRO-DIFFERENTIAL EQUATIONS FOR LIGHT NUCLEI

CHAPTER I

§ 1.1 NUCLEON-NUCLEUS SCATTERING

Let $\Phi(\widetilde{123, \ldots A})$ be the total antisymmetric wave function of A nucleons. In Φ the total isospin T and its z-component T_z will determine the nature of the target nucleus and projectile (nucleon), that is, its isobaric state. It is also characterized by the total angular momentum J, its z-component J_z and the total spin S.

Consider

$$\begin{aligned}\Phi(\widetilde{12 \ldots A}) = {} & F(1\text{-}23 \ldots A)\ \Phi(1,\widetilde{23 \ldots A}) \\ & - F(2\text{-}13 \ldots A)\ \Phi(2,\widetilde{13 \ldots A}) \\ & - F(3\text{-}21 \ldots A)\ \Phi(3,\widetilde{21 \ldots A}) - \text{etc.} \\ & \text{(all exchanges of 1 with 23...A)} \\ = {} & \widetilde{\Sigma} F(1\text{-}23 \ldots A)\ \Phi(1,\widetilde{23 \ldots A}) \qquad (1.1.1)\end{aligned}$$

$F(1\text{-}23 \ldots A)$ denotes the space function of nucleon 1 relative to the C.M.$_{\text{(centre of mass)}}$ of 23...A. $\Phi(1,\widetilde{23 \ldots A})$ is a function of space, spin and isospin variables of all nucleons 1,2...A except the space variables of nucleon 1.

We define the kinetic energy operator

$$\begin{aligned}T_{123 \ldots A} = {} & T_{1\text{-}23 \ldots A} + T_{2\text{-}34 \ldots A} + \cdots + T_{A-1,A} \\ = {} & T_{2\text{-}13 \ldots A} + T_{1\text{-}34 \ldots A} + \cdots + T_{A-1,A} \\ = {} & \text{etc. (all other similar combinations)} \\ = {} & \frac{-\hbar^2}{2M} \left(\frac{A}{A-1} \nabla^2_{1\text{-}23 \ldots A} + \frac{A-1}{A-2} \nabla^2_{2\text{-}34 \ldots A} + \cdots \right. \\ & \left. \cdots + \frac{2}{1} \nabla^2_{A-1,A} \right) \\ = {} & \frac{-\hbar^2}{2M} \left(\frac{A}{A-1} \nabla^2_{2\text{-}13 \ldots A} + \frac{A-1}{A-2} \nabla^2_{1\text{-}34 \ldots A} + \cdots \right. \\ & \left. \cdots + \frac{2}{1} \nabla^2_{A-1,A} \right) \\ = {} & \text{etc. (all other similar combinations)} \\ & \qquad (1.1.2)\end{aligned}$$

All the operators are hermitian which implies that any operator O can be expressed as

$$O = \vec{O} + \text{hermitian conjugate (h.c.)} \qquad (1.1.3)$$

Thus following Hochberg (1967), we put

$$T = \vec{T} + \overleftarrow{T}$$

$$= \frac{-\hbar^2}{2M} (\vec{\nabla}^2 + \overleftarrow{\nabla}^2) \qquad (1.1.4)$$

We assume that

$\Phi(1,\widetilde{23...A})$ satisfies a Schrödinger equation

$$(\vec{T}_{234...A} + \vec{V}_{234...A} - E_{A-1})\Phi(1,\widetilde{234...A}) = 0 \qquad (1.1.5)$$

and also its adjoint equation

$$\Phi^*(1,\widetilde{234...A})(\overleftarrow{T}_{234...A} + \overleftarrow{V}_{234...A} - E_{A-1}) = 0 \qquad (1.1.6)$$

where

$$V_{234...A} = V_{23} + V_{24} + \ldots \quad \ldots + V_{A-1,A} \qquad (1.1.7)$$

V_{ij} is the interaction operator between particles (i,j). The presence of the spin and isospin variables of nucleon 1 in $\Phi(1,\widetilde{23...A})$ reminds us that Φ is not the ground state wave function of the target nucleus consisting of A-1 nucleons (23...A) but some modification of it (a polarized state). If we choose $\Phi(1,\widetilde{23...A})$ to have the correct total spin and isospin of the target nucleus (23...A) in its ground state we can take as an approximation E_{A-1} to be the binding energy of this nucleus. The value of E_{A-1} is obtained by several authors including Sugie et al., 1957; Nagata et al., 1957; Hochberg et al., 1954; Massey et al., 1941 and H. Kanada et al., 1963 by a variational solution of equation (1.1.5). Since we assume an exact ground state solution of equation (1.1.5) we can use the experimental value E_{A-1}. The validity of this approximation will be discussed at the end of § 1.2.

We now assume that $\Phi(1,\widetilde{23\ldots A})$ satisfies the Schrödinger equation :

$$(T_{123\ldots A} + V_{123\ldots A} - E)\Phi(1,\widetilde{23\ldots A}) = 0 \qquad (1.1.8)$$

where E is the total energy in the C.M. system.

Multiplying on the left equation (1.1.8) by $\Phi^*(1,\widetilde{23\ldots A})$ and integrating and or summing over all variables of particles 23...A, we get

$$\int d\tau_{23\ldots A}\ \Phi^*(1,\widetilde{23\ldots A})(T_{123\ldots A} + V_{123\ldots A} - E)\ x$$
$$\tilde{\Sigma}F(1\text{-}23\ldots A)\Phi(1,\widetilde{23\ldots A}) = 0 \qquad (1.1.9)$$

Using equation (1.1.6) we can write equation (1.1.9) as

$$\int d\tau_{234\ldots A}\ \Phi^*(1,\widetilde{234\ldots A})(T_{1\text{-}23\ldots A} + V_{12} + V_{13} + \ldots$$
$$V_{1A} - E_n)\ x\ F(1\text{-}23\ldots A)\Phi(1,\widetilde{23\ldots A}) -$$
$$\int d\tau_{23\ldots A}\ \Phi^*(1,\widetilde{23\ldots A})(T_{123\ldots A} + V_{123\ldots A})$$
$$x \sum_{i\neq 1}\!\!\!\!\!\!\sim\ F(i\text{-}123..i\text{-}1,i\text{+}1,.A)\Phi(i,\widetilde{123\ldots i-1,i+1,\ldots A})$$
$$= 0 \qquad (1.1.10)$$

where we use

$$E = E_n + E_{A-1} \ldots \qquad (1.1.11)$$

and E_n is the incident nucleon kinetic energy in the C.M. system. Making use of symmetry properties of the integrals and variables of integration we can further modify the last equation to obtain

$$(T_{1\text{-}23\ldots A} - E_n)F(1\text{-}23\ldots A) + [(A\text{-}1)\int d\tau_{234\ldots A}\ x$$
$$\Phi^*(1,\widetilde{23\ldots A})V_{12}\ \Phi(1,\widetilde{23\ldots A})]\ F(1\text{-}23\ldots A) - (A\text{-}1)\ x$$
$$\int d\tau_{23\ldots A}\ \Phi^*(1.\widetilde{23\ldots A})(T_{1\text{-}23\ldots A} + V_{12} + V_{13} + \ldots$$
$$\ldots + V_{1A} - E_n)\Phi(2,\widetilde{13\ldots A})\ F(2\text{-}13\ldots A) = 0 \qquad (1.1.12)$$

This is the equation for the incident neutrons. A similar modification is required for the incident protons. The last integral can further be written

$$-(A-1)\int d\tau_{23\ldots A}\,\Phi^*(1,\widetilde{23\ldots A})(T_{1-23\ldots A}+V_{12}+(A-2)V_{13}-E_n)\Phi(2,\widetilde{13\ldots A})F(2-13\ldots A)$$

Using equations (1.1.5) and (1.1.6) we can write

$$\int d\tau_{23\ldots A}\,\Phi^*(1,\widetilde{23\ldots A})(T_{123\ldots A}+V_{123\ldots A}-E)\Phi(2,\widetilde{134\ldots A})x$$

$$F(2-134\ldots A)$$

$$=\int d\tau_{23\ldots A}\,\Phi^*(1,\widetilde{23\ldots A})(T_{2-13\ldots A}+V_{21}+V_{23}+\ldots$$

$$+V_{2A}-E_n)\Phi(2,\widetilde{134\ldots A})F(2-134\ldots A)$$

$$=\int d\tau_{23\ldots A}\,\Phi^*(1,\widetilde{23\ldots A})(\tfrac{1}{2}T_{1-23\ldots A}+\tfrac{1}{2}T_{2-13\ldots A}+V_{12}$$

$$+\tfrac{1}{2}(A-2)(V_{13}+V_{23})-E_n)\Phi(2,\widetilde{13\ldots A})F(2-13\ldots A) \qquad (1.1.13)$$

Thus we can simplify equation (1.1.12) using equation (1.1.13) to obtain

$$(T_{1-23\ldots A}-E_n)F(1-23\ldots A)+(A-1)[\int d\tau_{23\ldots A}\,\Phi^*(1,\widetilde{23\ldots A})\,x$$

$$V_{12}\Phi(1,\widetilde{23\ldots A})]F(1-23\ldots A)-(A-1)\int d\tau_{23\ldots A}\Phi^*(1,\widetilde{23\ldots A})\,x$$

$$[\tfrac{1}{2}T_{1-22\ldots A}+\tfrac{1}{2}T_{2-13\ldots A}+V_{12}+(A-2)(\tfrac{1}{2}V_{13}+\tfrac{1}{2}V_{23})-E_n]$$

$$x\ \Phi(2,\widetilde{13\ldots A})F(2-13\ldots A)=0 \qquad (1.1.14)$$

This is the final integro-differential equation in the dependent variable F and the independent vector-variable (1-23...A).

We now integrate and/or sum over all variables of nucleons except the radial component of the vector (1-23...A). This leads to a set of scalar equations in this radial component for given values of J, S and T. Therefore one type of potential and two types of kernel depend on the N-N interaction: all other terms in the equation merely depend on the number and types of nucleons (whether protons or neu-

trons) involved.

A further simplification (Hochberg) is possible and this will now be discussed.

§ 1.2 ALTERNATIVE FORM OF EQUATION

We now make use of the following identity:

$$0 = \int d\tau_{23\ldots A}\, \Phi^*(1,\widetilde{23\ldots A})(T_{134\ldots A} + V_{13} + V_{14} + \ldots + V_{A-1,A} - E_{A-1})\Phi(2,\widetilde{134\ldots A})$$

$$= \int d\tau_{23\ldots A}\, \Phi^*(1.\widetilde{23\ldots A})(T_{134\ldots A} + (A-2)V_{13} + {}^{k}C_2 V_{34} + {}^{z}C_2 V_{56} - E_{A-1})\Phi(2,\widetilde{13\ldots A}) \qquad (1.2.1)$$

where

$${}^{k}C_2 = {}^{A-2}C_2 - {}^{z}C_2 \qquad (1.2.2)$$

and z is the number of protons and 5,6 are a proton pair. This enables us to write equation (1.1.14) as

$$(T_{1-23\ldots A} - E_n)F(1-23\ldots A) + (A-1)\left[\int d\tau_{23\ldots A}\, \Phi^*(1,\widetilde{23\ldots A}) V_{12}\, \Phi(1,\widetilde{23\ldots A})\right]F(1-23\ldots A) - (A-q)\int d\tau_{23\ldots A}\, \Phi^*(1,\widetilde{23\ldots A})$$

$$\times \left[\tfrac{1}{2}T_{1-23\ldots A} + \tfrac{1}{2}T_{2-13\ldots A} + V_{12} - E_n - \tfrac{1}{2}T_{134\ldots A} - \tfrac{1}{2}T_{234\ldots A} + E_{A-1} - {}^{k}C_2 V_{34} - {}^{z}C_2 V_{56}\right]\Phi(2,\widetilde{134\ldots A})F(2-134\ldots A) \qquad (1.2.3)$$

where

$$q = z + 1 \qquad (1.2.4)$$

Equation (1.2.3) has the advantage that the kernel:

(i) is symmetric as before in equation (1.1.14);

(ii) involves one term V_{12} which can be thought of as the interaction between the particles (1,2) directly concerned in the scattering process;

(iii) involves two other terms V_{34} and V_{56} which describe the interaction between the particles of the target nucleus.

The feature (iii) is particularly useful if one assumes all particle pairs to be in "S" states relative to each other. Consequently both Tensor, Spin-Orbit and the Quadratic Spin-Orbit Forces will then give no contribution to the terms V_{34} and V_{56}.

We note that in equation (1.1.14) E_{A-1} does not appear explicitly and so the solution depends on choosing a reliable wave function Φ_{A-1} for nucleus (A-1). This will be some modification of the bound state functions Φ^{b}_{A-1} of nucleus (A-1) due to the proximity of the projectile nucleon.

Let the polarized bound state function be denoted by $\Phi^{b,p}_{A-1}$. Therefore $\Phi_{A-1} = \Phi^{b,p}_{A-1}$. In many calculations such as J. Irving (1951, 1952), A.C. Clark (1954), G. Abraham et al. (1955) and H. Kanada et al. (1963) a variational form of Φ^{b}_{A-1} was used and let it be denoted by $\Phi^{b,v}_{A-1}$. Neither $\Phi^{b,v}_{A-1}$ nor Φ^{b}_{A} are equal to Φ_{A-1}. It follows that both Φ^{b}_{A-1} and $\Phi^{b,v}_{A-1}$ can be used as approximations in the calculation and one cannot say a priori which is more accurate. Consequently the use of Φ^{b}_{A-1} instead of $\Phi^{b,v}_{A-1}$ need not necessarily reduce the accuracy. A better scheme would probably be, taking a variational form for Φ_{A-1} and using the stationary property of the phase shifts to determine a few parameters.

To sum up, the simplifications are essentially based on the use of equation (1.1.5) and its adjoint (1.1.6) leading to two alternative forms of the linear integro-differential equations, namely equations (1.1.14) and (1.2.3). Equation (1.1.5) was previously used in scattering problems such as Sugie et al. (1957), Massey et al. (1942),

E. Van Der Spuy (1956) and this reduced the algebra but led to symmetry difficulties which were eliminated by a second application of equation (1.1.5). The combined use of the equations (1.1.5) and (1.1.6) further reduces the algebraic and numerical work and avoids the symmetry difficulties.

We shall now give the results obtained for a few special cases. Three special cases will be considered. We shall consider only two of them in this section and the third will be dealt with fully in Chapter III.

Consider the following two special cases:

§ 1.3 NEUTRON-DEUTERON SCATTERING (n-d) PROBLEMS

Let $\Psi(\widetilde{12},3)$ be the resonating group wave function where particles 1,2 are neutrons and 3 is a proton. The formulation without isospin as mentioned earlier in this chapter is shortened for practical calculations.

The basic Schrödinger's equation is

$$(T_{123} - E + V_{12} + V_{13} + V_{23})(\Phi(\overline{23})F(1\text{-}23) - \Phi(\overline{13})F(2\text{-}13)) = 0 \qquad (1.3.1)$$

where we have written

$$\Psi(\widetilde{12},3) = \Phi(\overline{23})F(1\text{-}23) - \Phi(\overline{13})F(2\text{-}13) \qquad (1.3.2)$$

and $\Phi(\overline{23})$ etc. are symmetric in interchange of 2 and 3. T is the kinetic energy operator. E is the total energy of the system and V_{ij}'s are the interactions between particles i and j. We now use the deuteron equation:

$$(T_{23} + V_{23} - E_D)\Phi(\overline{23}) = 0 \qquad (1.3.3)$$

and its complex conjugate

$$\Phi^*(\overline{23})(T_{23} + V_{23} - E_D) = 0 \qquad (1.3.4)$$

where

$$E = E_n + E_D \tag{1.3.5}$$

and E_D, E_n being the deuteron binding energy and the incident neutron energy respectively (C.M. units).

Following the simplifications outlined in § 1.2, the equivalent of equation (1.2.3) is

$$\left[-\frac{\hbar^2}{2M}\,(3/2\,\nabla_r^2) - E_n\right] F(r) + \sum_{\text{spin}} \int d^3\,\underline{u}\;\Phi^*(\overline{23})\;(|\underline{u}|)\;\times$$

$$2V_{12}\;(|\underline{u}|)\;\Phi(\overline{23})(|\underline{u}|)F(r)$$

$$= \left(\frac{4}{3}\right)^3 \sum_{\text{spin}}' \int d^3\underline{r}'\;\Phi^*(\overline{23})(|\underline{u}|)V_{12}(|\underline{u}-\underline{v}|)\Phi(\overline{13})(|\underline{v}|)F(r')$$

$$+ \left(\frac{4}{3}\right)^3 \sum_{\text{spin}}' \int d^3\underline{r}'\,\Phi^*(\overline{23})(|\underline{u}|)\left\{E_D - E_n - \frac{\hbar^2}{2M}\left[\frac{2}{3}\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}\right) + \right.\right.$$

$$\left.\left.{}^8/_3\,\frac{\partial}{\partial \underline{u}} \cdot \frac{\partial}{\partial \underline{v}}\right]\right\}\Phi(\overline{13})(|\underline{v}|)F(r') \tag{1.3.6}$$

where

$$\left.\begin{aligned} \underline{u} &= \tfrac{4}{3}\,\underline{r}' + \tfrac{2}{3}\,\underline{r} \\ \underline{v} &= \tfrac{2}{3}\,\underline{r}' + \tfrac{4}{3}\,\underline{r} \end{aligned}\right\} \tag{1.3.7}$$

and $\underline{r}$, $\underline{r}'$ are the C.M. coordinates of particles 1,2 respectively. The scalar linear integro-differential equations are obtained by multiplying equation (1.3.6) on the left by $Y^{JS}(1)$ which is the eigen function of 1 having given eigen values J and S (total angular momentum and total spin respectively) and summing and integrating over all variables except the radial component of $\underline{r}$.

§ 1.4 NEUTRON-TRITON SCATTERING (n-T) PROBLEMS

Let 1,2,3 be the neutrons and 4 the proton. Then by the same procedure similar to § 1.3, the final equation for the n-T scattering can be written as

$$\{\int \Phi^*(-1)(T_{1-234} - E_n + 3V_{12})\Phi(-1)d\tau_{234}\}F(1)$$
$$- 2\int d\tau_{234}\Phi^*(-1)(T_{1-234} - T_{1-34} - T_{34} + E_T - E_n + V_{12}$$
$$- V_{34})\Phi(-2)F(2) = 0 \qquad (1.4.1)$$

where

$\Phi^*(-1)$ is $\Phi(\widetilde{234})$ etc. and E_T is the triton binding energy. Note that we have applied equation (1.2.3) to the two special cases considered above.

CHAPTER II

§ 2.1 FORMS OF THE NUCLEAR POTENTIAL

The N-N (nucleon-nucleon) interaction is known to include both central and non-central forces. According to Rosenfeld (1948, pp. 312-4) and, Okubo and Marshak (1958), the most general form of this interaction with the invariance and symmetry requirements must be a linear combination of the following terms:

(i) The Central Exchange Force

(ii) The Linear Spin-Orbit Force

$$S(r_{ij}) = V(\underline{r}_{ij})[(\underline{s}_i+\underline{s}_j).(\underline{r}_i-\underline{r}_j)\wedge(\underline{p}_i-\underline{p}_j)] \quad (2.1.1)$$

(iii) The Tensor Force

$$T(\underline{r}_{ij}) = V(\underline{r}_{ij})[3(\underline{\sigma}_i.\underline{r}_{ij})(\underline{\sigma}_j.\underline{r}_{ij})/r_{ij}^2 - (\underline{\sigma}_i.\underline{\sigma}_j)] \quad (2.1.2)$$

and

(iv) The Quadratic Spin-Orbit Force

$$Q(\underline{r}_{ij}) = V(\underline{r}_{ij})[(\underline{\sigma}_i.\underline{\sigma}_j)\underline{L}_{ij}^2 - Q_{ij}] \quad (2.1.3)$$

where

$$\underline{L}_{ij} = (\underline{r}_i-\underline{r}_j)\wedge(\underline{p}_i-\underline{p}_j) \quad (2.1.4)$$

$$Q_{ij} = \tfrac{1}{2}[(\underline{\sigma}_i.\underline{L}_{ij})(\underline{\sigma}_j.\underline{L}_{ij})+(\underline{\sigma}_j.\underline{L}_{ij})(\underline{\sigma}_i.\underline{L}_{ij})] \quad (2.1.5)$$

$V(\underline{r}_{ij})$ is a radial function, $\underline{S}_i$ is the Pauli Spin matrix vector for the i-th particle and $\underline{r}_i$ and $\underline{p}_i$ are its position and momentum vectors respectively.

The evidence for the existence of the non-central forces in the form of the linear spin-orbit and the tensor terms has been ~~explained~~ discussed by many authors (Signell and Marshak, 1957,

1958; Gammel and Thaler 1957). The necessity for the inclusion of the quadratic spin-orbit term is confirmed by the recent work of Hamada (1960, 1961) and Hamada and Johnston (1962) in order to produce all the available data of p-p and n-p below 300 MeV.

In order to take care of the exchange nature of these forces between nucleons in various states, combinations of projection operators are constructed in such a way that each operator will pick out the pair of nucleons in a certain state only (Sribhibhadh, 1966).

The projection operators are:

$$\frac{1}{4}\left({}^{\nu}w_{\pm} + {}^{\nu}b_{\pm}B_{ij} + {}^{\nu}m_{\pm}M_{ij} + {}^{\nu}h_{\pm}H_{ij}\right) , \qquad (2.1.6)$$

ν being 1 and 3 to represent the singlet and tripletstates respectively. $\pm$ representing the even and the odd parity states. B_{ij}, M_{ij} and H_{ij} are the usual Bartlett, Majorana and Heisenberg exchange operators for the nuclei i and j.

B_{ij} interchanges the spin of particles i and j

M_{ij} interchanges the spatial coordinates of particles i and j

H_{ij} interchanges both the spin and the spatial coordinates of particles i and j. The notation we shall use throughout this thesis is such that

$$M_{ij}B_{ij}H_{ij} = 1 \qquad (2.1.7)$$

The values of w, b, m and h are as follows:

$${}^{\nu}w_{\pm} = 1 \quad \text{for all, } \nu_{\pm}, \qquad (2.1.8)$$

$$\left.\begin{array}{l} {}^{1}b_{+} = -1, \quad {}^{1}b_{-} = -1, \quad {}^{3}b_{+} = 1, \quad {}^{3}b_{-} = 1, \\ {}^{1}m_{+} = 1, \quad {}^{1}m_{-} = -1, \quad {}^{3}m_{+} = 1, \quad {}^{3}m_{-} = -1, \\ {}^{1}h_{+} = -1, \quad {}^{1}h_{-} = 1, \quad {}^{3}h_{+} = 1, \quad {}^{3}h_{-} = -1. \end{array}\right\} \qquad (2.1.9)$$

The potential ~~wells~~ shape functions $V(\underline{r}_{ij})$ in this work are taken to be Gaussian forms whose parameters are determined by least squares fits to the Hamada and Johnston Potential (Hamada and Johnston, 1962). Two Gaussian terms are used for each potential well so that one may represent the short range contribution and the other the long range one.

The interaction can now be written in full as:

$$V_{ij} = \sum_{\lambda=1}^{4} \sum_{\nu=1}^{4} \frac{1}{4} (w + b_\nu B_{ij} + m_\nu M_{ij} + h_\nu H_{ij}) \, {}^{\nu}V_{\lambda}(\underline{r}_{ij}, \underline{\sigma}_i, \underline{\sigma}_j) \tag{2.1.10}$$

where

$$ {}^{\nu}V_{\lambda}(\underline{r}_{ij}, \underline{\sigma}_i, \underline{\sigma}_j) = \sum_{k=1}^{2} {}^{\lambda}U_k^{\nu} \exp\left[-{}^{\lambda}\mu_k^{\nu} r_{ij}^2\right] \times$$

$$\left[\delta_{\lambda,1} + \delta_{\lambda,2}\left\{\tfrac{1}{2}(\underline{\sigma}_i+\underline{\sigma}_j)\cdot\underline{L}_{ij}\right\} + \delta_{\lambda,3}\left\{3(\underline{\sigma}_i\cdot\underline{r}_{ij}) \times (\underline{\sigma}_j\cdot\underline{r}_{ij})/r_{ij}^2 - (\underline{\sigma}_i\cdot\underline{\sigma}_j)\right\} + \delta_{\lambda,4}\left\{(\underline{\sigma}_i\cdot\underline{\sigma}_j)\underline{L}_{ij}^2 - Q_{ij}\right\}\right] \tag{2.1.11}$$

$\delta_{\lambda,\lambda'}$ is the Kronecker delta, λ represents the k-th Gaussian term, λ takes the values 1,2,3 and 4 for the central forces, the linear-spin-orbit forces, the tensor forces and the quadratic spin-orbit forces respectively. ν = 1,2,3 and 4 to represent the triplet even state, the triplet odd state, the singlet even state and the singlet odd state respectively. The interaction given above is taken to be in the units in which

$$c = \hbar = 1. \tag{2.1.12}$$

§ 2.2 THE ALPHA PARTICLE WAVE FUNCTION

The wave function representing the He^4 system has to be constructed so that it is anti-symmetrical for interchange of the two neutrons and for the two protons respectively. The ground state of He^4 is of even parity and has a total angular moment J=0, so that the classification of possible states can be made using the rules for compounding angular momentum. Thus, the possible values of L are 0, 1 and 2. The possible states in operator form have been listed by Gerjuoy and Schwinger (1942), Irving (1953) and Abraham, Cohen and Roberts (1955). The ground state is therefore a mixture of ^1S_o-, ^3P_o- and ^5D_o- states. Of these, Irving (1953) retains only the principal S state and the principal D state. Only the D state is directly coupled to the S state by the tensor force. Of the six D states listed by Gerjuoy and Schwinger only one is completely symmetric in the space coordinates. This only is considered in this thesis, and in Irving's work this is taken as the principal D state. The principal P state will not be considered here for its contribution is quite negligible for a nuclear force of the type we are going to consider. Similarly we do not take into account the ^3P_o-state because we have

$$\begin{aligned}\langle {}^1S_o|V_T|{}^3P_o\rangle &= \langle {}^1S_o|V_{LS}|{}^3P_o\rangle = \langle {}^3P_o|V_T|{}^5D_o\rangle \\ &= \langle {}^3P_o|V_{LS}|{}^5D_o\rangle = \langle {}^1S_o|V_{LS}|{}^5D_o\rangle \\ &= 0 \qquad (2.2.1)\end{aligned}$$

while only

$$\langle {}^1S_o|V_T|{}^5D_o\rangle \quad \neq 0 \text{ is non-zero} \qquad (2.2.2)$$

Also, since the ^3P_o-state will appear only as a second approximation, it therefore follows that as the first approximation we can neglect the ^3P_o-state probability. The foregoing explains why we do not take into account the contribution of the ^3P_o-state in our scattering problems.

The alpha particle wave function $\psi(-1)$ can be written in the notation of Sugie, Hodgson and Robertson (1957) as

$$\psi(-1) = \sum_S \psi_{L,S,0}(-1) = \sum_{S,P} \psi^P_{L,S,0}(-1)$$
$$= \sum_{S,P} g^P_S(\underline{u},\underline{v},\underline{w}) w^P_S(\underline{u},\underline{v},\underline{w};\ \underline{\sigma}_2,\underline{\sigma}_4)\chi(\widetilde{23},\widetilde{45}) \qquad (2.2.3)$$

in which S=0 and S=2 are important. The superscript P distinguishes the many possible spin-angular wave functions; $\underline{u}$, $\underline{v}$ and $\underline{w}$ are the three independent internal space coordinates; and χ is the spin wave function of the singlet state. We define χ as

$$\chi(\widetilde{23},\widetilde{45}) = \tfrac{1}{2}(\alpha_2\beta_3-\beta_2\alpha_3)(\alpha_4\beta_5-\beta_4\alpha_5) = \chi(-1) \qquad (2.2.4)$$

In the S state there are two spin-angular wave functions, one corresponding to the state in which the spins of two similar particles couple to zero, and the other to the state in which they couple to one. In the ground state the former predominates and the latter will be neglected. The wave function of the alpha particle can therefore be written in the form

$$\psi(-1) = (\psi_S+C\psi_D)/(1+C^2)^{\frac{1}{2}} \qquad (2.2.5)$$

where

$$\psi_S = g_S(\underline{u},\underline{v},\underline{w})\chi \qquad (2.2.6)$$

and $$\psi_D = g_D(\underline{u},\underline{v},\underline{w})w_D\chi \qquad (2.2.7)$$

g_S and g_D represent the normalized spatial parts of the wave functions for the principal ^1S_o- and ^5D_o-state respectively.

w_D is defined by

$$w_D = \sum_{i>j=2}^{5} r_{ij}^2 S_{ij}$$

$$= 3(\underline{\sigma}_2\cdot\underline{r}_{23})(\underline{\sigma}_4\cdot\underline{r}_{45}) + 3(\underline{\sigma}_2\cdot\underline{r}_{45})(\underline{\sigma}_4\cdot\underline{r}_{23})$$

$$-2(\underline{\sigma}_2\cdot\underline{\sigma}_4)(\underline{r}_{23}\cdot\underline{r}_{45}) \qquad (2.2.8)$$

C^2 determines the amount of the D-state in the mixture. We assume that both ψ_S and ψ_D are normalized to unity, so that $\psi(-1)$ is then normalized to unity.

The radial parts ψ_S and ψ_D are of the form

$$g_S = N_S \exp\left(-\tfrac{1}{2}\alpha \sum_{i>j=2}^{5} r_{ij}^2\right) \qquad (2.2.9)$$

and

$$g_D = N_D \exp\left(-\tfrac{1}{2}\beta \sum_{i>j=2}^{5} r_{ij}^2\right) \qquad (2.2.10)$$

where N_S and N_D are the normalization constants. The radial parts are assigned different variation parameters, α and β respectively.

§2.3 THE FIVE-BODY WAVE FUNCTION

In quantum mechanics the superposition of stationary states is used in molecular theory and J.A. Wheeler (1937) applying this to nuclear binding energy or scattering problems developed the method of the resonating group structures. This is the method we are going to apply to our five-body problem of neutron-alpha scattering ($n\text{-}He^4$). This method

specifies a wave function consisting of the product of the incompatible states and the sum of the compatible ones on a statistical basis.

J.A. Wheeler postulates that a given system of n nucleons, subdivides into groups of stable nuclei and nucleons at any instant of time. Thus

$$\begin{aligned}\Psi(123\ldots n) = {} & w_1 \Phi_1(n_1^1)\Phi_2(n_2^1) \ldots \Phi_\alpha(n_\alpha^1) \\ & + w_2 \Phi_1(n_1^2)\Phi_2(n_2^2) \ldots \Phi_\beta(n_\beta^2) \\ & + \ldots . \\ & + w_\varkappa \Phi_1(n_1^\varkappa)\Phi_2(n_2^\varkappa) \ldots \Phi_\gamma(n_\gamma^\varkappa)\end{aligned}$$

where for example $\Phi_1(n_1^1)$ represents the wave function of a stable nucleus with n_1 nucleons and $\Phi_2(n_2^1)$ the wave function of a stable nucleus with n_2 nucleons etc. such that

$n_1^1 + n_2^1 + \ldots + n_\alpha^1 = n$ etc. and w_1, w_2, etc. are the "weights" proportional to the probability of each configuration (related to binding energy).

In quantum mechanics any system which ~~consists of~~ are active in non-central forces only the total angular momentum J and its z-component J_z with their respective eigen values J and M respectively will be constants of motion, but the orbital angular momentum $\underline{L}$ and the total spin $\underline{S}$ are not conserved (Dirac).

Consider a five-body problem. We can split the five particle problem into deuterons, tritons and the alpha particles with their respective weights. However, since the alpha particle is strongly bound compared to deuterons and tritons we shall consider its contribution only. The spatial coordinates in the five-body problem of n-He^4 scattering are depicited below.

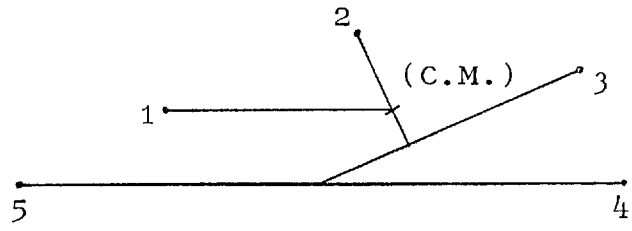


Fig. I

Particles 1, 2 and 3 are neutrons and 4 and 5 are protons.

§2.4 NEUTRON-ALPHA PARTICLE SCATTERING

Consider the problem of n-He^4 scattering depicited below symbolically:

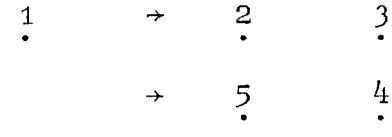


Fig. II

where we have used the number 1 to represent the coordinates of the incident neutrons, 2 and 3 the neutrons in the helium nucleus and 4 and 5 the nuclear protons, 2, 3, 4 and 5 represents the alpha particle.

Since protons and neutrons are fermions, the wave function representing the motion of the system must be antisymmetric in 1, 2 and 3 and also in 4 and 5. We may now write down the complete wave function in the resonating group method which describes the system using Hochberg's notation (1953) in the form:

$$\Psi = \psi(-1)\varphi(1) + \psi(-2)\varphi(2) + \psi(-3)\varphi(3) \qquad (2.4.1)$$

where $\psi(-i)$ is the antisymmetrized wave function of the target nucleus which does not contain the i^{th} particle and φ is the wave function of the incident neutron. The wave

function of the incident neutron can be decomposed into partial waves by writing it in the form:

$$\varphi = \sum_{\ell, J=\ell\pm\frac{1}{2}} \{f_{\ell J(r)}/r\}\chi^{m}_{\ell J}(\theta,\varphi,s) \qquad (2.4.2)$$

where (r,θ,φ) are the spherical polar coordinates of the neutron relative to the centre-of-mass (C.M.) of the alpha particle and $\chi^{m}_{\ell J}$ is the spin-angular wave function of the neutrons. Since the spin of the alpha particle is zero, the magnetic quantum number, m, is also the magnetic quantum number of the whole system.

Using the notation of Buckingham and Massey (1941), the alpha particle wave function can be expanded in eigen functions of J and M as follows:

$$\Psi_M = \sum_{J=\frac{1}{2}}^{\infty} \sum_{\ell=J-\frac{1}{2}}^{J+\frac{1}{2}} \frac{1}{r_1} f_{\ell JM(r_1)} [C_{JM\ell,M+\frac{1}{2}} Y_{\ell,M+\frac{1}{2}}(\theta_1,\varphi_1)\beta_1 + C_{JM\ell,M-\frac{1}{2}} Y_{\ell,M-\frac{1}{2}}(\theta_1,\varphi_1)\alpha_1] \qquad (2.4.3)$$

$M\hbar$ being the z-component of the total angular momentum, $C_{J\ell M}$ the appropriate Clebsch-Gordon coefficients and $Y_{\ell,M}$ the spherical harmonics. Using the notation of Hochberg et al. (1968), each of the eigen functions may be expressed in terms of substates characterized by the quantum numbers ℓ and S of the orbital angular momentum and the total spin. Thus, we write the complete wave function as:

$$\Psi_M = \sum_S \psi(-1)\, F^S_{JM}\, F(1\text{-}2345) \qquad (2.4.4)$$

where

$$F^S_{JM}(1\text{-}2345) = \sum_{\ell=|J-S|}^{J+S} Y_{JM\ell}(1,\overline{2345};\ \Omega)\, \frac{1}{r}\, f^S_{JM\ell}(r) \qquad (2.4.5)$$

$$Y^{S}_{JM\ell}(1,\overline{2345};\ \Omega) = \sum_{m=M-S}^{M+S} C^{S}_{J\ell Mm}\ Y_{\ell M(\Omega)}\chi^{S}_{M-m}(1,\overline{2345}) \qquad (2.4.6)$$

Ω being the solid angle of $\underline{r}$.

For each J and M, in the doublet spin state ($S=\frac{1}{2}$) for example, we put

$$\chi^{\frac{1}{2}}_{(1)} = [\chi^{\frac{1}{2}}_{\frac{1}{2}}(1,\overline{234}5);\ \chi^{\frac{1}{2}}_{-\frac{1}{2}}(1,\overline{234}5)], \qquad (2.4.7)$$

$$Y^{\frac{1}{2}}_{JM\ell(\Omega)} = \begin{bmatrix} C^{\frac{1}{2}}_{JM(J-\frac{1}{2})(M-\frac{1}{2})}\ Y^{J-\frac{1}{2}}_{M+\frac{1}{2}}(\theta,\varphi) & , \\ C^{\frac{1}{2}}_{JM(J+\frac{1}{2})(M-\frac{1}{2})}\ Y^{J+\frac{1}{2}}_{M-\frac{1}{2}}(\theta,\varphi) & \\ C^{\frac{1}{2}}_{JM(J-\frac{1}{2})(M+\frac{1}{2})}\ Y^{J-\frac{1}{2}}_{M+\frac{1}{2}}(\theta,\varphi) & , \\ C_{JM(J+\frac{1}{2})(M+\frac{1}{2})}\ Y^{J+\frac{1}{2}}_{M+\frac{1}{2}}(\theta,\varphi) & \end{bmatrix} \qquad (2.4.8)$$

This is a 2 x 2 matrix.

$$F_{JM}(r) = \begin{bmatrix} f^{\frac{1}{2}}_{JM\ J-\frac{1}{2}}(r) \\ f^{\frac{1}{2}}_{JM\ J+\frac{1}{2}}(r) \end{bmatrix} \qquad (2.4.9)$$

Thus, equation (2.4.5) can now be rewritten in the form:

$$F^{S}_{JM}(1\text{-}2345) = \frac{1}{r}\,\chi YF \qquad (2.4.10)$$

Here Y always refers to $Y^{S}_{JM\ell(\Omega)}$ which involves no spin functions whereas $Y^{S}_{JM\ell}(1,\overline{234}5;\ \Omega)$ does, as shown by its argument and will always be written in full.

§2.5 THE HARD CORES OF THE POTENTIALS

The nuclear potentials of Hamada and Johnston which are used in this thesis contain hard cores in all states of the interacting nucleons. The radii of the cores are assumed to be the same and small ($r_c \sim 0.485 \times 10^{-13}$ cm).

Brueckner (1958), discussing the hard core, shows that physically acceptable solutions of two body problems, can be

obtained if the expression $rV(r)\varphi(r)$ behaves like a Dirac delta function for $0 < r < r_c$, where $\varphi(r)$ is the two-body wave function and the hard core potential V is infinite for $0 < r < r_c$. It follows that $\varphi(r)$ vanishes for $0 < r < r_c$. This represents a ~~great~~ difficulty in the analysis of the five-body scattering problems.

Following the method of Brueckner applied to a two-body scattering problem, the Schrödinger equation involves integrals of the form:

$$\int \Psi^*(-1)V(r_{12})\Psi(-1)d\tau_{-1} \ .$$

This integral has to be divided into two regions corresponding to $|r_{12}| < r_c$ and $|r_{12}| > r_c$ if we consider the hard cores of the potential.

However, taking $V(r) \sim (r^2-r_c^2)w(r)$ in two nucleon attractive states and $V(r) \sim -(r^2+r_c^2)w(r)$ in two nucleon repulsive states the calculation greatly simplifies and this was here adopted.

CHAPTER III

§3.1 FORMULATION OF NEUTRON-ALPHA (n-He^4) SCATTERING PROBLEMS

The formulation we are going to use is based on the two modifications (Hochberg) of deriving the integro-differential equations for light nuclei using the method of the resonating groups as given in Chapter I. We start with the basic Schrodinger equation for the wave function Ψ given by

$$(T_{12345} + \sum_{i>j=1}^{5} V_{ij})\Psi(\widetilde{123},\widetilde{45}) = E\Psi(\widetilde{123},\widetilde{45}) \qquad (3.1.1)$$

where E is the total energy of the system in the C.M. system. E is given by

$$E = E_n + E_\alpha \qquad \text{where}$$

E_n is the energy of the incident neutron, and
E_α is the energy of the alpha ground state, that is, the binding energy of the alpha particle.

T_{12345} is the kinetic energy operator and V_{12345} the potential energy.

We may now write the kinetic energy operator T_{12345} as:

$$\begin{aligned} T_{12345} &= T_{1-2345} + T_{2-345} + T_{3-45} + T_{45} \\ &= T_{2-1345} + T_{1-345} + T_{3-45} + T_{45} \\ &= \text{etc. (all other similar combinations)} \\ &= \frac{-\hbar^2}{2M}\left(\frac{5}{4}\nabla^2_{1-2345} + {}^4/_3\,\nabla^2_{2-345} + {}^3/_2\,\nabla^2_{3-45} + {}^2/_1\nabla^2_{45}\right) \\ &= \frac{-\hbar^2}{2M}\left(\frac{5}{4}\nabla^2_{2-1345} + {}^3/_3\,\nabla^2_{1-345} + {}^3/_2\,\nabla^2_{3-45} + {}^2/_1\nabla^2_{45}\right) \\ &= \text{etc. (all other similar combinations)} \qquad (3.1.2) \end{aligned}$$

The complete wave function describing the scattering problems can be written in the resonating group method using Hochberg's notation (1953) in the form

$$\Psi(\widetilde{123},\widetilde{45}) \equiv F(1\text{-}2345)\Phi(\widetilde{2345}) + F(2\text{-}1345)\Phi(\widetilde{1345}) + F(3\text{-}2145)\Phi(\widetilde{2145})$$
$$\equiv \Psi(-1)\varphi(1) + \Psi(-2)\varphi(2) + \Psi(-3)\varphi(3) \qquad (3.1.3)$$

where

$\psi(-i)$ is the antisymmetrized wave function of the target nucleus which does not contain the i^{th} particle and φ is the wave function of the incident neutrons. Using equation (2.4.2) in Chapter II, we write φ as:

$$\varphi = \sum_{\ell,\, J=\ell\pm\frac{1}{2}} \{f_{\ell J(r)}/r\}\chi^{m}_{\ell J}\ (\theta,\varphi,S) \qquad (3.1.4)$$

(r,θ,φ) and $\chi^{m}_{\ell J}$ have already been defined.

We shall now assume that $\Phi(1,\widetilde{2345})$ satisfies a Schrödinger wave equation for the alpha-particle, that is,

$$(T_{2345} + V_{2345} - E_{\alpha})\Phi(1,\widetilde{2345}) = 0 \qquad (3.1.5)$$

and also its adjoint equation

$$\Phi^{*}(1,\widetilde{2345})(T_{2345} + V_{2345} - E_{\alpha}) = 0 \qquad (3.1.6)$$

We now assume further that $\Phi(1,\widetilde{2345})$ satisfies the Schrödinger equation given by

$$(T_{12345} + V_{12345} - E)\Phi(1,\widetilde{2345}) = 0 \qquad (3.1.7)$$

Multiplying equation (3.1.7) on the left by $\Phi^{*}(1,\widetilde{2345})$ and integrating and/or summing over all variables of particles 2, 3, 4 and 5, we obtain

$$\int d\tau_{-1}\Phi^{*}(1,\widetilde{2345})(T_{12345} + \sum_{i>j=1}^{5} V_{ij} - E)\ x$$
$$\Sigma F(1\text{-}2345)\Phi(1,\widetilde{2345}) = 0 \qquad (3.1.8)$$

where $d\tau_{-1}$ refers to an integration over the alpha (2,3,4,5) configuration space. Using equation (3.1.6) we can write equation (3.1.8) as:

$$(T_{1-2345} - E_n + \sum_{j=2}^{5} V_{1j})\Phi(\widetilde{2345})F(1-2345)$$

$$= (T-E + \sum_{i>j=1}^{5} V_{ij})\Phi(\widetilde{1345})F(2-1345)+(T-E+ \sum_{i>j=1}^{5} V_{ij}) \times$$

$$\Phi(\widetilde{2145})F(3-2145) \qquad (3.1.9)$$

Making use of the symmetry properties of the integrals and variables of integration we can further modify equation (3.1.9) to obtain

$$\int \Phi^*(\widetilde{2345})(T_{1-2345} - E_n + 4V_{12})\Phi(\widetilde{2345})F(1-2345)d\tau_{-1}$$

$$= -2\int \Phi^*(\widetilde{2345})(T_{1-2345} - E_n + \sum_{j=2}^{5})\Phi(\widetilde{3145})F(2-3145)d\tau_{-1}$$

(3.1.10)

Thus the equation for $f_{\ell J(r)}$ is given by

$$-\frac{\hbar^2}{2M}\left[\frac{d^2}{dr^2}+k^2-\frac{\ell(\ell+1)}{r^2}\right] f_{\ell J(r)}$$

$$= 4\int d\tau_{-1}d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1)\ V_{12}\psi(-1)\chi_{\ell J}^{m}(1)f_{\ell J(r)}$$

$$+2\int d\tau_{-1}d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1) \sum_{j=2}^{5} V_{1j}\psi(-2)\chi_{\ell J}^{m}(2) \times$$

$$\{f_{\ell J(r')}/r'\}r + 2\int d\tau_{-1}d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1)e^2/r_{45} \times$$

$$\psi(-2)\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}/r'\}r \ + 2\int d\tau_{-1}d\Omega\Psi(-1) \times$$

$$\overline{\chi}_{\ell J}^{m}(1)[-\nabla^2_{1-2345}-k^2]\psi(-2)\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}/r'\}r$$

(3.1.11)

$$\text{where}\quad k^2 = (2M'/h^2)E_n \qquad M' = (4/5)M \qquad \underline{r} = \underline{r}_1 - 1/4(\underline{r}_2 + \underline{r}_3 + \underline{r}_4 + \underline{r}_5) \qquad \underline{r}' = \underline{r}_2 - 1/4(\underline{r}_1 + \underline{r}_3 + \underline{r}_4 + \underline{r}_5) \qquad (3.1.12)$$

This is in agreement with the work of H. Kanada et al.(1963). The last integral in equation (3.1.10) can further be written in the form

$$-2\int\varphi^*(\widetilde{2345})(T_{2-1345}-E_n+V_{21}+V_{22}+V_{24}+V_{25})\Phi(\widetilde{1345})F(2-1345)d\tau_{-1}$$

$$= -\int\Phi(\widetilde{2345})(T_{1-2345}+T_{2-1345}-2E_n+2V_{12}+3(V_{13}+V_{23}))\Phi(\widetilde{1345})\ x$$

$$F(2-1345)d\tau_{-1} \qquad (3.1.13)$$

Thus the kernel is symmetrical in interchanging particles 1 and 2 (that is $1 \longleftrightarrow 2$). Thus the only potential terms to be worked out are V_{12} and V_{13}. As in equation (3.1.11) the equation for $f_{\ell J(r)}$ is given by

$$-\frac{\hbar^2}{2M'}\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right]f_{\ell J(r)} = 4\int d\tau_{-1}d\Omega_1\Psi(-1)\overline{\chi}_{\ell J}^{m}(1)V_{12}\psi(-1)$$

$$\chi_{\ell J}^{m}(2)f_{\ell J(r)} + \int d\tau_{-1}d\Omega_1\Psi(-1)\overline{\chi}_{\ell J}^{m}(1)\ (2V_{12}+3(V_{13}+V_{23}))\Psi(-2)\ x$$

$$\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}/r'\}r \quad + \int d\tau_{-1}d\Omega_1\Psi(-1)\overline{\chi}_{\ell J}^{m}(1)\ x$$

$$\left[-\nabla^2_{1-2345} - \nabla^2_{2-1345} - 2k^2\right]\psi(-2)\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}/r'\}r +$$

$$2\int d\tau_{-1}d\Omega_1\Psi(-1)\overline{\chi}_{\ell J}^{m}(1)e^2/r_{45}\psi(-2)\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}r/r'\}$$

(3.1.14)

Alternatively we replace $3(V_{13}+V_{23})$ by

$$3(V_{13}+V_{23}) = 2E_\alpha - T_{1345} - T_{2345} - 4V_{34} - 2V_{45}$$

We now rewrite equation (3.1.14) as

$$\frac{\hbar^2}{2M'}\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right]f_{\ell J(r)} = 4\int d\tau_{-1} d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1) \times$$

$$V_{12}\psi(-1)\chi_{\ell J}^{m}(1)f_{\ell J(r)} + 2\int d\tau_{-1} d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1) \times$$

$$(V_{12}-V_{34}-V_{45})\psi(-2)\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}/r'\}r$$

$$+2\int d\tau_{-1} d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1)e^2/r_{45}\psi(-2)\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}/r'\}r$$

$$+\int d\tau_{-1} d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1)[-\nabla^2_{1-2345}-\nabla^2_{2-1345}-\varkappa^2] \times \psi(-2)\chi_{\ell J}^{m}(2)$$

$$\times \{f_{\ell J(r')}/r'\}r + \left(\frac{16}{15}\right)\int d\tau_{-1} d\Omega_1 \Psi(-1)\overline{\chi}_{\ell J}^{m}(1) \times$$

$$[-\nabla^2_{1-345}-\nabla^2_{2-345}-9/4\nabla^2_{3-45} -3\nabla^2_{45}]\psi(-2)\chi_{\ell J}^{m}(2)\{f_{\ell J(r')}/r'\}r$$

(3.1.15)

where

$$\varkappa^2 = (2M'/h^2)(E_n-E_\alpha). \qquad (3.1.16)$$

Note that in deriving equations (3.1.11), (3.1.14) and (3.1.15) we have assumed that $\Phi(\widetilde{2345})$ satisfies the alpha particle wave equation. If we now assume that the functions $\Phi(\widetilde{2345})$ while not being necessarily exact solutions of the alpha particle ground state equation, are nevertheless good variational approximations, then equation (1) reads

$$(T_{1-2345}-E_n+\sum_{j=2} V_{ij})\Phi(\widetilde{23,45})F(1-2345) = (T-E+\sum_{i>j=1}^{5} V_{ij}) \times$$

$$\Phi(\widetilde{13,45})F(2-2345)+(T-E+\sum_{i>j=1}^{5} V_{ij})\Phi(\widetilde{21,45})F(3-2145).$$

i.e. $$(T_{1-2345}-E_n+\sum_{j=2}^{5} V_{ij})\Phi(\widetilde{2345})F(1-2345)$$

$$= 2(T-E+\sum_{i>j=1}^{5} V_{ij})\Phi(\widetilde{1345})F(2-1345) \qquad (3.1.17)$$

Premultiplying equation (3.1.17) by $\Phi^*(\widetilde{2345})$ on the left, summing over the spins, and integrating over all the

relative spatial coordinates except $\underline{r}$, we obtain the equation for $f_{\ell J(r)}$ as:

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] f_{\ell J(r)} = \int \Psi(-1)\overline{\chi}_{\ell J}{}^{m}(1) \times$$

$$\sum_{j=2}^{5} U_{ij}\Psi(-1)\chi_{\ell J}{}^{m}(1) f_{\ell J(r)} d\tau_{-1} d\Omega_1$$

$$+ 2\int \Psi(-1)\overline{\chi}_{\ell J}{}^{m}(1) \sum_{i>j=1}^{5} U_{ij}\Psi(-2)\chi_{\ell J}{}^{m}(2)\{f_{\ell J(r')}\underline{r}/r'\} d\tau_{-1} d\Omega_1$$

$$- 2\int \Psi(-1)\overline{\chi}_{\ell J}{}^{m}(1)[\ K.E + \varkappa^2\ ]\ \Psi(-2)\chi_{\ell J}{}^{m}(2)\{f_{\ell J(r')}\underline{r}/r'\} \times$$

$$d\tau_{-1}\, d\Omega_1 \quad + \quad \text{Coulomb terms} \qquad (3.1.18)$$

where $k^2 = (2M^1/\hbar^2)E_n$, $M^1 = (4/5)M$, $\varkappa^2 = 2M^1/h^2(E_n + E_\alpha)$

$$U_{ij} = (2M^1/\hbar^2)V_{ij}$$

$$\text{and } K.E = \frac{-\hbar^2}{2M}\left(\frac{5}{4}\nabla^2_{1-2345} + \frac{4}{3}\nabla^2_{2-345} + \frac{3}{2}\nabla^2_{3-45} + \frac{2}{1}\nabla^2_{45}\right) \qquad (3.1.19)$$

The results of solving equations (3.1.11), (3.1.14) and (3.1.15) in terms of phase-shifts and cross-sections for the n-He^4 scattering problems will be compared with the numerical results of equation (3.1.19) in terms of the phase-shifts and total cross-sections in this thesis.

§3.2 METHOD OF PRESENTATION

The resulting integrals are of two types which we classify as "direct" and "indirect". The direct integrals involve the outside neutron (coordinate $\underline{r}$). They may therefore be evaluated completely. The indirect integrals contain func-

tions of $\underline{r}$ and $\underline{r}'$ and must therefore be left in the form of undetermined integrals. The final part of the calculation consists in solving the resulting integro-differential equations in the function $f^{M}_{\ell J}$. This has to be done numerically.

In the following chapters we shall use the standard notation for the nuclear potentials and the wave functions defined in the previous sections often without comment. We shall also use the standard notation for coordinates given in Appendix II.

The evaluation of the direct terms, indirect terms, kinetic energy terms and the Coulomb terms will be dealt with in two parts, namely

i) The S-S terms - pre and post multiplying alpha wave functions are both in the S-state;

ii) the S-D and D-S terms - one of the wave functions is in the S-state and the other the D-state.

The D-D terms will be neglected due to the small percentage of the D-admixture (about 4%).

Owing to the large amount of analysis involved in some parts of the calculation, it is not always practicable to give every step explicitly. Also some of the suffices are omitted wherever there is no risk of confusion.

PART II

NEUTRON-ALPHA SCATTERING

CHAPTER IV(A)

THE CENTRAL FORCE TERMS (S-S INTERACTION)

§ 4.1 FORMULATION

In this chapter we extend the n-He^4 scattering equations to cover the generalized potentials of Hamada and Johnston (1962) given by:

$$V(r_{ij}) = \sum_{\lambda=1}^{4} \sum_{\nu=1}^{4} \{\tfrac{1}{4}(w+b_\nu B_{ij} + m_\nu M_{ij} + h_\nu H_{ij})\}^\nu \times V_\lambda(\underline{r}_{ij}, \underline{\sigma}_i, \underline{\sigma}_j) + \frac{e^2}{r_{ij}^2} \qquad (4.1.1)$$

where ${}^\nu V_\lambda(\underline{r}_{ij}, \underline{\sigma}_i, \underline{\sigma}_j)$ are defined in Chapter II. In this chapter we shall consider the contribution of central force terms to the n-He^4 scattering problem, namely the interaction of the type:

$$V(r_{ij}) = \sum_{\lambda=1}^{4} \sum_{\nu=1}^{4} \tfrac{1}{4}(w+b_\nu B_{ij} + m_\nu M_{ij} + h_\nu H_{ij}) \times \sum_{\varkappa=1}^{2} {}^\lambda U_\varkappa^\nu \exp\left[-{}^\lambda\mu_\varkappa^\nu r_{ij}^2\right] + \frac{e^2}{r_{ij}^2} \qquad (4.1.2)$$

where B, M and H are the usual Bartlett, Majorana and Heisenberg exchange operators for the nuclei i and j respectively. e is the Coulomb electronic charge.

As already shown in §3.1, by equation (3.1.14), the equation for $f_{\ell J(r)}$ is given by

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] f_{\ell J(r)} = \int \Psi(-1)\overline{\chi}_{\ell J}{}^m(1) \times$$

$$\sum_{j=2}^{5} V_{1j}\Psi(-1)\chi_{\ell J}{}^{m}(1)f_{\ell J(r)}d\tau_{-1}\,d\Omega_1$$

$$+2\int\Psi(-1)\overline{\chi}_{\ell J}{}^{m}(1)\sum_{i>j=1}^{5} V_{ij}\Psi(-2)\chi_{\ell J}{}^{m}(2)\{f_{\ell J(r')}r/r'\}d\tau_{-1}d\Omega_1$$

$$-2\int\Psi(-1)\overline{\chi}_{\ell J}{}^{m}(1)\,[\,K.E+\kappa^2\,]\,\Psi(-2)\chi_{\ell J}{}^{m}(2)\{f_{\ell J(r')}r/r'\}d\tau_{-1}d\Omega_1$$

(4.1.3)

where V_{ij} are defined by equation (4.1.2).

For the sake of accuracy it is necessary to do the analysis in a ~~completely sys-~~ tematic way~~ if we are to avoid missing sections of the work~~. Hence we divide the evaluation of each term into four stages as follows:

(i) Spin Summations

(ii) Integrations over complete vectors

(iii) Integrations over spherical harmonics

(iv) Final results.

(i) SPIN SUMMATIONS

In carrying out the spin summations, the following rules for evaluating the spin products will be used. Consider the spin functions $\chi_{\widetilde{\ell m},\widetilde{no}}$, $\chi_{\widetilde{ij},\widetilde{\kappa p}}$. Pair all ℓm, no and ij, ij,κp and every pair gives $+^1/4$ if in the same relative position and $-^1/4$ if in different relative position. For example, suppose ℓ=i and n=κ, then $\chi_{\widetilde{\ell m},\widetilde{no}}\cdot\chi_{\widetilde{\ell j},\widetilde{np}}$ gives $+^1/4$ (pair(ℓ,n)). If ℓ=j and n=p, then the product of $\chi_{\widetilde{\ell m},\widetilde{no}}\cdot\chi_{\widetilde{i\ell},\widetilde{\kappa p}}$ is $^-1/4$ (pair (ℓ,n)).

Note that ℓ only pairs with no

m " " " no

Note that n only pairs with ℓm

p " " " ℓm

and the same for ij, $\varkappa p$.

Consider for example the product of $\chi(\widetilde{23},\widetilde{45}).\chi(\widetilde{23},\widetilde{41})$. Here the pairs are (24), (34). Therefore the value is $+\frac{1}{2}$ etc.

Making use of the above rules, then, after the spin summations the integro-differential equation in (4.1.3) now becomes

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] f_{\ell J(r)} = (4w + 2b - m - 2h)U_{c(r)} f_{\ell J(r)}$$

$$+ \int \{(4m + 2h - w - 2b)Q_{c(r,r')} + (m + w) P_{c(r,r')} +$$

$$+ (\frac{E_n}{E_\alpha} - \frac{17}{15}) N_{c(r,r')} + S_{c(r,r')} + C_{45(r,r')}\} x$$

$$f_{\ell J(r')} r\, r'\, dr' d\Omega \qquad (4.1.4)$$

where

$$U_c = \frac{8M}{5\hbar^2} \int V(|\underline{v} - {}^3/_4 \underline{\rho}_2|)|\varphi(\underline{\rho}_2, \underline{\rho}_3, \underline{\rho}_4)|^2 \, d\underline{\rho}_2 d\underline{\rho}_3 d\underline{\rho}_4$$

$$Q_c = (\frac{16}{15})^3 \frac{8M}{5\hbar^2} \int \varphi^*(\underline{u}, \underline{\rho}_3, \underline{\rho}_4) V(|\underline{u} - \underline{v}|) \varphi(\underline{v}, \underline{\rho}_3, \underline{\rho}_4) d\underline{\rho}_3 d\underline{\rho}_4$$

$$N_c = (\frac{16}{15})^3 \frac{8M}{5\hbar^2} E_\alpha \int \varphi^*(\underline{u}, \underline{\rho}_3, \underline{\rho}_4) \varphi(\underline{v}, \underline{\rho}_3, \underline{\rho}_4) d\underline{\rho}_3 d\underline{\rho}_4$$

$$P_c = (\frac{16}{15})^3 \frac{8M}{25\hbar^2} \int \varphi^*(\underline{u}, \underline{\rho}_3, \underline{\rho}_4) \varphi(\underline{v}, \underline{\rho}_3, \underline{\rho}_4) \{V(|\underline{u} - {}^2/_3 \, \underline{\rho}_3|) +$$

$$+ V(|\underline{v} - {}^2/_3 \, \underline{\rho}_3|) + 17v(|\underline{\rho}_4|)\} \, d\underline{\rho}_3 d\underline{\rho}_4$$

$$S_c = (\frac{16}{15})^3 \int \left[\frac{128}{225} \nabla_{\underline{u}} \varphi^*(\underline{u}, \underline{\rho}_3, \underline{\rho}_4) . \nabla_{\underline{v}} \varphi(\underline{v}, \underline{\rho}_3 . \underline{\rho}_4) -\right.$$

$$- 17(\frac{4}{15})^2 \varphi^*(\underline{u}, \underline{\rho}_3 . \underline{\rho}_4) \{{}^9/_8 \nabla^2_{3-45} + {}^3/_2 \nabla^2_{45}\} x$$

$$\left. \varphi(\underline{v}, \underline{\rho}_3, \underline{\rho}_4)\right] d\underline{\rho}_3 d\underline{\rho}_4$$

$$C_{45} = \frac{8M}{5\hbar^2} e^2 \left(\frac{16}{15}\right)^3 \int \varphi^*(\underline{u}, \underline{\rho}_3, \underline{\rho}_4)\varphi(\underline{v}, \underline{\rho}_3, \underline{\rho}_4) \frac{1}{r_{45}} d\underline{\rho}_3 d\underline{\rho}_4 \qquad (4.1.5)$$

If we do not assume that $\widetilde{\varphi(2345)}$ satisfies the alpha particle wave equation as in equation (3.1.18) we have the following integro-differential equations:

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right] f_{\ell J(r)} = (4w + 2b - m - 2h) \times$$

$$\int V_{12} |\varphi(-1)|^2 d\tau_{-1} f_{\ell J(r)} + (4m + 2h - w - 2b) \times$$

$$\int \varphi^*(-1) V_{12} \varphi(-2) f_{\ell J(r')} dr' - 3(w + m) \times$$

$$\int \varphi^*(-1) \left[V_{13} + V_{23} + V_{45} \right] \varphi(-2) f_{\ell J(r')} d\tau_{-1} +$$

$$\int \varphi^*(-1) \{\nabla_2^2 - \varkappa^2 - C_{45}\} \varphi(-2) f_{\ell J(r')} d\tau_{-1} +$$

$$\int \varphi^*(-1) f_{\ell J(r')} \left\{\frac{8}{5} \nabla_{45}^2 + \frac{6}{5} \nabla_{3,45}^2 + \frac{16}{15} \nabla_{1,345}^2\right\} \varphi(-2) d\tau_{-1}$$

where

$$V_{ij} = \frac{8M}{5\hbar^2} V_{ij}, \quad K^2 = \frac{8M}{5\hbar^2} E_n, \quad \varkappa^2 = \frac{8M}{5\hbar^2} (E_\alpha + E_n)$$

$$\text{and} \quad C_{45} = \frac{8M}{5\hbar^2} \frac{e^2}{r_{45}} \qquad (4.1.6)$$

We shall consider both equations (4.1.5) and (4.1.6) in this chapter. The choice of coordinates is given in the Appendix II.

(ii) INTEGRATIONS OVER COMPLETE VECTORS

We shall consider direct and indirect terms separately.

§ 4.2 DIRECT INTEGRATIONS

From equations (4.1.5) and (4.1.6) we see that the contribution from the central force is the same and is given by:

$$c_{D_{s-s(r)}}^{12} = \frac{8M}{5\hbar^2}\,(4w + 2b - m - 2h)\int V(|\underline{v} - \tfrac{3}{4}\underline{\rho}_2|)\,|\varphi^*(\underline{\rho}_2,\underline{\rho}_3,\underline{\rho}_4)|^2 \times d\underline{\rho}_2 d\underline{\rho}_3 d\underline{\rho}_4 \qquad (4.2.1)$$

Consider the following integral

$$\int V(|\underline{v} - \tfrac{3}{4}\underline{\rho}_2|)\,|\varphi(\underline{\rho}_2,\underline{\rho}_3,\underline{\rho}_4)|^2\, d\underline{\rho}_2 d\underline{\rho}_3 d\underline{\rho}_4$$

where $$V(|\underline{v} - \tfrac{3}{4}\underline{\rho}_2|) \equiv U(r_{12}) = \sum_{k=1}^{2} {}^{c}U_{\kappa}^{\nu}\, \exp\left[-{}^{c}\mu_{\kappa} r_{12}^2\right] \qquad (4.2.2)$$

and

$$|\varphi(\underline{\rho}_2,\underline{\rho}_3,\underline{\rho}_4)|^2 = \frac{N_S^2}{1+c^2}\, \exp\left[-\alpha(3\rho_2^2 + \frac{8\rho_3^2}{3} + 2\rho_4^2)\right] \qquad (4.2.3)$$

N_S is a normalisation factor and is given by

$$N_S^2 = \left(\frac{16\alpha^3}{\pi^3}\right)^{3/2} \qquad (4.2.4)$$

We now consider

$$\int |\varphi(\underline{\rho}_2,\underline{\rho}_3,\underline{\rho}_4)|^2\; V(|\underline{v} - {}^{3}/_{4}\,\underline{\rho}_2|)\, d\underline{\rho}_2 d\underline{\rho}_3 d\underline{\rho}_4$$

$$= \frac{N_S^2}{1+c^2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{c}U_{\kappa}^{(\nu)} \int \exp\left[-\alpha(3\rho_2^2 + \frac{8\rho_3^2}{3} + 2\rho_4^2) - {}^{c}\mu_{\kappa}^{(\nu)}\,(\underline{r} - {}^{3}/_{4}\underline{\rho}_2)^2\right] d\underline{\rho}_2 d\underline{\rho}_3 d\underline{\rho}_4$$

$$= \frac{N_S^2}{1+c^2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{c}U_{\kappa}^{(\nu)} \int \exp\left[-\lambda(\underline{\rho}_2 - \gamma\underline{r})^2 - \frac{8\alpha\rho_3^2}{3} - 2\alpha\rho_4^2 - p_{\kappa} r^2\right] \times d\underline{\rho}_2 d\underline{\rho}_3 d\underline{\rho}_4 \qquad (4.2.5)$$

$$= \frac{1}{1+c^2} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} \left(\frac{16\alpha}{16\alpha+3^{c}\mu_{\kappa}^{(\nu)}}\right)^{3/2} \exp(-p_{\kappa} r^2) \qquad (4.2.6)$$

where

$$\left.\begin{aligned} \lambda &\equiv \frac{3}{16}\left(16\alpha + 3^{c}\mu_{\kappa}^{(\nu)}\right) \\ \gamma &\equiv \frac{4^{c}\mu_{\kappa}^{(\nu)}}{16\alpha + 3^{c}\mu_{\kappa}^{(\nu)}} \end{aligned}\right\} \qquad (4.2.7)$$

and

$$p \equiv \frac{16\alpha^{c}\mu_{\kappa}^{(\nu)}}{16\alpha+3^{c}\mu_{\kappa}^{(\nu)}}$$

Thus equation (4.2.1) becomes

$$c_{D_{s-s}}^{(12)} = \frac{8M}{5\hbar^2} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (4w+2b-m-2h) \frac{c_{\mu_{\kappa}}^{(\nu)}}{1+c^2} \left(\frac{16\alpha}{16\alpha+3^{c}\mu_{\kappa}^{(\nu)}}\right)^{3/2}$$

$$x \exp\left[-p_{\kappa} r^2\right] \qquad (4.2.8)$$

4.3 INDIRECT INTEGRATIONS

We shall now consider the contribution from the central force terms to the indirect terms. We shall first of all consider the indirect integrals which arise from equation (4.1.5) and then consider afterwards those from equation (4.1.6).

Consider the integral

$$\int V(|\underline{s}'-\underline{s}|)\varphi^*(\underline{s}',\underline{u},\underline{\rho})\varphi(\underline{s},\underline{u},\underline{\rho})\,d\underline{u}\,d\underline{\rho}$$

where

$$V(|\underline{s}'-\underline{s}|) = U_{(r_{12})} = \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} {}^{c}\mu_{\kappa}^{(\nu)} \exp\left[-{}^{c}\mu_{\kappa}^{(\nu)}\, r_{12}^2\right]$$

$$\varphi^*(\underline{s}',\underline{u},\underline{\rho})\varphi(\underline{s},\underline{u},\underline{\rho}) = \frac{N_S^2}{1+c^2} \exp\left[-\frac{3\alpha}{2}(s'^2+s^2) - \frac{8\alpha u^2}{3} - 2\alpha\rho^2\right] \qquad (4.3.1)$$

Therefore

$$\int V(|\underline{s}'-\underline{s}|)\Phi^*(\underline{s}',\underline{u},\underline{\rho})\Phi(\underline{s},\underline{u},\underline{\rho})\,d\underline{u}\,d\underline{\rho}$$

$$= \frac{N_S^2}{1+c^2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{c}U_{\kappa}^{(\nu)} \int \exp\left[-3\alpha/2(s'^2+s^2) - \frac{8\alpha u^2}{3} - 2\alpha\rho^2 - {}^{c}\mu_{\kappa}^{(\nu)}(\underline{s}'-\underline{s})^2\right] d\underline{u}\,d\underline{\rho}$$

$$= \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{1}{1+c^2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{c}U_{\kappa}^{(\nu)} \exp\left[-\frac{3\alpha}{2}(s^{12}+s^2) - {}^{c}\mu_{\kappa}^{(\nu)}(\underline{s}'-\underline{s})^2\right]$$

$$= \left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}} \frac{1}{1+c^2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{c}U_{\kappa}^{(\nu)} \exp\left[-\frac{8}{75}(17\alpha + 6{}^{c}\mu_{\kappa}^{(\nu)})(r^2+r'^2) - \frac{32}{75}(4\alpha - 3{}^{c}\mu_{\kappa}^{(\nu)})\underline{r}.\underline{r}'\right] \qquad (4.3.2)$$

Thus

$${}^{c}I_{s-s}^{(12)} = \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} (4m+2h-w-2b) \frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^2} \left(\frac{3\alpha}{\pi}\right)^{3/2} x$$

$$\exp\left[-\frac{8}{75}(17\alpha+6{}^{c}\mu_{\kappa}^{(\nu)})(r^2+r'^2) - \frac{32}{75}(4\alpha-3{}^{c}\mu_{\kappa}^{(\nu)})\,x\right.$$

$$\left.\underline{r}.\underline{r}'\right] \qquad (4.3.3)$$

We now consider the contributions from the interactions $V_{(13)}$ and $V_{(23)}$.

Consider the following integral due to the interaction $V_{(13)}$

$${}^{c}I_{s-s}^{(13)} = \frac{N_S^2}{1+c^2} \left(\frac{16}{15}\right)^3 \frac{8M}{25\hbar^2} (w+m) \int \exp\left[-\frac{3\alpha}{2}(s'^2+s^2) - \frac{8\alpha u^2}{3} - 2\alpha\rho^2\right] V(|\underline{s}' - {}^{2}/_{3}\,\underline{u}|)\,d\underline{u}\,d\underline{\rho} \qquad (4.3.4)$$

where

$$V(|\underline{s}'-{}^2/3\ \underline{u}|) = \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{c}U_{\kappa}^{(\nu)} \exp\left[-\ {}^{c}\mu_{\kappa}^{(\nu)}(\underline{s}'-{}^2/3\ \underline{u})^2\right] \tag{4.3.5}$$

Thus equation (4.3.4) becomes

$$\begin{aligned} {}^{c}I_{s-s}^{(13)} &= \left(\frac{16}{15}\right)^3 \frac{8M}{25\hbar^2}(w+m)\left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} \left(\frac{6\alpha}{6\alpha+{}^{c}\mu_{\kappa}^{(\nu)}}\right)^{3/2} x \\ &\quad \exp\left[-\frac{3\alpha}{2}(s'^2+s^2) - \frac{6\alpha\,{}^{c}\mu_{\kappa}^{(\nu)}s'^2}{6\alpha+{}^{c}\mu_{\kappa}^{(\nu)}}\right]\frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^2} \\ &= \left(\frac{16}{15}\right)^3 \frac{8M}{25\hbar^2}(w+m)\left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} \frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^2}\ \eta_{\kappa}^{3/2}\ x \\ &\quad \exp\left[-\frac{4}{75}\eta_{\kappa}\{(34\alpha+27\ {}^{c}\mu_{\kappa}^{(\nu)})r'^2 + \right. \\ &\quad \left.(34\alpha+7\,{}^{c}\mu_{\kappa}^{(\nu)})r^2\} - \zeta_{\kappa}\ \underline{r}.\underline{r}'\right] \end{aligned} \tag{4.3.6}$$

where $\eta_{\kappa} \equiv \dfrac{6\alpha}{6\alpha+{}^{c}\mu_{\kappa}^{(\nu)}}$ and $\zeta_{\kappa} \equiv \dfrac{128\alpha}{25}\left(\dfrac{2\alpha+{}^{c}\mu_{\kappa}^{(\nu)}}{6\alpha+{}^{c}\mu_{\kappa}^{(\nu)}}\right)$ (4.3.7)

We deduce from equation (4.3.6) above the interaction $V_{(23)}$ which is given by

$$\begin{aligned} {}^{c}I_{s-s}^{(23)} &= \left(\frac{16}{15}\right)^3 \frac{8M}{25\hbar^2}(w+m)\left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} \frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^2}\ \eta_{\kappa}^{3/2}\ x \\ &\quad \exp\left[-\frac{4}{75}\eta_{\kappa}\{(34\alpha+27{}^{c}\mu_{\kappa}^{(\nu)})r^2\right. \\ &\quad \left.+\ (34\alpha+7{}^{c}\mu_{\kappa}^{(\nu)})r'^2\} - \zeta_{\kappa}\ \underline{r}.\underline{r}'\right] \end{aligned} \tag{4.3.8}$$

Consider the interaction potential $V_{(45)}$, i.e.

$$\begin{aligned} {}^{c}I_{s-s}^{(45)} &= 17\left(\frac{16}{15}\right)^3 \frac{8M}{25\hbar^2}(w+m) \int \varphi^*(\underline{s}',\underline{u},\underline{\rho})V(|\underline{\rho}|)\ x \\ &\quad \varphi(\underline{s},\underline{u},\underline{\rho})\ d\underline{u}\ d\underline{\rho} \end{aligned} \tag{4.3.9}$$

Now consider the following integral:

$$\int \varphi^*(\underline{s}',\underline{u},\underline{\rho})V(|\underline{\rho}|)\varphi(\underline{s},\underline{u},\underline{\rho})\, d\underline{u}\, d\underline{\rho}$$

$$= \frac{N_S^2}{1+c^2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} c_{U_\kappa}^{(\nu)} \int \exp\left[-\frac{3\alpha}{2}(s'^2+s^2) - \frac{8\alpha u^2}{3} - (2\alpha + {}^{c}\mu_\kappa^{(\nu)})\rho^2\right] du\, d\rho$$

$$= \left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} \frac{c_{U_\kappa}^{(\nu)}}{1+c^2} \left(\frac{2\alpha}{2\alpha + {}^{c}\mu_\kappa^{(\nu)}}\right)^{3/2} \exp\left[-\frac{136\alpha}{75}(r^2+r'^2) - \frac{128\alpha}{75}\,\underline{r}.\underline{r}'\right] \qquad (4.3.10)$$

Hence equation (4.3.9) becomes

$${}^{c}I_{s-s}^{(45)} = 17\left(\frac{16}{15}\right)^3 \frac{8M}{25\hbar^2} \left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} (w+m) \frac{c_{U_\kappa}^{(\nu)}}{1+c^2} \left(\frac{2\alpha}{2\alpha + {}^{c}\mu_\kappa^{(\nu)}}\right)^{3/2}$$

$$x \exp\left[-\frac{136\alpha}{75}(r^2+r'^2) - \frac{128\alpha}{75}\,\underline{r}.\underline{r}'\right] \qquad (4.3.11)$$

$$= 17\left(\frac{16}{15}\right)^3 \frac{8M}{25\hbar^2} \left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} (w+m) \frac{c_{U_\kappa}^{(\nu)}}{1+c^2} \; x$$

$$\left(\frac{2\alpha}{2\alpha + {}^{c}\mu_\kappa^{(\nu)}}\right)^{3/2} \exp\left[-\frac{136\alpha}{75}(r^2+r'^2) - \varepsilon\,\underline{r}.\underline{r}'\right] \qquad (4.3.12)$$

where

$$\varepsilon \equiv \frac{128\alpha}{75} \qquad (4.3.13)$$

(iii) INTEGRATIONS OVER SPHERICAL HARMONICS

§ 4.4 We use the formula given in Appendix III for performing the integrations over spherical harmonics. Thus

$$\int Y_{\ell m}^*(\theta,\varphi) e^{-\delta \underline{r}.\underline{r}'} d\Omega = \frac{4\pi}{\delta r r'} Y_{\ell' m'}^*(\theta',\varphi') \vartheta_{\ell+\frac{1}{2}}(\delta r r') \qquad (4.4.1)$$

and define a diagonal matrix

$$[\mathcal{J}_{\ell+\frac{1}{2}}(x)] = \begin{bmatrix} \mathcal{J}_{J-S+\frac{1}{2}}(x) & & \\ & \mathcal{J}_{J-S+3/2}(x) & \\ & & \ddots \\ & & & \mathcal{J}_{J+S+\frac{1}{2}}(x) \end{bmatrix} \qquad (4.4.2)$$

for all J if $S = \frac{1}{2}$.

We now define

$$\exp[-\zeta\, \underline{r}.\underline{r}'] = 4\pi \sum_{L=0}^{\infty} \sum_{M=-L}^{L} q_L(\zeta_{rr'})\, Y_L^M(\theta,\varphi)\overline{Y}_L^M(\theta',\varphi') \qquad (4.4.3)$$

where

$$q_\ell(\zeta rr') = i^\ell j_\ell(i\zeta rr')$$

j_ℓ is the spherical Bessel function of order ℓ. Using the orthormality of the Clebsch-Gordon coefficients, we have

$$\int \overline{\chi}(-1)\chi_{\ell J}{}^m(1) \sum_M Y_L^M(\Omega)\overline{Y}_L^M(\Omega')\chi_{\ell J}{}^m(2)\chi(-2)d\Omega d\Omega' = -\tfrac{1}{2}\,\delta_{\ell L}. \qquad (4.4.4)$$

Also

$$\left.\begin{aligned} rr'q_\ell(\lambda rr') &= \frac{1}{\lambda}\,\mathcal{J}_{\ell+\frac{1}{2}}(\lambda rr') \\ \underline{r}.\underline{r}'q_\ell(\lambda rr')rr' &= -\frac{1}{\lambda}\left[\frac{\ell}{\lambda}\,\mathcal{J}_{\ell+\frac{1}{2}}(\lambda rr') - rr'\mathcal{J}_{\ell+3/2}(\lambda rr')\right] \end{aligned}\right) \qquad (4.4.5)$$

Define $\lambda_\nu \equiv \frac{32}{75}(4\alpha - 3{}^u\mu_\nu^{(\nu)})$.

Then equation (4.3.3) becomes

$${}^cI_{s-s}(12) = \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2} \sum_{\nu=1}^{2} \sum_{\nu=1}^{4} (4m+2h-w-2b)\, \frac{{}^cU_\nu^{(\nu)}}{1+c^2} \left(\frac{3\alpha}{\pi}\right)^{3/2} x$$

$$\exp\left[-\frac{8}{75}\,(17\alpha + 6{}^c\mu_\nu^{(\nu)})(r^2+r'^2) - \lambda_\nu \underline{r}.\underline{r}'\right] \qquad (4.4.6)$$

On performing the angular integration of equation (4.4.6) we have

$$ {}^{c}I^{12}_{s-s} = -2\left(\frac{16}{15}\right)^{3} \frac{8M}{5\hbar^{2}} \left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (4m+2h-w-2b)\ x $$

$$ \frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^{2}} \int \bar{\chi}(-1)\bar{\chi}_{\ell J}{}^{m}(1) \exp\left[-\frac{8}{75}(17\alpha+6\,{}^{c}\mu_{\kappa}^{(\nu)})(r^{2}+r'^{2})-\lambda_{\kappa}\underline{r}.\underline{r}'\right] x $$

$$ \sum_{M} Y_{L}^{M}(\Omega)\ \bar{Y}_{L}^{M}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2)rr'\ d\Omega d\Omega' $$

$$ = \left(\frac{16}{15}\right)^{3}\left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{M}{\hbar^{2}} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (4m+2h-w-2b) \frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^{2}}\ x $$

$$ \left(\frac{15\pi}{4\alpha-3\,{}^{c}\mu_{\kappa}^{(\nu)}}\right) \exp\left[-\frac{8}{75}(17\alpha+6\,{}^{c}\mu_{\kappa}^{(\nu)})(r^{2}+r'^{2})\right] \vartheta_{\ell+\frac{1}{2}}(\lambda_{\kappa}rr') \qquad (4.4.7) $$

On performing the angular integration of equation (4.3.6) we have

$$ {}^{c}I^{13}_{s-s} = \left(\frac{16}{15}\right)^{3}\left(\frac{3\alpha}{\pi}\right)/32\ \frac{M}{\hbar^{2}} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (w+m) \frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^{2}} \frac{3\pi}{2(2\alpha+{}^{c}\mu_{\kappa}^{(\nu)})} $$

$$ x\ \eta_{\kappa}^{\frac{1}{2}} \Big[\exp -\frac{4}{75}\eta_{\kappa}\Big[\{(34\alpha+7\,{}^{c}\mu_{\kappa}^{(\nu)})r^{2} $$

$$ + (34\alpha+27\,{}^{c}\mu_{\kappa}^{(\nu)})r'^{2}\}\Big]\Big] \vartheta_{\ell+\frac{1}{2}}(\zeta_{\kappa}rr') \qquad (4.4.8) $$

Similarly ${}^{c}I^{(23)}_{s-s}$ can be obtained from equation (4.4.8) by the interchange $r \overset{\rightarrow}{\leftarrow} r'$.

From equation (4.3.12) we have

$$ {}^{c}I^{45}_{(s-s)} = \left(\frac{16}{15}\right)^{3} \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{M}{\hbar^{2}} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (w+m) \frac{{}^{c}U_{\kappa}^{(\nu)}}{1+c^{2}} \left(\frac{2\alpha}{2\alpha+{}^{c}\mu_{\kappa}^{(\nu)}}\right)^{3/2} $$

$$ x \exp\left[-\frac{136\alpha}{75}(r^{2}+r'^{2})\right] \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') \qquad (4.4.9) $$

(iv) THE CENTRAL FORCE TERMS (FINAL RESULTS)

§ 4.5 From equation (4.1.5) we have the following contributions from the central force terms.

$$U_c = \frac{1}{1+c^2}\left(\frac{512}{5}\right)\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}\frac{M}{\hbar^2}\,{}^cU_\kappa^{(\nu)}\left(\frac{\alpha}{16\alpha+3\,{}^c\mu_\kappa^{(\nu)}}\right)^{3/2}\exp[-p_\kappa r^2]$$

$$Q_c = \left(\frac{16}{15}\right)^3\left(\frac{3\alpha}{\pi}\right)^{3/2}\frac{1}{1+c^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}\frac{M}{\hbar^2}\,{}^cU_\kappa^{(\nu)}\,\frac{15\pi}{4\alpha-3\,{}^c\mu_\kappa^{(\nu)}}\,x$$

$$\exp\left[-\frac{8}{75}\left(17\alpha+6\,{}^c\mu_\kappa^{(\nu)}\right)(r^2+r'^2)\right]\vartheta_{\ell+\frac{1}{2}}(\lambda_\kappa rr')$$

$$P_c = \left(\frac{16}{15}\right)^3\left(\frac{3\alpha}{\pi}\right)^{3/2}\frac{1}{1+c^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}\frac{M}{\hbar^2}\,{}^cU_\kappa^{(\nu)}\,\frac{3\pi}{2(2\alpha+{}^c\mu_\kappa^{(\nu)})}\,\eta_\kappa^{\frac{1}{2}}\,x$$

$$\left[\exp\left(-\frac{4}{75}\eta_\kappa\right)\{(34\alpha+27\,{}^c\mu_\kappa^{\nu})r^2+(34\alpha+7\,{}^c\mu_\kappa^{\nu})r'^2\}+\right.$$

$$\left.\exp\left(-\frac{4}{75}\eta_\kappa\right)\{(34\alpha+7\,{}^c\mu_\kappa^{\nu})r^2+(34\alpha+27\,{}^c\mu_\kappa^{\nu})r'^2\}\right]\vartheta_{\ell+\frac{1}{2}}(\zeta_\kappa rr')$$

$$+\left(\frac{16}{15}\right)^3\left(\frac{3\alpha}{\pi}\right)^{3/2}\frac{1}{1+c^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}\frac{M}{\hbar^2}\,{}^cU_\kappa^{\nu}\,\frac{51\pi}{4\alpha}\left(\frac{2\alpha}{2\alpha+{}^c\mu_\kappa^{\nu}}\right)^{3/2}$$

$$x\exp\left[-\frac{136\alpha}{75}(r^2+r'^2)\right]\vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') \qquad (4.5.1)$$

The results of the indirect terms which arise from equation (4.1.6) are similar to those of equation (4.1.5) and the results can be obtained directly from equation (4.5.1).

The calculations of the indirect terms due to the energy terms, that is, the N-kernel and the S-kernels (the kinetic energy kernels) will be discussed in Chapter VII.

CHAPTER IV (B)

THE COULOMB FORCE TERMS (S-S INTERACTION)

There is a contribution to the direct and the exchange integrals.

§ 4.6 DIRECT INTEGRATION

The direct integral is given by

$$c_D{}^{coul.}_{s-s(r)} = \frac{8M}{5\hbar^2} e^2 \int |\varphi(\underline{\rho}_2, \underline{\rho}_3, \underline{\rho}_4)|^2 \frac{1}{\underline{\rho}_4} d\underline{\rho}_2 d\underline{\rho}_3 d\underline{\rho}_4 \, f_{\ell J(r)} \tag{4.6.1}$$

where

$$|\varphi(\underline{\rho}_2, \underline{\rho}_3, \underline{\rho}_4)|^2 = \frac{N_S^2}{1+c^2} \exp\left[-\alpha\left(3\rho_2{}^2 + \frac{8\rho_3{}^2}{3} + 2\rho_4{}^2\right)\right]$$

The above integral is easily evaluated and the result is

$$c_D{}^{coul.}_{s-s(r)} = \frac{8M}{5\hbar^2} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} 2e^2 \frac{1}{1+c^2} f_{\ell J(r)} \tag{4.6.2}$$

dropping the $f_{\ell J(r)}$, we have

$$c_D{}^{coul.}_{s-s(r)} = \frac{16M}{5\hbar^2} e^2 \frac{1}{1+c^2} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} \tag{4.6.3}$$

§4.7 INDIRECT INTEGRATION

The indirect integral is given by

$$c_I{}^{coul.}_{s-s(r)} = \frac{8M}{5\hbar^2} r \int \varphi^*(\widetilde{2345}) \frac{2}{\underline{\rho}}, \varphi(\widetilde{1345}) f_{(r')} \, d\tau_{-1} \tag{4.7.1}$$

This is due to two exchange integrals $\int \varphi^*(\widetilde{2345}) \frac{1}{\underline{\rho}}, \varphi(\widetilde{1345}) F(2) d\tau_{-1}$ and $\int \varphi^*(\widetilde{2345}) \frac{1}{\underline{\rho}}, \varphi(\widetilde{1245}) F(3) d\tau_{-1}$.

These two last integrals are the same as shown in Chapter I.

Thus

$$c I^{coul.}_{s-s(r)} = -\left(\frac{16}{15}\right)^3 \frac{8Me^2}{5\hbar^2} \frac{N_S^2}{1+c^2} \int \frac{1}{\rho} \exp\left[-\frac{3\alpha}{2}(s'^2+s^2) - \frac{8\alpha u^2}{3} - 2\alpha\rho^2\right] f_{\ell J(r')}\, rr'dr'\, du\, d\rho \qquad (4.7.2)$$

$$= -\frac{1}{1+c^2} \left(\frac{16}{15}\right)^3 \frac{8Me^2}{5\hbar^2} \left(\frac{6\alpha^2}{\pi^2}\right)^{3/2} \exp\left[-\frac{3\alpha}{2}(s'^2+s^2)\right] x \int \frac{1}{\rho} e^{-2\alpha\rho^2}\, d\rho rr'dr$$

$$= -\frac{1}{1+c^2} \frac{16Me^2}{5\hbar^2} \left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} \int \exp\left[-\frac{3\alpha}{2}(s'^2+s^2)\right] x\, rr'dr\, f_{\ell J(r')}$$

$$= -\frac{1}{1+c^2} \frac{16Me^2}{5\hbar^2} \left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} \int \exp\left[-\frac{136\alpha}{75}(r^2+r'^2) - \frac{128\alpha}{75}\, \underline{r}.\underline{r}'\right] f_{\ell J(r')}\, rr'dr' \qquad (4.7.3)$$

On performing the angular integration the above integral leads to

$$c I^{coul.}_{s-s(r)} = -\frac{1}{1+c^2} \left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} e^2 \frac{M}{5\hbar^2}\, x$$

$$\frac{15\pi}{2\alpha} \int \exp\left[-\frac{136\alpha}{75}(r^2+r'^2)\right] \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr')\, f_{\ell J(r')}\, dr' \qquad (4.7.4)$$

where $\varepsilon \equiv \frac{128\alpha}{75}$ (4.7.5)

Equation (4.7.4) can also be written as

$$c I^{coul.}_{s-s(r)} = -\frac{1}{1+c^2} \left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}} \frac{32}{15} \varepsilon^2 \left\{\frac{4M'}{\varepsilon}\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} e^2\right\} x$$

$$\exp\left[-\frac{17}{16}\varepsilon(r^2+r'^2)\right] \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') \qquad (4.7.6)$$

where

$$M' = \frac{15}{8\alpha} \frac{M}{\hbar^2} \qquad (4.7.7)$$

CHAPTER V

THE SPIN-ORBIT FORCE TERMS (S-S INTERACTION)

§ 5.1 FORMULATION

The alpha particle (hereinafter referred to as He^4) is of spin zero and thus coupled equations do not arise in the analysis of the collision. The vector sum of the spins of the incident and target nuclei is $\frac{1}{2}$ for n-He^4 scattering. Since He^4 is spin saturated, the incident neutron can assume two possible directions of spin $+\frac{1}{2}$ and $-\frac{1}{2}$ and therefore this is a case of "doublet splitting".

For a given total angular momentum J, there are two relative angular momenta, namely $J+\frac{1}{2}$ and $J-\frac{1}{2}$. Thus any state J will be split into $\ell = J+\frac{1}{2}$ and $\ell = J-\frac{1}{2}$ ($\underline{J}=\underline{L}+\underline{S}$). In particular the state of scattering for $\ell = 1$ will split into $J = 3/2$ and $J = \frac{1}{2}$. The parities of the systems corresponding to these two momenta are ~~quite~~ different and they do not mix. This means that the orbital angular momentum is also a good quantum number. It should be pointed out that this is no longer true if the polarization of the He^4 is taken into account during the scattering processes.

The full wave function of the problem as given previously is

$$\psi_M(\widetilde{12}3,\widetilde{45}) = \sum_{1,2,3} \sum_{J=\frac{1}{2}}^{\infty} \sum_{\ell=J-\frac{1}{2}}^{J+\frac{1}{2}} \varphi_{\ell JM}(-1)\, f_{J\ell M}(1) \times$$

$$\sum_{m=M-\frac{1}{2}}^{M+\frac{1}{2}} C_{J\ell Mm} Y_{\ell m}(1)\, \chi_{M-m}(1,\widetilde{23},\widetilde{45}) \qquad (5.1.1)$$

For a doublet state characterized by $J,M(J_z = M)$ there are two possible ℓ values $\ell = J+\frac{1}{2}$, $\ell=J-\frac{1}{2}$ and two possible values of the quantum number $m=M+\frac{1}{2}$, $M-\frac{1}{2}$. $Y_{\ell,m}$ is a tesseral harmonic. The coefficients $C_{J\ell Mm}$ are found from the condition that J^2 is an eigen value $(J(J+1))$ of the wave function chosen and further

$$\sum_{m=M-\frac{1}{2}}^{M+\frac{1}{2}} C^2_{J\ell Mm} = 1 \qquad (5.1.2)$$

Several researchers including Hughes and Le Couteur (1950), Inglis (1953), Elliot (1953), Hochberg (1953), Sack et al. (1954), Hochberg et al. (1954,1955), Van de Spuy (1956), Y. Takamura and R. Tamaji (1961) and H. Kanada et al. (1963) have considered the scattering of N-He^4 (nucleon-alpha particle) in terms of the vector spin-orbit force either of the type:

$$V(r_{ij}) = \frac{1}{\hbar^2} (\underline{s}_i+\underline{s}_j).\{(\underline{r}_i-\underline{r}_j)\wedge(\underline{p}_i-\underline{p}_j)\}V_{Ls}(r_{ij}) \qquad (5.1.3)$$

or $$V(r_{ij}) = (1 + \beta\underline{I}.\underline{\sigma})\ V_{Ls}(r_{ij}) \qquad (5.1.4)$$

or $$V(r_{ij}) = (1 - \beta\underline{I}.\underline{\sigma}\ \frac{1}{r}\frac{d}{dr})\ V_{Ls}(r_{ij}) \qquad (5.1.5)$$

The $\underline{s}_i$ is the vector spin of the i^{th} particle and is defined in terms of the Pauli spin vector $\underline{\sigma}$ as:

$$\underline{\sigma}_i = \frac{2}{\hbar}\underline{s}_i \qquad (5.1.6)$$

$\underline{p}_i$ refers to the i^{th} particle momentum. The analytic forms of these potential wells were taken to be of square-, Gauss- and exponential-form. For example, Hochberg (1953) used equation (5.1.4) with a square well potential and found that the S and P phase-shifts obtained agree quite

well with those determined experimentally. He chose

$$\left.\begin{aligned} V(r) &= V_o \quad \text{for } r < a \\ &= 0 \quad \text{for } r > a \end{aligned}\right\} \qquad (5.1.7)$$

The values of his parameters are V_o = -70.9 MeV, its radius a = 2.5f and β = 0.150. Bürgel (1952) made similar calculation and found that the best agreement with experiment when V_o = -33.0 MeV, a = 2.55f and β = 0.103. Sack et al. calculated the S and P phase shifts for p-He^4 scattering using N-N interaction of the form given by equation (5.1.5) having a spin-orbit term of the Thomas type. Calculations were made for square, Gauss and exponential wells. They found that the exponential well gave a P-phase splitting increasing too rapidly with energy, the square well a P-phase splitting increasing too slowly with energy and the Gaussian well a satisfactory overall fit.

In this chapter we shall extend our generalized potential outlined in Chapter IV to include potentials of the type given by equation (5.1.3) applied to equations (3.1.14) and (3.1.18) respectively. The radial dependence of the potentials $V_{Ls}(r)$ are assumed to be of double Gaussian shape ~~function~~ obtained by a least squares fit from the Hamada and Johnston's potential. This enables one to carry the calculation analytically further than with other shapes, while at the same time giving a close approximation to the actual shape of potential and the wave functions.

§5.2 (i) THE SPIN SUMMATIONS

We shall use the spin functions $\chi(\widetilde{23},\widetilde{45})$ and $\chi(\widetilde{13},\widetilde{45})$ defined in Chapter II. For simplicity we shall work with the Pauli spin operator $\underline{\sigma}_i = \frac{2}{\hbar}\underline{s}_i$, rather than $\underline{s}_i$ themselves. Now for each of the five $\underline{\sigma}_i$, there are ten possible spin products, five for the direct terms and five for the indirect terms.

The following relationships together with those listed in Chapter IV are used to simplify the spin products which arise from the problems:

(i) $\underline{\sigma}_i\chi(\widetilde{ij}) = -\underline{\sigma}_j\chi(\widetilde{ij})$ for any pair i,j.

(ii) We may interchange the particle suffices in a spin product in any way without altering its value, for the complete expression is independent of suffices.

(iii) Using (i) and (ii) we have

$$\chi^*(\widetilde{ij}).\underline{\sigma}_i\chi(\widetilde{ij}) = 0 \quad \text{for all } i,j.$$

(iv) $\underline{\sigma}_i^+ = \underline{\sigma}_i$, $\underline{\sigma}_i^+$ is the complex conjugate transpose of $\underline{\sigma}_i$.

From equation (3.1.14) using equation (5.1.3) and ~~taking into account~~ remembering that the spin-orbit force contributes only in the triplet states of n-He^4 scattering, we obtain the following integro-differential equations for direct and indirect terms respectively.

$$(a)\quad {}^{Ls}D_{s-s(r)} = \frac{8M}{5\hbar^2}\int dr d\Omega\,[\,\varphi(-1)\chi(1)Y(\Omega)\,]^*\sum_\nu (w-\tfrac{1}{2}m)_\nu \times$$

$$ {}^{\nu}V_{Ls}(12)\;\varphi(-1)\chi(1)Y(\Omega)f_{\ell J(r)} \qquad (5.2.1)$$

The potential in this case is

$$\sum_{\nu}\sum_{\kappa} {}^{Ls}U_{\kappa}^{\nu} \exp\left[-{}^{Ls}\mu_{\kappa}^{\nu} r_{12}^2\right] = \sum_{\nu} (w-\tfrac{1}{2}m)_{\nu} {}^{\nu}V_{Ls}(12) \qquad (5.2.2)$$

and

$$(b)\ {}^{Ls}I^{12}_{s-s(r)} = \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2}\, 2\int dr'd\Omega\ [\varphi(-1)\chi(1)Y(\Omega)]^* \times$$

$$\sum_{\nu} (w-2m)_{\nu} {}^{\nu}V_{Ls}(12)\varphi(-2)\chi(2)Y(\Omega')f_{\ell J(r')}\, rr'\, d\underline{u}d\underline{\rho}d\Omega' \qquad (5.2.3)$$

and the potential is defined in a similar way as in equation (5.2.2)

§5.3 (ii) INTEGRATIONS OVER COMPLETE VECTORS

We consider first the direct integration. Consider equation (5.2.1). Writing the spin-orbit operator in full, we have

$${}^{Ls}D^{12}_{s-s(r)} = \frac{8M}{5\hbar^2} N_S^2 \frac{1}{2i} \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} 4(w-\tfrac{1}{2}m)_{\nu} \frac{{}^{Ls}U_{\kappa}^{\nu}}{1+c^2} \times$$

$$\int \exp\left[-\left(\frac{8\alpha u^2}{3} + 2\alpha\rho^2\right)\right] d\underline{u}d\underline{\rho} \int \exp\left[-\frac{3\alpha v^2}{2} - {}^{Ls}\mu_{\kappa}^{\nu}(\underline{r}-^3/_4\underline{v})^2\right]$$

$$\times\ \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[(\underline{\sigma}_1+\underline{\sigma}_2).\left\{(\underline{r}-^3/_4\underline{v})\wedge\left(\frac{5}{4}\frac{\partial}{\partial\underline{r}} - \frac{\partial}{\partial\underline{v}}\right)\right\}\right] \times$$

$$\exp\left[-\frac{3\alpha v^2}{2}\right] \times \chi_{\ell J}{}^{m}(1)\chi(-1)\, d\underline{r}d\underline{v}d\Omega\ . \qquad (5.3.1)$$

Using the relation that $\Sigma\chi^*(-1)\underline{\sigma}_2\chi(-1) = 0$, we have

$${}^{Ls}D^{12}_{s-s(r)} = \frac{8M}{5\hbar^2} N_S^2 \frac{1}{2i} \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w-\tfrac{1}{2}m)_{\nu} \frac{{}^{Ls}U_{\kappa}^{\nu}}{1+c^2} \int \exp\left[-\left(\frac{8\alpha u^2}{3}\right.\right.$$

$$\left.\left. + 2\alpha\rho^2\right)\right] d\underline{u}d\underline{\rho} \int \exp\left[-\frac{3\alpha v^2}{2} - {}^{Ls}\mu_{\kappa}^{\nu}(\underline{r}-^3/_4\underline{v})^2\right] \times$$

$$\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\underline{\sigma}_1.\left[\frac{5}{4}\underline{r}\wedge\frac{\partial}{\partial\underline{r}} - \frac{15}{16}\underline{v}\wedge\frac{\partial}{\partial\underline{r}} - \underline{r}\wedge\frac{\partial}{\partial\underline{r}} + \frac{3}{4}\underline{v}\wedge\frac{\partial}{\partial\underline{v}}\right] \times$$

$$e^{-\frac{3\alpha v^2}{2}} \chi_{\ell J}{}^{m}(1)\chi(-1)d\underline{v}d\underline{r}d\Omega\ . \qquad (5.3.2)$$

Consider $\exp\left[-3\alpha v^2 - {}^{Ls}\mu_{\kappa}^{\nu}\,(\underline{r}-{}^{3}/_{4}\,\underline{v})^2\right]$

$$= \exp\left[-\frac{16\alpha\ {}^{Ls}\mu_{\kappa}^{\nu}\ r^2}{16\alpha + 3^{Ls}\mu_{\kappa}^{\nu}} - \lambda\ (\underline{v}-\gamma\underline{r})^2\right]$$

where $\lambda \equiv \frac{3}{16}\ (16\alpha + 3^{Ls}\mu_{\kappa}^{\nu})$

$$\gamma \equiv \frac{4^{Ls}\mu_{\kappa}^{\nu}}{16\alpha + 3^{Ls}\mu_{\kappa}^{\nu}} \qquad (5.3.3)$$

Consider the following integral

$$\int \ldots\ \underline{v}\ \exp\ (-\lambda(\underline{v}-\gamma\underline{r})^2)\,d\underline{v}$$

This integral is proportional to r.

Thus

$$\int \ldots\ \underline{r}\wedge\frac{\partial}{\partial\underline{v}}\ \ldots \propto \int \ldots\ \underline{r}\wedge\underline{v}\ \ldots\ldots \propto \int \ldots\ \underline{r}\wedge\underline{r}\ \ldots = 0$$

Similarly

$$\int \ldots\ \underline{v}\wedge\frac{\partial}{\partial\underline{v}}\ \ldots \propto \int \ldots\ \underline{v}\wedge\underline{v}\ \ldots\ldots\ldots = 0$$

Hence, the only integral which survives in equation (5.3.2) is

$${}^{Ls}D^{12}_{s-s(r)} = -\frac{4M}{5\hbar^2}\ N_S^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w-\tfrac{1}{2}m)_{\nu}\ \frac{{}^{Ls}U_{\kappa}^{\nu}}{1+c^2} \int \exp\left[-\frac{8\alpha u^2}{3}\right.$$

$$\left. + 2\alpha\rho^2)\right]\chi^*(-1)\chi_{\ell J}{}^{m}(1)\ d\underline{u}d\underline{\rho} \int \exp\left[-\frac{16\alpha\ {}^{Ls}\mu_{\kappa}^{\nu}\ r^2}{16\alpha + 3^{Ls}\mu_{\kappa}^{\nu}} -\right.$$

$$\left.\lambda\,(\underline{v}-\gamma\underline{r})^2\right]\, i\underline{\sigma}_1\cdot\left(\frac{5}{4}\ \underline{r}\wedge\frac{\partial}{\partial\underline{r}} - \frac{15}{16}\ \underline{v}\wedge\frac{\partial}{\partial\underline{r}}\right)\ \chi_{\ell J}{}^{m}(1)\chi(-1)\,d\underline{r}d\underline{v}d\Omega \qquad (5.3.4)$$

$$= -\frac{8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 2\left(\frac{16\alpha}{16\alpha + 3^{Ls}\mu_{\kappa}^{\nu}}\right)^{3/2}\ (1-\tfrac{3}{4}\gamma)\ (w-\tfrac{1}{2}m)_{\nu}\ x$$

$$\frac{{}^{Ls}U_{\kappa}^{\nu}}{1+c^2} \exp\left[-\frac{16\alpha\,{}^{Ls}\mu_{\kappa}^{\nu}\, r^2}{16\alpha + 3^{\,{}^{Ls}\mu_{\kappa}^{\nu}}}\right] \int \chi^*(-1)\bar{\chi}_{\ell J}{}^{m}(1)\ \frac{5}{4}\ i\ \underline{\sigma}.\underline{r}\wedge\frac{\partial}{\partial\underline{r}}\ x$$

$$\chi_{\ell J}{}^{m}(1)\chi(-1)\ d\Omega \qquad (5.3.5)$$

Define $\underline{L} = \frac{1}{i}\left(\underline{r}\wedge\frac{\partial}{\partial\underline{r}}\right)$

Since $\underline{J} = \underline{L} + \underline{S}$, therefore $2\underline{L}.\underline{S} = \underline{J}.\underline{\sigma}$

$$= J(J+1)-L(L+1)-S(S+1) \quad \text{etc.} \qquad (5.3.6)$$

In our case $S = \frac{1}{2}$. Thus we may write

$$i\ \underline{\sigma}.\underline{r}\wedge\frac{\partial}{\partial\underline{r}} = \underline{L}.\underline{\sigma}$$

Hence $$||\ \underline{\sigma}\ \ell\ || = \begin{cases} 0 & \text{for } J=\frac{1}{2}, \text{ and } \ell = 0 \\ \ell & \text{for } J=\ell+\frac{1}{2} \\ -(\ell+1) & \text{for } J=\ell-\frac{1}{2} \end{cases} \qquad (5.3.7)$$

Thus equation (5.3.5) now becomes

$${}^{Ls}D_{s-s(r)}^{12} = \frac{8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}(w-\tfrac{1}{2}m)_{\nu}\ \frac{{}^{Ls}U_{\kappa}^{\nu}}{1+c^2}\ \frac{5}{2}\ ||\ \underline{\sigma}\ \underline{\ell}\ ||\ P_{Ls(\kappa)}^{5/2}$$

$$x\ \exp\left[-P_{Ls(\kappa)}\ {}^{Ls}\mu_{\kappa}^{\nu}\ r^2\right]\ . \qquad (5.3.8)$$

where

$$P_{Ls(\kappa)} \equiv \frac{16\alpha}{16\alpha + 3^{\,{}^{Ls}\mu_{\kappa}^{\nu}}}\ . \qquad (5.3.9)$$

§ 5.4 INDIRECT INTEGRATION

We shall now consider the indirect integration which arises from equation (5.2.3). Writing the spin-orbit operator in full we have the following integral:

$${}^{Ls}I_{s-s(r)}^{12} = \frac{N_S{}^2}{1+c^2}\ \frac{8M}{5\hbar^2}\ \frac{1}{2i}\ \left(\frac{16}{15}\right)^3\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}2(w-2m)_{\nu}\ x$$

$$^{Ls}U_{\mu}^{\nu} \int \chi^*(-1)\bar{\chi}_{\ell J}{}^{m}(1)\ \exp\left[-\frac{3\alpha s'^2}{2} - \frac{16}{25}\,{}^{Ls}\mu_{\mu}^{\nu}\,(\underline{r}-\underline{r}')^2 - \frac{4\alpha u^2}{3} - \alpha\rho^2\right](\underline{\sigma}_1+\underline{\sigma}_2).\{(\underline{r}-\underline{r}')\wedge(\frac{\partial}{\partial \underline{r}} - \frac{\partial}{\partial \underline{r}'})\}\ \exp\left[-\frac{3\alpha s^2}{2} - \frac{4\alpha u^2}{3} - \alpha\rho^2\right]\chi_{\ell J}{}^{m}(2)\chi(-2)f_{\ell J(r')}\ rr'\ dr'\ d\underline{u}d\underline{\rho}d\Omega \qquad (5.4.1)$$

where $\underline{s} = \frac{16}{15}\,\underline{r} + \frac{4}{15}\,\underline{r}'$, $\underline{s}' = \frac{16}{15}\,\underline{r}' + \frac{4}{15}\,\underline{r}$ (5.4.2)

Consider

$$\int \exp\left[-\frac{3\alpha s'^2}{2} - \frac{16}{25}\ {}^{Ls}\mu_{\mu}^{\nu}\ (\underline{r}-\underline{r}')^2\right](\underline{\sigma}_1+\underline{\sigma}_2).(\underline{r}-\underline{r}')\wedge(\frac{\partial}{\partial \underline{r}} - \frac{\partial}{\partial \underline{r}'})\ x$$

$$\exp\left[-\frac{3\alpha}{2}\,s^2\right] f_{\ell J(r')}\ rr'\ dr'\ d\underline{u}d\underline{\rho}$$

We can separate the above integral into two parts. We first of all consider the following integral (1st part).

$$\int \exp\{-\frac{3\alpha}{2}\,s'^2 - \frac{16}{25}\ {}^{Ls}\mu_{\mu}^{\nu}(\underline{r}-\underline{r}')^2\}(\underline{\sigma}_1+\underline{\sigma}_2).(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}}\ x$$

$$e^{-\frac{3\alpha s^2}{2}}\ f_{\ell J(r')}\ rr'\ dr d\underline{u}d\underline{\rho}$$

$$= \frac{64\alpha}{15}\int \exp\{-\frac{3\alpha}{2}(s^2+s'^2) - \frac{16}{25}\,{}^{Ls}\mu_{\mu}^{\nu}\ (\underline{r}-\underline{r}')^2\}\ (\underline{\sigma}_1+\underline{\sigma}_2)\ x$$

$$(\underline{r}'\wedge\underline{r})\ f_{\ell J(r')}\ rr'\ dr' d\underline{u}d\underline{\rho} \qquad (5.4.3)$$

We now consider the second part of the integral, namely

$$-\int \exp\{-\frac{3\alpha}{2}\,s'^2 - \frac{16}{25}\,{}^{Ls}\mu_{\mu}^{\nu}\ (\underline{r}-\underline{r}')^2\}\ (\underline{\sigma}_1+\underline{\sigma}_2).(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}'}\ x$$

$$e^{-\frac{3\alpha s^2}{2}}\ f_{\ell J(r')}\ rr'\ dr' d\underline{u}d\underline{\rho}.$$

Applying Green's Theorem, the above integral becomes

$$\frac{64\alpha}{15}\int\exp\left[-\frac{3\alpha}{2}(s^2+s'^2)-\frac{16}{25}\,{}^{Ls}\mu_{\varkappa}^{\nu}\,(\underline{r}-\underline{r}')^2\right](\sigma_1+\underline{\sigma}_2)\ x$$

$$(\underline{r}\wedge\underline{r}')f_{\ell J(r')}\ rr'\ dr'\ d\underline{u}d\underline{\rho}\ .$$

Thus

$${}^{Ls}I^{12}_{ss(r)} = \left(\frac{16}{15}\right)^3\left(\frac{3\alpha}{\pi}\right)^{3/2}\frac{128\alpha}{15}\,\frac{8M}{5\hbar^2}\sum_{\varkappa=1}^{2}\sum_{\nu=3}^{4}(w-2m)_{\nu}\ x$$

$$\frac{{}^{Ls}U_{\varkappa}^{\nu}}{1+c^2}\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\exp\left[-\frac{8}{75}(17\alpha+6\,{}^{Ls}\mu_{\varkappa}^{\nu})(r^2+r'^2)-\right.$$

$$\left.\frac{32}{75}(4\alpha-3\,{}^{Ls}\mu_{\varkappa}^{\nu})\,\underline{r}.\underline{r}'\right]i(\underline{\sigma}_1+\underline{\sigma}_2).(\underline{r}\wedge\underline{r}')\chi_{\ell J}{}^{m}(2)\chi(-2)\ x$$

$$f_{\ell J(r')}\ rr'dr'd\Omega. \qquad (5.4.4)$$

§ 5.5 (iii) INTEGRATION OVER SPHERICAL HARMONICS

In performing the integration over spherical harmonics of equation (5.4.4), we shall consider first the following integration by parts, viz.

$$\left[\int\varphi(\underline{r},\underline{r}')\ \underline{r}\wedge\frac{\partial}{\partial\underline{r}'}\ f(r')d\underline{r}'\right]_{x'} = \iiint\varphi(xx')\ \varphi(yy')\varphi(zz')\ x$$

$$\left[y\frac{\partial}{\partial z'}-z\frac{\partial}{\partial y'}\right]f(x')\ dx'dy'dz$$

$$= -\iiint f(r')dx'dy'dz'\left(y\frac{\partial}{\partial z'}-z\frac{\partial}{\partial y'}\right)\varphi(xx')\varphi(yy')\varphi(zz')$$

$$= \left[-\iiint(r')d\underline{r}'\ \underline{r}\wedge\frac{\partial}{\partial\underline{r}'}\ \varphi(\underline{r},\underline{r}')\right]_{x'} \qquad (5.5.1)$$

Since $\varphi(xx') \to 0$ as $x' \to \pm\infty$ etc.

For example, consider the following integral

$$\int f\ (r')d\underline{r}'\ d^{\Omega}\ \underline{r}\wedge\frac{\partial}{\partial\underline{r}'}\ e^{-\delta(r^2+r'^2)-\varepsilon\underline{r}.\underline{r}'}$$

$$= -\int f(r')\, dr' d^{\Omega} 2\delta \underline{r} \wedge \underline{r}' \; e^{-\delta(r^2+r'^2)-\varepsilon \underline{r}.\underline{r}'}$$

Thus

$$-2\delta \underline{r}' \wedge \underline{r} \; e^{-\delta(r^2+r'^2)-\varepsilon \underline{r}.\underline{r}'} = 2\delta \frac{1}{\varepsilon} \underline{r}' \wedge \frac{\partial}{\partial \underline{r}'} \; e^{-\delta(r^2+r'^2)-\varepsilon \underline{r}.\underline{r}'} \tag{5.5.2}$$

Hence

$$\int f(r') d\underline{r}' d\Omega \; \underline{r} \wedge \underline{r}' \; e^{-\delta(r^2+r'^2)-\varepsilon \underline{r}.\underline{r}'} = -\frac{1}{\varepsilon} \int f(r') d\underline{r}' d^{\Omega} \; x$$

$$\underline{r}' \wedge \frac{\partial}{\partial \underline{r}'} \; e^{-\delta(r^2+r'^2)-\varepsilon \underline{r}.\underline{r}'} \tag{5.5.3}$$

Thus in general we have the following transformation:

$$\int \varphi \; \underline{r}' \wedge \underline{r} \; \psi f d\tau = \int \psi f \underline{r}' \wedge \underline{r} \varphi d\tau = -\frac{1}{\varepsilon} \int \psi f \underline{r}' \wedge \frac{\partial}{\partial \underline{r}'} \; \varphi d\tau$$

$$= \frac{1}{\varepsilon} \int \varphi \underline{r}' \wedge \frac{\partial}{\partial \underline{r}'} \; \psi f d\tau \tag{5.5.4}$$

Note that the last equation is obtained by integration by parts.

$$\text{Define} \quad \lambda_{Ls(n)} = \frac{32}{75} (4\alpha - 3^{Ls}\mu_n^{\nu}) \tag{5.5.5}$$

Then we have from equation (5.4.4) using the above formulae in carrying out the integration over spherical harmonics:

$$^{Ls}I^{12}_{ss(r)} = \left(\frac{16}{15}\right)^2 \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{128\alpha}{15} \frac{8M}{5\hbar^2} \sum_{n=1}^{2} \sum_{\nu=3}^{4} 2(w-2m)_{\nu} \; x$$

$$\frac{^{Ls}U_n^{\nu}}{1+c^2} \; \frac{1}{\lambda_{Ls(n)}} \int \overline{\chi}(-1) \overline{\chi}_{\ell J}{}^{m}(1) \exp\left[-\frac{8}{75}(17\alpha + 6^{Ls}\mu_n^{\nu})(r^2+r'^2)\right.$$

$$\left. - \lambda_{Ls(n)} \underline{r}.\underline{r}'\right] (\underline{\sigma}_3 . \underline{L}) \chi_{\ell J}{}^{m}(2) \chi(-2) f_{\ell J(r')} \; rr' dr' d\Omega.$$

$$= -\left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \sum_{n=1}^{2} \sum_{\nu=3}^{4} (w-2m)_{\nu} \frac{M}{\hbar^2} \frac{^{Ls}U_n^{\nu}}{1+c^2} \; x$$

$$\left(\frac{20\alpha}{4\alpha-3^{Ls}\mu_{\nu}^{\nu}}\right)\frac{15\pi}{4\alpha-3^{Ls}\mu_{\nu}^{\nu}}\;||\underline{\sigma}\;\underline{\ell}||\int\exp\left[-\frac{8}{75}(17\alpha+6^{Ls}\mu_{\nu}^{\nu})\,x\right.$$

$$\left.(r^2+r'^2)\right]\mathcal{J}_{\ell+\frac{1}{2}}(\lambda_{Ls(\nu)}rr')\,f_{\ell J(r')}\,dr'. \qquad (5.5.6)$$

(iv) FINAL SPIN-ORBIT S-S TERMS

§5.6 From equation (3.1.14) we have the total contributions from the spin-orbit S-S terms as:

$$wLs\,f_{\ell J(r)} + \int k_{Ls}^{\lambda\ell}(r,r')\,f_{\ell J(r')}\,dr'$$

where

$$wLs(r) = \frac{M}{\hbar^2}\sum_{\nu=1}^{2}\sum_{\nu=3}^{4}(4w-2m)_{\nu}\frac{^{Ls}U_{\nu}^{\nu}}{1+c^2}\;||\underline{\sigma}\;\underline{\ell}||\;P_{Ls(\nu)}^{5/2}\;x$$

$$\exp\left[-P_{Ls(\nu)}\;^{Ls}\mu_{\nu}^{\nu}\,r^2\right]$$

$$k_{Ls}^{\lambda\ell}(r,r') = -\left(\frac{16}{15}\right)^3\left(\frac{3\alpha}{\pi}\right)^{3/2}\frac{M}{\hbar^2}\sum_{\nu=1}^{2}\sum_{\nu=3}^{4}(w-2m)_{\nu}\;x$$

$$\frac{^{Ls}U_{\nu}^{\nu}}{1+c^2}\left(\frac{20\alpha}{4\alpha-3^{Ls}\mu_{\nu}^{\nu}}\right)\frac{15\pi}{4a-3^{Ls}\mu_{\nu}^{\nu}}\;||\underline{\sigma}\;\underline{\ell}||\;x$$

$$\exp\left[-\frac{8}{75}(17\alpha+6^{Ls}\mu_{\nu}^{\nu})(r^2+r'^2)\right]\mathcal{J}_{\ell+\frac{1}{2}}(\lambda_{Ls(\nu)}rr') \qquad (5.6.1)$$

where

$$P_{Ls(\nu)} \equiv \frac{16\alpha}{16\alpha+3^{Ls}\mu_{\nu}^{\nu}}$$

$$\lambda_{Ls(\nu)} \equiv \frac{32}{75}(4\alpha - 3^{Ls}\mu_{\nu}^{\nu})$$

$$||\underline{\sigma}\;\underline{\ell}|| = \begin{cases} 0 \text{ for } J=\frac{1}{2} \text{ and } \ell=0 \\ \ell \text{ for } J=\ell+\frac{1}{2} \\ -(\ell+1) \text{ for } J=\ell-\frac{1}{2} \end{cases} \qquad (5.6.2)$$

The contribution of the spin-orbit terms from equation (3.1.18) is found to be the same as that from equation (3.1.14).

CHAPTER VI

THE QUADRATIC SPIN-ORBIT FORCE TERMS (S-S INTERACTION)

§ 6.1 FORMULATION

In this chapter we consider fully the contribution of the quadratic spin-orbit force to n-He^4 scattering. So far only one publication has taken into account the effect of the quadratic spin-orbit force on light nuclei at low energies. Hochberg et al. (1968) considered a three body problem consisting of central, non-central exchange, linear spin-orbit, tensor and quadratic spin-orbit forces in terms of phase-shifts using the recent Hamada and Johnston potential whose parameters are determined by the Least Squares fit. At low incident neutron energies, the S- and D-phases obtained by them have opposite sign to the corresponding phases obtained by other workers including Christian and Gammel (1953), de Borde and Massey (1955), Buckingham et al. (1952), Burke and Robertson (1957) and Elwyn et al. (1962). Their P-phases have the same sign and at energies up to about 3 MeV they differ only slightly. Their values of the P-phases for $J=\frac{1}{2}$ and $J=^3/2$ for the doublet case are nearly the same. The large discrepancies in the phases are attributed to the completely different nature of the nuclear interaction used.

In this chapter we extend the work of Hochberg et al. (1968) to a five body problem. Because of the considerable amount of analysis involved in the case of the quadratic spin-orbit force, we shall limit our considerations only to the S-S interactions. The improved version of the

nucleon-interaction given by Hamada and Johnston (1962) whose form of the quadratic spin-orbit term we now use.

We shall now consider the direct ${}^{Qs}D_{s-s(r)}$ and the indirect ${}^{Qs}I_{s-s(r)}$ interactions due to the quadratic spin-orbit force which arise from equations (3.1.14) and (3.1.18) respectively which are of the form:

$$ {}^{Qs}D_{s-s(r)} = \frac{8M}{5\hbar^2} r\int d\underline{s}d\Omega \left[\varphi(1)\chi(1)Y(\Omega)\right] * V_{LQs}(12)\ \varphi(1)\chi(1)\ x $$

$$ Y(\Omega)\ \frac{1}{r}\ f_{\ell J(r)} \qquad (6.1.1) $$

and

$$ {}^{Qs}I_{s-s(r)} = \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2} r\int d\underline{r}'d\underline{\rho}d\underline{\rho}'d\Omega \left[\varphi(1)\chi(1)Y(\Omega)\right]* x $$

$$ V_{LQs}(12)\varphi(2)\chi(2)Y(\Omega')\ \frac{1}{r'}\ f_{\ell J(r')} \qquad (6.1.2) $$

where

$$ \left.\begin{aligned} Qs(12) &= (\underline{\sigma}_1\cdot\underline{\sigma}_2)\underline{L}_{12}^2 - Q_{12} \\ \text{and}\quad Q_{12} &= \tfrac{1}{2}\left[(\underline{\sigma}_1\cdot\underline{L}_{12})(\underline{\sigma}_2\cdot\underline{L}_{12})+(\underline{\sigma}_2\cdot\underline{L}_{12})(\underline{\sigma}_1\cdot\underline{L}_{12})\right] \end{aligned}\right\} \qquad (6.1.3) $$

$$ \text{and}\quad i\underline{L}_{12} = (\underline{r}_1-\underline{r}_2)\wedge\left(\frac{\partial}{\partial\underline{r}_1} - \frac{\partial}{\partial\underline{r}_2}\right) \qquad (6.1.4) $$

Due to the complexity of the operators, we shall try to simplify the integrals by considering the spin first.

§6.2 (i) THE SPIN SIMPLIFICATION

We define the following spin functions $\chi(1,\widetilde{23},\widetilde{45})$ and $\overline{\chi}(1,\widetilde{23},\widetilde{45})$ as follows:

$$ \left.\begin{aligned} \chi(1,\widetilde{23},\widetilde{45}) &= \tfrac{1}{2}\alpha_1(\alpha_2\beta_3-\beta_2\alpha_3)(\alpha_4\beta_5-\beta_4\alpha_5) \equiv \chi^{\frac{1}{2}}_{+\frac{1}{2}} \\ \overline{\chi}(1,\widetilde{23},\widetilde{45}) &= \tfrac{1}{2}\beta_1(\alpha_2\beta_3-\beta_2\alpha_3)(\alpha_4\beta_5-\beta_4\alpha_5) \equiv \chi^{\frac{1}{2}}_{-\frac{1}{2}} \end{aligned}\right\} \qquad (6.2.1) $$

where the α's and β's are the usual spin functions of the individual nucleons obeying the law $\alpha_i\beta_j = \delta_{ij}$ and δ_{ij} is the

usual Kronecker Delta.

We use the following relations:

$$\begin{aligned}
&(a)\ \Sigma\chi^*(1,\widetilde{23},\widetilde{45})(\underline{\sigma}_i\cdot\underline{\sigma}_j)\chi(1,\widetilde{23},\widetilde{45}) = 0 \text{ for any pair } i,j = 1,2,3,4,5;\\
&\quad \chi^* \quad " \quad " \quad \overline{\chi} \quad " = 0 \quad " \quad "\\
&\quad \overline{\chi} \quad " \quad " \quad \chi \quad " = 0 \quad " \quad "\\
&\quad \overline{\chi}^* \quad " \quad " \quad \overline{\chi} \quad " = 0 \quad " \quad "
\end{aligned} \tag{6.2.2}$$

and

$$\begin{aligned}
&(b)\ \Sigma\chi^*(1,\widetilde{23},\widetilde{45})(\underline{\sigma}_i\cdot\underline{\sigma}_j)\chi(2,\widetilde{31},\widetilde{45}) = -\,{}^3/2[\delta] \text{ for } i,j = 1,2;1,3;2,3;\\
&\qquad = 0\,[\delta] \text{ otherwise}\\
&\quad \Sigma\chi^*(1,\widetilde{23},\widetilde{45})(\underline{\sigma}_i\cdot\underline{\sigma}_j)\overline{\chi}(2,\widetilde{31},\widetilde{45}) = 0\,[\delta] \text{ for any pair } i,j = 1,2,3,4,5;\\
&\quad \Sigma\overline{\chi}^* \quad " \quad " \quad \chi(2,\widetilde{31},\widetilde{45}) = 0\,[\delta] \quad " \quad "\\
&\quad \Sigma\overline{\chi}^* \quad " \quad " \quad \overline{\chi} \quad " = -\,{}^3/2[\delta] \text{ for } i,j = 1,2;1,3;2,3;\\
&\qquad = 0\,[\delta] \text{ otherwise}
\end{aligned} \tag{6.2.3}$$

$$\begin{aligned}
\text{Thus } &\langle\chi^*(1,\widetilde{23},\widetilde{45})\,|(\underline{\sigma}_1\cdot\underline{\sigma}_2)L^2|\,\chi(1,\widetilde{23},\widetilde{45})\rangle\\
&= \langle\overline{\chi}^*(1,\widetilde{23},\widetilde{45})\,|(\underline{\sigma}_1\cdot\underline{\sigma}_2)|\,\overline{\chi}(1,\widetilde{23},\widetilde{45}\rangle L^2\\
&= 0
\end{aligned} \tag{6.2.4}$$

We now write Q_{12} in the form

$$Q_{12} = {}^1/3\ S_{12}(\underline{L},\underline{L}) + {}^1/3\ (\underline{\sigma}_1\cdot\underline{\sigma}_2)L^2 \tag{6.2.5}$$

and so $\langle\chi_1^*\,|Q_{12}|\,\chi_1\rangle = {}^1/3\langle\overline{\chi}_1^*\,|(\underline{\sigma}_1\cdot\underline{\sigma}_2)|\,\overline{\chi}_1\rangle L^2 = 0$ (6.2.6)

$S_{ij}(\underline{L},\underline{L})$ is the usual tensor operator which is defined by

$$S_{ij}(\underline{L},\underline{L}) = 3(\underline{\sigma}_i\cdot\underline{L})(\underline{\sigma}_j\cdot\underline{L}) - (\underline{\sigma}_i\cdot\underline{\sigma}_j)\,L^2 \tag{6.2.7}$$

and $[\delta]$ is a 2x2 unit matrix.

(ii) INTEGRATION OVER COMPLETE VECTORS

We consider first the direct integrations which arise from equations (3.1.14) and (3.1.18) respectively. In fact, we are going to consider the direct integrations from equation (3.1.14) and the results for equation (3.1.18) can be deduced from the results we obtain from equation (3.1.14).

§6.3 DIRECT INTEGRATIONS

The only direct term which gives a non-vanishing contribution after spin summation is given by

$$Qs_{D}{}^{12}_{s-s(r)} = \frac{8M}{5\hbar^2} r \int dr d\Omega \,[\varphi(-1)\chi(1)Y(\Omega)]^* \sum_{\nu} 2(m-2b)_{\nu} \; x$$

$$^{\nu}V_{LL}(12)Qs(12)\,\varphi(-1)\chi(2)Y(\Omega') \frac{1}{r} f_{\ell J(r)} \qquad (6.3.1)$$

Writing the quadratic spin-orbit operator in full, we have

$$Qs_{D}{}^{12}_{s-s(r)} = \frac{8M}{5\hbar^2} r N_S{}^2 \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} 4(m-2b)_{\nu} \frac{LL_U{}^{\nu}_{\kappa}}{1+c^2} \int Y^*_{J\ell M}(1) \; x$$

$$\exp\left[-\frac{\alpha}{2}(3v^2 + \frac{8u^2}{3} + 2\rho^2) - LL_{\mu}{}^{\nu}_{\kappa}\,(\underline{r} - {}^3/_4\,\underline{v})^2\right](\underline{\sigma}_1\cdot\underline{\sigma}_2)\frac{L^2_{12}}{3} \; x$$

$$\sum_{J\ell} Y_{J\ell M}(2) \exp\left[-\frac{\alpha}{2}(3v^2 + \frac{8u^2}{3} + 2\rho^2)\right]\frac{1}{r} f_{\ell Jm(r)} \; d\underline{v}d\underline{u}d\underline{\rho}d\Omega \qquad (6.3.2)$$

where

$$i\underline{L}_{12} = (\underline{r} - {}^3/_4\,\underline{v})\wedge({}^5/_4\,\frac{\partial}{\partial\underline{r}} - \frac{\partial}{\partial\underline{v}}) \qquad (6.3.3)$$

Using the following relations

$$\left.\begin{aligned} \underline{\sigma}_1\chi(\widetilde{13}) &= -\underline{\sigma}_3\chi(\widetilde{13}) \\ \underline{\sigma}_2\chi(\widetilde{23}) &= -\underline{\sigma}_3\chi(\widetilde{23}) \\ (\underline{\sigma}\cdot\underline{\sigma}) &= 3 \end{aligned}\right\} \qquad (6.3.4)$$

we have

$$Qs_{D}{}^{12}_{s-s(r)} = \frac{8M}{5\hbar^2} rN_S^2 \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} 4(m-2b)_\nu \frac{LL_U{}^\nu_\kappa}{1+c^2} \int Y^*_{\ell JM}(1) \times$$

$$\exp\left[-\frac{\alpha}{2}(3v^2 + \frac{8u^2}{3} + 2\rho^2) - {}^{LL}\mu^{\nu}_{\kappa}(\underline{r} - {}^3/4\ \underline{v})^2\right] L_{12}^2 \times$$

$$\sum_{J,\ell} Y_{J\ell M}(2) \exp\left[-\frac{\alpha}{2}(3v^2 + \frac{8u^2}{3} + 2\rho^2)\right] \frac{1}{r} f_{\ell JM}(r)\ d\underline{v}d\underline{u}d\underline{\rho}d\Omega \qquad (6.3.5)$$

Consider the following expressions

$$\int Y^*_{J\ell m}(1) \exp(-\frac{3\alpha}{2}v^2)\ {}^{LL}V_{LL}(12)\ L_{12}^2 \sum_{J,\ell} Y_{J\ell m}(2) \times$$

$$\exp\left(-\frac{3\alpha}{2}v^2\right) f_{\ell Jm(r)}\ d\underline{v}d\Omega \qquad (6.3.6)$$

$$(i)^2 L_{12}^2 \exp(-\frac{3\alpha}{2}v^2)$$

$$= (i)\underline{L}_{12} \cdot \left[{}^5/4(\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{r}} - (\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{v}}\right] \exp(-\frac{3\alpha}{2}v^2)$$

$$= \frac{25}{16}(\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{r}} \cdot (\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{r}} \exp(-\beta v^2) \quad .. \quad A$$

$$+ \frac{5\beta}{2}(\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{r}} \cdot (\underline{r} \wedge \underline{v}) \exp(-\beta v^2) \quad .. \quad B$$

$$- \frac{5}{4}(\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{r}} \cdot (\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{r}} \exp(-\beta v^2) \quad .. \quad C$$

$$- 2\beta(\underline{r} - {}^3/4\ \underline{v}) \wedge \frac{\partial}{\partial \underline{r}} \cdot (\underline{r} \wedge \underline{v}) \exp(-\beta v^2) \quad .. \quad D \qquad (6.3.7)$$

We shall now consider the above expressions term by term.

$$A = \frac{25}{16}\left[(\underline{r} \wedge \frac{\partial}{\partial \underline{r}}) \cdot (\underline{r} \wedge \frac{\partial}{\partial \underline{r}}) - \frac{3}{4}(\underline{r} \wedge \frac{\partial}{\partial \underline{r}}) \cdot (\underline{v} \wedge \frac{\partial}{\partial \underline{r}}) - \frac{3}{4}(\underline{v} \wedge \frac{\partial}{\partial \underline{r}}) \cdot (\underline{r} \wedge \frac{\partial}{\partial \underline{r}}) + \right.$$

$$\left.\frac{9}{16}(\underline{v} \wedge \frac{\partial}{\partial \underline{r}}) \cdot (\underline{v} \wedge \frac{\partial}{\partial \underline{r}})\right] \exp(-\beta v^2)$$

$$= \frac{25}{16}\left[L^2 r(i)^2 - {}^3/4\ (\underline{r} \wedge \frac{\partial}{\partial \underline{r}}) \cdot (\underline{v} \wedge \frac{\partial}{\partial \underline{r}}) - {}^3/4(\underline{v} \wedge \frac{\partial}{\partial \underline{r}}) \cdot (\underline{r} \wedge \frac{\partial}{\partial \underline{r}})\right.$$

$$+ \ {}^{9}/16 \ (\underline{v}\wedge\frac{\partial}{\partial\underline{r}}).(\underline{v}\wedge\frac{\partial}{\partial\underline{r}})\Big] \exp\ (-\beta v^2) \qquad (6.3.8)$$

From equations (6.3.6) and (6.3.8) after $d\underline{v}$ integration, we have

$$A \ \rightarrow \ (\frac{\pi}{\lambda})^{3/2} \ \frac{25}{16}\Big[(i)^2(L^2 r - {}^{3}/4\gamma L^2\underline{r}) - {}^{3}/4 \ \gamma\underline{r}\wedge\frac{\partial}{\partial\underline{r}} \cdot \underline{r}_c\wedge\frac{\partial}{\partial\underline{r}}$$

$$+ \ {}^{9}/16 \ \gamma^2 \ \underline{r}\wedge\frac{\partial}{\partial\underline{r}} \cdot \underline{r}_c\wedge\frac{\partial}{\partial\underline{r}} + {}^{9}/16\lambda \ (\frac{\partial}{\partial\underline{r}})^2\Big] \qquad (6.3.9)$$

Using $(\underline{r}\wedge\frac{\partial}{\partial\underline{r}}).(\underline{r}\wedge\frac{\partial}{\partial\underline{r}}) = (\underline{r}\wedge\frac{\partial}{\partial\underline{r}}).(\underline{r}_c\wedge\frac{\partial}{\partial\underline{r}}) + \underline{r}.\frac{\partial}{\partial\underline{r}} - 3\underline{r}.\frac{\partial}{\partial\underline{r}}$

it follows that

$$(\underline{r}\wedge\frac{\partial}{\partial\underline{r}}).(\underline{r}_c\wedge\frac{\partial}{\partial\underline{r}}) = (\underline{r}\wedge\frac{\partial}{\partial\underline{r}}).(\underline{r}\wedge\frac{\partial}{\partial\underline{r}}) + 2\underline{r}.\frac{\partial}{\partial\underline{r}}$$

$$= (i)^2 \ L^2_{\underline{r}} + 2\underline{r}.\frac{\partial}{\partial\underline{r}} \qquad (6.3.10)$$

Thus

$$A \ \rightarrow \ (\frac{\pi}{\lambda})^{3/2} \ (i)^2 \ \frac{25}{16} \ (1 - {}^{3}/4\gamma)^2 \ L^2_{\underline{r}} - \frac{75}{32} \ \gamma \ \underline{r}.\frac{\partial}{\partial r}$$

$$+ \ 2(\frac{15}{16})^2 \ \gamma^2 \ \underline{r}.\frac{\partial}{\partial\underline{r}} + (\frac{15}{16})^2 \ \frac{1}{\lambda} \ (\frac{\partial}{\partial\underline{r}})^2 \qquad (6.3.11)$$

$$B = \frac{5\beta}{2}\Big[(\underline{r} - {}^{3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{r}} \ .\underline{r}\wedge\underline{v}\Big]\exp(-\beta v^2)$$

$$= \frac{5\beta}{2}\Big[\{r^2\underline{v}.\frac{\partial}{\partial\underline{r}} - \underline{r}.\underline{v} \ \underline{r}.\frac{\partial}{\partial\underline{r}} - 2\underline{r}.\underline{v}\} - \frac{3}{4}\{(\underline{r}.\underline{v})\underline{v}.\frac{\partial}{\partial\underline{r}} -$$

$$v^2\underline{r}.\frac{\partial}{\partial\underline{r}} - 2v^2\}\Big] \exp(-\beta v^2) \qquad (6.3.12)$$

After $d\underline{v}$ integration

$$B \ \rightarrow \ \frac{5\beta}{2}\Big[-2\gamma(1 - \frac{3\gamma}{4})r^2 + \frac{9}{4\lambda} + \frac{3}{4\lambda} \ \underline{r}.\frac{\partial}{\partial\underline{r}} \ \Big](\frac{\pi}{\lambda})^{3/2} \qquad (6.3.13)$$

$$C = - \frac{5}{4}\Big[(\underline{r} - {}^{3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{v}} \cdot (\underline{r} - {}^{3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{r}} \ \Big] \exp(-\beta v^2)$$

$$= -\frac{5}{4}\left[(\underline{r}\underline{r}^{-3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{v}}\cdot(\underline{r}\underline{r}^{-3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{r}} - 2\beta(\underline{r}\underline{r}^{-3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{r}}\cdot(\underline{r}\wedge\underline{v})\right]\exp(-\beta v^2) \quad (6.3.14)$$

$$D = -2\beta\left[(\underline{r}\underline{r}^{-3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{v}}\cdot(\underline{r}\wedge\underline{v})\right]\exp(-\beta v^2)$$

$$= -\left[(\underline{r}\underline{r}^{-3}/4\underline{v})\wedge\frac{\partial}{\partial\underline{v}}\cdot(2\beta\underline{r}\wedge\underline{v}) - (2\beta)^2(\underline{r}\wedge\underline{v})\cdot(\underline{r}\wedge\underline{v})\right]\exp(-\beta v^2) \quad (6.3.15)$$

Thus from C and D, we have

$$C+D \rightarrow \left[\frac{5\beta}{2}\left(\frac{6}{8\lambda}\,\underline{r}\cdot\frac{\partial}{\partial\underline{r}}\right) + 4\beta^2 r^2/\lambda - (1-\underline{r}^{3}/4\gamma)\left(\frac{15}{8}\underline{r}\cdot\frac{\partial}{\partial\underline{r}} + 4\beta r^2\right)\right] \quad (6.3.16)$$

after $d\underline{v}$ integration.

Collecting all terms, the integral becomes

$$Qs\,D^{12}_{s-s(r)} = -\frac{8M}{5\hbar^2}\,N_S{}^2\sum_{\mu=1}^{2}\sum_{\nu=1}^{4}2(m-2b)_\nu\,\frac{LL_U{}^\nu_\mu}{1+c^2}\left(\frac{\pi}{\lambda}\right)^{3/2} x$$

$$\exp\left[-\frac{16\alpha\,LL_\mu{}^\nu_\mu\,r^2}{16\alpha + 3\,LL_\mu{}^\nu_\mu}\right]\int\exp\left[-2\alpha\left(\frac{4}{3}u^2+\rho^2\right)\right]Y^*_{J\ell M}(1)\left[(i)^2 x\right.$$

$$\frac{25}{16}\left(1-\frac{3}{4}\gamma\right)^2 L_r{}^2 + \frac{135\alpha}{16\lambda} - 6\alpha\left(1-\frac{3}{4}\gamma\right)\left(1+\frac{5}{4}\gamma\right)r^2 + \frac{9}{\lambda}\alpha^2 r^2 +$$

$$\left.\frac{15}{8}\left\{\frac{3\alpha}{\lambda} - \left(1+\frac{5}{4}\gamma\right)\left(1-\frac{3}{4}\gamma\right)\right\}\underline{r}\cdot\frac{\partial}{\partial\underline{r}} + \frac{1}{\lambda}\left(\frac{15}{16}\right)^2\left(\frac{\partial}{\partial\underline{r}}\right)^2\right] x$$

$$\sum_{J,\ell} Y_{J\ell M}(2)\,f_{\ell JM(r)}\,du\,d\rho\,d\Omega$$

$$= -\frac{8M}{5\hbar^2}\,r\sum_{\mu=1}^{2}\sum_{\nu=1}^{4}2(m-2b)_\nu\,\frac{LL_U{}^\nu_\mu}{1+c^2}\,P^{3/2}_{LL(\mu)}\exp\left[-P_{LL(\mu)}\,x\right.$$

$$\left.LL_\mu{}^\nu_\mu\,r^2\right]\int Y^*_{J\ell M}(1)\left[(i)^2\,\frac{25}{16}\,(1-\underline{r}^{3}/4\,\gamma)^2\,L^2_{\underline{r}} + \frac{135\alpha}{16\lambda} -\right.$$

$$- 6\alpha(1+\tfrac{5}{4}\gamma)(1-\tfrac{3}{4}\gamma)r^2 + \tfrac{9}{\lambda}\alpha^2 r^2 + \tfrac{15}{8}\{\tfrac{3\alpha}{\lambda} - (1+\tfrac{5}{4}\gamma)\times$$

$$(1-\tfrac{3}{4}\gamma)\}\underline{r}.\frac{\partial}{\partial \underline{r}} + \frac{1}{\lambda}(\tfrac{15}{16})^2(\frac{\partial}{\partial \underline{r}})^2\Big] \sum_{J,\ell} Y_{J\ell M}(2)\, f_{J\ell M}(r)\, \frac{1}{r}\, d\Omega \,. \qquad (6.3.17)$$

where

$$\left.\begin{aligned} \lambda &\equiv {}^3/16\ (16\alpha + 3^{LL}\mu_{\nu}^{\nu}) \\ \gamma &\equiv \frac{4^{LL}\mu_{\nu}^{\nu}}{16\alpha+3^{LL}\mu_{\nu}^{\nu}} \\ P_{LL(\nu)} &\equiv \frac{16\alpha}{16\alpha+3^{LL}\mu_{\nu}^{\nu}} \end{aligned}\right\} \qquad (6.3.18)$$

$$\left.\begin{aligned} \text{Now}\quad L^2 rYf &= fL^2 rY \\ \underline{r}.\frac{\partial}{\partial \underline{r}}\, Yf &= f\underline{r}.\frac{\partial}{\partial \underline{r}}\, Y + Y\underline{r}\,\frac{\partial f}{\partial r} \\ \frac{\partial}{\partial \underline{r}}.\frac{\partial}{\partial \underline{r}}\, Yf &= \frac{\partial}{\partial \underline{r}}.f\,\frac{\partial}{\partial \underline{r}}\, Y + \frac{\partial}{\partial \underline{r}}.\underline{r}\; Y(\frac{1}{r}\,\frac{\partial f}{\partial r}) \\ &= f\,\frac{\partial^2}{\partial r^2}\, Y + \frac{2}{r}\,\frac{\partial f}{\partial r}\, Y + \frac{\partial^2 f}{\partial r^2}\, Y \end{aligned}\right\} \qquad (6.3.19)$$

§ 6.4 THE RADIAL WAVE FUNCTION

We define $F(r) = \frac{1}{r} f(r)$.

Hence

$$\left.\begin{aligned} F'' &= \frac{1}{r} f'' - \frac{2}{r^2} f' + \frac{2}{r^3} f \\ \text{and so} & \\ L^2 rYF &= FL^2 rY \\ (\underline{r}.\frac{\partial}{\partial \underline{r}})YF &= rYF' \\ (\frac{\partial}{\partial \underline{r}})^2 YF &= F\,\frac{\partial^2}{\partial r^2}\, Y + \frac{2}{r}\, YF' + YF'' \end{aligned}\right\} \qquad (6.4.1)$$

Hence

$$
\left.
\begin{aligned}
L^2 rYF &= \ell(\ell+1)\,\frac{1}{r}\,fY \\
(\underline{r}.\frac{\partial}{\partial \underline{r}})YF &= (f' - \frac{1}{r}\,f)Y \\
(\frac{\partial}{\partial \underline{r}})^2\ YF &= \left[\frac{1}{r}\,f'' - \frac{\ell(\ell+1)f}{r^3}\right] Y
\end{aligned}
\right\} \qquad (6.4.2)
$$

Hence the matrix elements of Qs(12) for the direct terms are

$$
{}^{Qs}D^{12}_{s-s(r)} = -\frac{8M}{5\hbar^2} \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(m-2b)_\nu \frac{{}^{LL}U^{\nu}_{\varkappa}}{1+c^2}\ P^{3/2}_{LL(\varkappa)}\ x
$$

$$
\exp\left[-P_{LL(\varkappa)}\ {}^{LL}\mu^{\nu}_{\varkappa}\ r^2\right] \left\{\left[\left\{\frac{25}{16}\left(1-\frac{3}{4}\gamma\right)^2 + \left(\frac{15}{16}\right)^2 \frac{1}{\lambda r^2}\right\} \ell(\ell+1) - \left(\frac{135\alpha}{16\lambda} + 2\sigma r^2 + 2\eta\right)\right] f_{\ell J(r)} + 2\eta r f'_{\ell J(r)} - \left(\frac{15}{16}\right)^2 \frac{1}{\lambda}\, f''_{\ell J(r)}\right\} \qquad (6.4.3)
$$

where

$$
\left.
\begin{aligned}
\sigma &\equiv 3\alpha\left[\frac{3\alpha}{2\lambda} - \left(1+\frac{5}{4}\gamma\right)\left(1-\frac{3}{4}\gamma\right)\right] \\
\eta &\equiv \frac{15}{16}\left[\left(1+\frac{5}{4}\gamma\right)\left(1-\frac{3}{4}\gamma\right) - \frac{3\alpha}{\lambda}\right]
\end{aligned}
\right\} \qquad (6.4.4)
$$

§6.5 THE INDIRECT INTEGRATION

There are ten pairs of the exchange S-S terms. L_{13}, L_{14}, L_{24}, L_{34} and L_{45} vanish either after the spin summations or after the integration over complete vectors. Since $\underline{L}_{14} = \underline{L}_{15}$, $\underline{L}_{24} = \underline{L}_{25}$ and $\underline{L}_{34} = \underline{L}_{35}$ and since $\underline{L}_{13}$ is invariant under the interchange of permutation of 1 and 2, it therefore follows that $\underline{L}_{23}$ must vanish after integration over complete vectors since it does not vanish after spin summations. Thus the only non-vanishing term comes from $\underline{L}_{12}$ and this will be considered fully in this chapter.

The evaluation of the indirect integration will be done in two sections:

(a) for the operator $\underline{L}_{12}^2$ and

(b) for the operator Q_{12}.

(ii) INTEGRATION OVER COMPLETE VECTORS

(a) The doublet indirect term ${}^{Qs}I^{(12)}_{s-s(r)}$ is given by

$$
{}^{Qs}I^{(12)}_{s-s(r)} = \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2} N_S^2 \, r \sum_{\mu=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \frac{LL_U{}^\nu_\mu}{1+c^2} \; x
$$

$$
\int Y^*_{J\ell M}(1) \exp\left[-\alpha/2(3s'^2+8\rho^2/3+2\rho'^2) - {}^{LL}\mu^\nu_\mu \left[\frac{4}{5}(\underline{r}-\underline{r}')\right]^2\right] x
$$

$$
(-3/2)L_{12}^2 \sum_{J,\ell} Y_{J\ell M}(2) \exp\left[-\frac{\alpha}{2}(3s^2+8\rho^2/3+2\rho'^2)\right] x
$$

$$
\frac{1}{r'} f_{\ell J(r')} \, d\underline{r}' d\underline{\rho} d\underline{\rho}' d\Omega \; . \qquad (6.5.1)
$$

THE MATRIX ELEMENTS OF $\underline{L}_{12}^2$

We now write $i\underline{L}_{12} = (\underline{r}-\underline{r}') \wedge \left(\frac{\partial}{\partial \underline{r}} - \frac{\partial}{\partial \underline{r}'}\right)$ (6.5.2)

Consider space coordinates only. We have on the right of the operator $\underline{L}_{12}$ the function:

$$
\exp\left[-\frac{\alpha}{2}(3s^2+8\rho^2/3+2\rho'^2)\right] Y(\Omega') \frac{1}{r'} f(r')
$$

and on its left

$$
\exp\left[-\frac{\alpha}{2}(3s'^2+8\rho^2/3+2\rho'^2) - {}^{LL}\mu^\nu_\mu \, r_{12}^2\right] Y^*(\Omega)
$$

where

$$
\left.\begin{aligned} \underline{s} &= \frac{16}{15}\underline{r} + \frac{4}{15}\underline{r}' \\ \text{and} \\ \underline{s}' &= \frac{4}{15}\underline{r} + \frac{16}{15}\underline{r}' \end{aligned}\right\} \qquad (6.5.3)
$$

Since $i\underline{L}_{12}$ is independent of $\underline{\rho}$ and $\underline{\rho}'$, we can perform the integrations over $\underline{\rho}$ and $\underline{\rho}'$. Thus, we have

$$Qs_{I^{12}_{s-s(r)}} = (\frac{16}{15})^3 \frac{8M}{5\hbar^2} r N_S^2 \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \frac{LL_U{}^\nu_\varkappa}{1+c^2} (\frac{3\pi^2}{16\alpha^2})^{3/2} x$$

$$\int d\underline{r}' d\Omega \exp\left[-\frac{3\alpha}{2} s'^2 - LL_\mu{}^\nu_\varkappa r_{12}^2\right] Y^*(\Omega)\left[-\frac{3}{2} L_{12}^2\right] Y(\Omega') x$$

$$\exp\left[-\frac{3\alpha}{2} s^2\right] \frac{1}{r'} f(r') \qquad (6.5.4)$$

The following steps will be applied in the derivation of the kernel:

(i) Differentiation with respect to $\underline{r}$ on $\exp(-\frac{3\alpha}{2} s^2)$

We have $\underline{s} = \frac{4}{15}(4\underline{r} + \underline{r}')$

We now write

$$\exp(-\frac{3\alpha}{2} s^2) = \exp\left[-\frac{8\alpha}{75}(4\underline{r}+\underline{r}')^2\right]$$

as $\exp[-\nu(4\underline{r}+\underline{r}')^2]$

where $\nu = \frac{8\alpha}{75}$ (6.5.5)

It therefore follows that

$$\frac{\partial}{\partial \underline{r}} \exp[-\nu(4\underline{r}+\underline{r}')^2] = -8\nu(4\underline{r}+\underline{r}') \exp[-\nu(4\underline{r}+\underline{r}')^2]$$

and so $(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}} \exp[-\nu(4\underline{r}+\underline{r}')^2]$

$$= 40\nu(\underline{r}' \wedge \underline{r}) \exp[-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.5.6)$$

(ii) Integration by parts with respect to $\underline{r}'$ (in order to transfer the unknown $f(r')$ to the left of the operator) followed by differentiation with respect to $\underline{r}'$.

Since $\underline{s}' = \frac{4}{15}(\underline{r} + 4\underline{r}')$

and $\underline{r}_{12} = \frac{4}{5}(\underline{r}-\underline{r}')$

we have the following results

$$\frac{\partial}{\partial \underline{r}'} \exp\left[-\frac{3\alpha}{2}s'^2 - LL_{\mu\varkappa}^{\nu} r_{12}^2\right]$$

$$= \frac{\partial}{\partial \underline{r}'} \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2\right]$$

$$= (\eta'\underline{r} + \xi\underline{r}') \exp\left[-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}'^2\right] \qquad (6.5,7)$$

where

$$\left.\begin{aligned} \lambda' &\equiv \frac{16}{25} LL_{\mu\varkappa}^{\nu} \\ \xi &\equiv -2(16\nu + \lambda') \\ \eta' &\equiv -2(4\nu - \lambda') \end{aligned}\right\} \qquad (6.5.8)$$

We thus obtain two operator identities

$$\underline{r} \wedge \frac{\partial}{\partial \underline{r}'} \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2\right]$$

$$= \xi(\underline{r}\wedge\underline{r}') \exp\left[-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2\right] \qquad (6.5.9)$$

and

$$\underline{r}' \wedge \frac{\partial}{\partial \underline{r}'} \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2\right]$$

$$= \eta'(\underline{r}'\wedge \underline{r}) \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2\right] \qquad (6.5.10)$$

The foregoing results for steps (i) and (ii) will now be used (often implicitly) in evaluating the matrix elements of the operators $\underline{L}_{12}^2$ and Q_{12}.

Consider

$$i\underline{L}_{12} \exp\left[-\nu(4\underline{r}+\underline{r}')^2\right] = \left[40\nu\underline{r}'\wedge \underline{r} - (\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}'}\right] \times \exp\left(-\nu(4\underline{r}+\underline{r}')^2\right)$$

$$(i)^2\underline{L}_{12} \exp\left[-\nu(4\underline{r}+\underline{r}')^2\right]$$

$$= \left[40\nu(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}} \cdot(\underline{r}'\wedge \underline{r}\right) \qquad (i)$$

$$-(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}}\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'} \qquad \text{(ii)}$$

$$-40\nu(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\cdot(\underline{r}'\wedge\underline{r}) \qquad \text{(iii)}$$

$$+(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'} \qquad \text{(iv)}$$

$$\ldots]\quad \exp\,[-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.5.11)$$

We now consider the expressions on the r.h.s. of equation (6.5.11) one by one.

$$(i) = 40\nu\,[\,(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}}\cdot(\underline{r}'\wedge\underline{r})]\,\exp\,[-\nu(4\underline{r}+\underline{r}')^2]$$

$$= 40\nu\,[\,40\nu\{r^2r'^2-(\underline{r}.\underline{r}')^2\}+2(\underline{r}.\underline{r}'-r'^2)]\;x$$

$$\exp\,(-\nu(4\underline{r}+\underline{r}')^2) \qquad (6.5.12)$$

We now consider (ii)

$$(ii) = [(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}}\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}]\,\exp\,(-\nu(4\underline{r}+\underline{r}')^2)$$

$$= [-8\nu(4\underline{r}+\underline{r}').\frac{\partial}{\partial\underline{r}'}(\underline{r}-\underline{r}')^2+8\nu\frac{\partial}{\partial\underline{r}'}\cdot(\underline{r}-\underline{r}')(\underline{r}-\underline{r}')\cdot$$

$$(4\underline{r}+\underline{r}'_c)-2\frac{\partial}{\partial\underline{r}'}\cdot(\underline{r}-\underline{r}')]\,\exp\,[-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2]$$

on using Green's Theorem.

$$= [-16\nu(4r^2-3\underline{r}.\underline{r}'-r'^2)-2\{\eta'r^2+(\xi-\eta')\underline{r}.\underline{r}'-\xi r'^2\}+$$

$$6+40\nu(\xi+\eta')\{(\underline{r}.\underline{r}')^2-r^2r'^2\}]\;x$$

$$\exp\,[-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2] \qquad (6.5.13)$$

Consider (iii)

$$(iii) = -40\nu\,[(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\cdot(\underline{r}'\wedge\underline{r})]\,\exp\,[-\nu(4\underline{r}+\underline{r}')^2]$$

Using Green's Theorem, (iii) now becomes

$$40\nu\ [(\underline{r}'\wedge\underline{r}).(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}]\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2]$$

$$= -40\nu\ [(\xi+\eta')(\underline{r}'\wedge\underline{r}).(\underline{r}'\wedge\underline{r})]\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2-$$

$$\lambda'(\underline{r}-\underline{r}')^2\ ]$$

$$= 40\nu(\xi+\eta')\ [(\underline{r}.\underline{r}')^2-r^2r'^2]\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2\ -$$

$$\lambda'(\underline{r}-\underline{r}')^2\ ] \qquad (6.5.14)$$

Consider now the last expression, that is, (iv)

$$(iv) = -\ [(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\ .(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}]\ \exp\ [-\nu(4\underline{r}+\underline{r}')^2]$$

Using Green's Theorem, (iv) becomes

$$(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\ (\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2\ ]$$

$$= -(\xi+\eta')(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\ .(\underline{r}'\wedge\underline{r})\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2\ -$$

$$\lambda'(\underline{r}-\underline{r}')^2\ ]$$

$$= [(\xi+\eta')^2\{r^2r'^2-(\underline{r}.\underline{r}')^2\}+2(\xi+\eta')(r^2-\underline{r}.\underline{r}')\ ]\ x$$

$$\exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2] \qquad (6.5.15)$$

Combining the above four terms, we obtain

$$\{[\ (40\nu)^2\ -\ 80\nu(\xi+\eta')+(\xi+\eta)^2\ ]\ (r^2r'^2-(\underline{r}.\underline{r}')^2\ -\ 64\nu(r^2\ -$$

$$2\underline{r}.\underline{r}'\ +\ r'^2)\ +\ 2\xi(r^2-2\underline{r}.\underline{r}'\ +\ r'^2)\ +\ 6\}\ x$$

$$\exp\ [-\nu(4\underline{r}+\underline{r}')^2-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2\ ] \qquad (6.5.16)$$

§6.6 (iii) INTEGRATION OVER SPHERICAL HARMONICS

As seen above, the $d\Omega d\Omega'$ integration will have a term containing $(\underline{r}.\underline{r}')^2$ which may be dealt with in the same manner as $(\underline{r}.\underline{r}')$.

Using the following relations due to the orthonormality of the Clebsch-Gordon Coefficients

$$\int \sum_M Y_L^M(\Omega)\, \overline{Y}_L^M(\Omega')\, \exp[-\varepsilon \underline{r}.\underline{r}']\, \underline{r}.\underline{r}'\, d\Omega d\Omega'$$

$$= -4\pi \frac{\partial}{\partial \varepsilon} \int \sum_M Y_L^M(\Omega)\, \overline{Y}_L^M(\Omega') \sum_{L=0}^{\infty} \sum_{M=-L}^{L} q_{L(\varepsilon rr')}\, x$$

$$Y_L^M(\Omega)\, \overline{Y}_L^M(\Omega')\, d\Omega d\Omega'$$

$$= -4\pi \frac{\partial}{\partial \varepsilon} q_{\ell(\varepsilon rr')} \qquad (6.6.1)$$

on using the fact that

$$\int \sum_M Y_L^M(\Omega)\, \overline{Y}_L^M(\Omega')\, d\Omega\, \Omega' = \delta_{\ell L}$$

$$q_{\ell(\varepsilon rr')} = i^{\ell} j_{\ell(i\varepsilon rr')} \qquad (6.6.2)$$

where j_ℓ is the spherical Bessel function of order ℓ.

$$\text{Also} \int \sum_M Y_L^M(\Omega)\, \overline{Y}_L^M(\Omega')(\underline{r}.\underline{r}')^2 \exp[-\varepsilon \underline{r}.\underline{r}']\, d\Omega d\Omega'$$

$$= 4\pi \frac{\partial^2}{\partial \varepsilon^2} q_{\ell(\varepsilon rr')} \qquad (6.6.3)$$

Now we define

$$\lambda q_\ell(\lambda) = \vartheta_{\ell+\frac{1}{2}}(\lambda) = i^{\ell} \left(\frac{\pi x}{2i}\right)^{\frac{1}{2}} J_{\ell+\frac{1}{2}}(ix) \qquad (6.6.4)$$

$$\frac{\partial}{\partial \varepsilon} q_{\ell(\varepsilon rr')} = -\frac{1}{\varepsilon}\left[\frac{\ell+1}{\varepsilon rr'} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') + \vartheta_{\ell-\frac{1}{2}}(\varepsilon rr')\right] \qquad (6.6.5)$$

where

$$\vartheta_{\ell-\frac{1}{2}}(\varepsilon rr') = \vartheta_{\ell+3/2}(\varepsilon rr') - \frac{2\ell+1}{\varepsilon rr'} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') \qquad (6.6.6)$$

and so

$$rr' \frac{\partial}{\partial \varepsilon} q_{\ell(\varepsilon rr')} = \frac{1}{\varepsilon}\left[\frac{\ell}{\varepsilon} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') - rr' \vartheta_{\ell+3/2}(\varepsilon rr')\right] \qquad (6.6.7)$$

Similarly we deduce from the last two expressions the following result

$$rr' \frac{\partial^2}{\partial \varepsilon^2} q_{\ell(\varepsilon rr')} = \frac{1}{\varepsilon}\left[\left\{\frac{\ell(\ell-1)}{\varepsilon^2} + r^2 r'^2\right\} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') + \frac{2rr'}{\varepsilon} \vartheta_{\ell+3/2}(\varepsilon rr')\right] \qquad (6.6.8)$$

Hence in general we have

$$\int d\Omega d\Omega' \; Y^*_{\ell,m}(\theta,\varphi)(\underline{r}.\underline{r}')^n \; Y_{\ell' m'}(\theta',\varphi') \exp(-\varepsilon \underline{r}.\underline{r}')$$

$$= \frac{4\pi}{\varepsilon rr'} \; r^n r'^n \; P^n_\varepsilon \; \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') \; \delta\ell\ell' \; \delta mm' \qquad (6.6.9)$$

where

$$r^n r'^n P^n_\varepsilon \; \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') \equiv (-1)^n \varepsilon \frac{d^n}{d\varepsilon^n}\left[\frac{1}{\varepsilon} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr')\right] \qquad (6.6.10)$$

Note that $\frac{d}{d\varepsilon} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') = \frac{\ell+1}{\varepsilon} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') - rr' \vartheta_{\ell+3/2}(\varepsilon rr')$

(6.6.11)

We therefore deduce the following results from the above expressions

$$\left.\begin{aligned} &\text{(i)} \quad \vartheta'_{\ell+\frac{1}{2}}(\lambda) = \frac{\ell+1}{\lambda} \vartheta_{\ell+\frac{1}{2}}(\lambda) - \vartheta_{\ell+3/2}(\lambda) \\ &\text{(ii)} \quad \vartheta''_{\ell+\frac{1}{2}}(\lambda) = \left[\frac{\ell(\ell+1)}{\lambda^2} + 1\right] \vartheta_{\ell+\frac{1}{2}}(\lambda) \text{ etc.} \end{aligned}\right\} \qquad (6.6.12)$$

where $\vartheta'_{\ell+\frac{1}{2}}(x)$ is written for $\frac{d}{dx} \vartheta_{\ell+\frac{1}{2}}(x)$ etc.

Hence the indirect integral of the operator $\underline{L}_{12}$ becomes

$$Qs_{I_{s-s(r)}} L_{12} = \left(\frac{16}{15}\right)^3 \left(\frac{3}{2}\right)^4 \left(\frac{\alpha}{3\pi}\right)^{3/2} \frac{8M}{5h^2} \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \; x$$

$$\frac{LL_{U^\nu_\varkappa}}{1+c^2} \; \frac{75\pi}{4\alpha - 3^{LL}\mu^\nu_\varkappa} \int \left[(6-2\zeta(r^2+r'^2) - \left(\frac{w}{\lambda_{LL(\varkappa)}}\right)^2 \ell(\ell-1) - \right.$$

$$4\zeta \frac{\ell}{\lambda_{LL(\varkappa)}}) \vartheta_{\ell+\frac{1}{2}}(\lambda_{LL(\varkappa)}rr') + 2(2\zeta - \frac{\omega^2}{\lambda_{LL(\varkappa)}})rr' \vartheta_{\ell+3/2} \times$$

$$(\lambda_{LL(\varkappa)}rr')] \exp [- \frac{8}{75} (17\alpha + 6^{LL}\mu_{\varkappa}^{\nu})(r^2+r'^2)] f_{\ell J(r')} dr' \qquad (6.6.13)$$

where

$$\left.\begin{aligned} \omega_{ij} &\equiv \frac{64}{15} (\alpha_i + \alpha_j) \\ \zeta_{ijk} &\equiv \frac{32}{75} (8\alpha_i + 8\alpha_j + 3^{LL}\mu_{\varkappa}^{\nu}) \\ \lambda_{LL(\varkappa)} &\equiv \frac{32}{75} (4\alpha - 3^{LL}\mu_{\varkappa}^{\nu}) \end{aligned}\right\} \qquad (6.6.14)$$

and

$$\alpha_i = \alpha_j = \alpha$$

§6.7 THE MATRIX ELEMENTS OF $Q_{12}(r_{12}^2)$

So far we have been considering the matrix elements of $\underline{L}_{12}$. We shall now consider in this section the matrix elements of Q_{12}. We shall follow the same procedure as in the case of $\underline{L}_{12}$.

Again, we put

$$Q_{12}(\underline{r}_{12}^2) \equiv \tfrac{1}{2}(q_{12} + q_{21}) \qquad (6.7.1)$$

$$i\underline{L}_{12} = (\underline{r}-\underline{r}') \wedge (\frac{\partial}{\partial \underline{r}} - \frac{\partial}{\partial \underline{r}'})$$

$$i\underline{\sigma}_2 \cdot \underline{L}_{12} \exp [-\nu(4\underline{r}+\underline{r}')^2] = [40\nu \underline{\sigma}_2 \cdot \underline{r}' \wedge \underline{r} - \underline{\sigma}_2 \cdot (\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}'}]$$

$$\times \exp [-\nu(4\underline{r}+\underline{r}')^2]$$

Therefore $(i)^2 (\underline{\sigma}_1 \cdot \underline{L}_{12})(\underline{\sigma}_2 \cdot \underline{L}_{12}) \exp [-\nu(4\underline{r}+\underline{r}')^2]$

$$= [40\nu [\underline{\sigma}_1 \cdot (\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}}][\underline{\sigma}_2 \cdot \underline{r}' \wedge \underline{r}] \qquad A_{12}$$

$$+ [\underline{\sigma}_1 \cdot (\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}}][-\underline{\sigma}_2 \cdot (\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}'}] \qquad B_{12}$$

$$+ 40\nu\,[-\underline{\sigma}_1\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}},\,][\,\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r}] \qquad C_{12}$$

$$+ [-\underline{\sigma}_1\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}},\,][-\underline{\sigma}_2\cdot(\underline{r}'\wedge\underline{r})\wedge\frac{\partial}{\partial\underline{r}'},] \qquad D_{12}$$

$$\ldots]\quad \exp\,[-\nu(4\underline{r}+\underline{r}')^2\,] \qquad (6.7.2)$$

Consider the term A_{12}

$$A_{12} = [(40\nu)^2(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})+40\nu(\underline{\sigma}_1\wedge(\underline{r}-\underline{r}'))\cdot(\underline{\sigma}_2\wedge\underline{r}')]\,x$$

$$\exp\,[-\nu(4\underline{r}+\underline{r}')^2]$$

$$= 40\nu\,[40\nu(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})+(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}-\underline{r}')\cdot\underline{r}'-(\underline{\sigma}_1\cdot\underline{r}')$$

$$x\ \underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\,]\exp\,[-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.7.3)$$

Hence

$$\tfrac{1}{2}(A_{12}+A_{21}) = \Big[(40\nu)^2\,\tfrac{1}{2}[(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})+(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})]$$

$$-\ (40\nu)\tfrac{1}{2}[(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r}')+(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\underline{r}')-2(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}.\underline{r}')]$$

$$+\ (40\nu)[(\underline{\sigma}_1\cdot\underline{r}')(\underline{\sigma}_2\cdot\underline{r}')-(\underline{\sigma}_1\cdot\underline{\sigma}_2)r'^2\,]\Big]\ \exp\,[-\nu(4\underline{r}+\underline{r}')^2]$$

$$(6.7.4)$$

$$\text{Put } U_{12} \equiv (\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r}) = U_{21} \qquad (6.7.5)$$

$$T_{12}(\underline{A},\underline{B}) \equiv \tfrac{1}{2}\,[(\underline{\sigma}_1\cdot\underline{A})(\underline{\sigma}_2\cdot\underline{B})+(\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_1\cdot\underline{B})-2(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{A}.\underline{B})]$$

$$= T_{21}(\underline{A},\underline{B}) \qquad (6.7.6)$$

Hence

$$\tfrac{1}{2}(A_{12}+A_{21}) = 40\nu[\,40\nu U_{12}-T_{12}(\underline{r},\underline{r}') + T_{12}(\underline{r}',\underline{r}')]\,x$$

$$\exp\,[-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.7.7)$$

$$B_{12} = \Big[[\,(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}-\underline{r}')\cdot\frac{\partial}{\partial\underline{r}'} - \underline{\sigma}_2\cdot(\underline{r}-\underline{r}')(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}'},)] -$$

$$40\nu(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})\ \underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'} + 8\nu[(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}-\underline{r}')^2 -$$

$$\underline{\sigma}_1\cdot(\underline{r}-\underline{r}')\underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\,]\Big]\ \exp\,[-\nu(4\underline{r}+\underline{r}')^2]$$

$$B_{12} = \Big[[(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}-\underline{r}') \cdot \frac{\partial}{\partial \underline{r}'} - \underline{\sigma}_2\cdot(\underline{r}-\underline{r}')(\underline{\sigma}_1\cdot \frac{\partial}{\partial \underline{r}'})]$$

$$-40\nu(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})\underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}'} + 8\nu\,[(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}-\underline{r}')^2 -$$

$$\underline{\sigma}_1\cdot(\underline{r}-\underline{r}')\underline{\sigma}_2\cdot(\underline{r}-\underline{r}')]\Big]\exp[-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.7.8)$$

Hence $\frac{1}{2}(B_{12}+B_{21}) = \Big[T_{12}(\underline{r}',\frac{\partial}{\partial \underline{r}'}) - T_{12}(\underline{r},\frac{\partial}{\partial \underline{r}'}) +$

$$8\nu\,[2T_{12}(\underline{r},\underline{r}')-T_{12}(\underline{r},\underline{r})-T_{12}(\underline{r}',\underline{r}')] - 40\nu\tfrac{1}{2}[(\underline{\sigma}_1\cdot$$

$$\underline{r}'\wedge\underline{r})\ \underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}'} + \underline{\sigma}_2\cdot(\underline{r}'\wedge\underline{r})\underline{\sigma}_1\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}'}]\Big] \ x$$

$$\exp\,[-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.7.9)$$

$$C_{12} = \Big[-40\nu(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})\underline{\sigma}_1\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}'} + 40\nu(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}-\underline{r}')\cdot$$

$$\underline{r}-(\underline{\sigma}_1\cdot\underline{r})\underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\Big]\exp\,(-\nu(4\underline{r}+\underline{r}')^2) \qquad (6.7.10)$$

Therefore

$$\tfrac{1}{2}(C_{12}+C_{21}) = 40\nu\tfrac{1}{2}\Big[\{(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}) + (\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})\ x$$

$$(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})\}-\{(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})+(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})\ x$$

$$(\underline{\sigma}_2\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})\}\Big]\exp\,[-\nu(4\underline{r}+\underline{r}')^2] +40\nu\,[T_{12}(\underline{r},\underline{r}') -$$

$$T_{12}(\underline{r},\underline{r})]\ \exp\,[-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.7.11)$$

$$\tfrac{1}{2}(D_{12}+D_{21}) = \tfrac{1}{2}\Big[(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_2\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})+(\underline{\sigma}_2\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})$$

D_1

$$+(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})+(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})\ x$$

$$(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}) \qquad D_2$$

$$-\{(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})+(\underline{\sigma}_2\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})\ x$$

$$(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})\} \qquad D_3$$

$$-\{(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})(\underline{\sigma}_2\cdot\underline{r}\wedge\frac{\partial}{\partial\underline{r}'})+(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial\underline{r}'})\} \qquad D_4$$

$$\ldots\ ]\ \exp\ [-\nu(4\underline{r}+\underline{r}')^2] \qquad (6.7.12)$$

By using Green's Theorem, B, C and D will operate on

$$\exp\ [-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2]$$

$$\frac{\partial}{\partial\underline{r}'},\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2]$$

$$= (\xi\underline{r}' + \eta\underline{r})\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2]$$

$$\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'},\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2]$$

$$= \eta(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2]$$

Hence

$$\exp\ [\nu(\underline{r}+4\underline{r}')^2+\lambda'(\underline{r}-\underline{r}')^2]\ (\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})\ x$$

$$\exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2]$$

$$= \eta^2(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})-\eta\{(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\underline{r}')-(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r}')\}$$

Thus $\exp[\nu(\underline{r}+4\underline{r}')^2+\lambda'(\underline{r}-\underline{r}')^2]\ D_2\ \exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2]$

$$= \eta^2U_{12} + \eta T_{12}(\underline{r},\underline{r}') \qquad (6.7.13)$$

Consider

$$\exp\ [\nu(\underline{r}+4\underline{r}')^2+\lambda'(\underline{r}-\underline{r}')^2]\ (\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial\underline{r}'})(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})\ x$$

$$\exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2\ ]$$

$$= -\eta\xi(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})-\eta\{(\underline{\sigma}_1\cdot\underline{\sigma}_2)r^2-(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r})\}$$

Hence

$$\exp\ [\nu(\underline{r}+4\underline{r}')^2+\lambda'(\underline{r}-\underline{r}')^2]\ D_3\exp\ [-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2]$$

$$= -\eta\xi U_{12} + \eta T_{12}(\underline{r},\underline{r}) \qquad (6.7.14)$$

We now consider

$$\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}'} \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2 \right]$$

$$= \xi(\underline{\sigma}_2 \cdot \underline{r} \wedge \underline{r}') \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2 \right]$$

Hence

$$\exp\left[\nu(\underline{r}+4\underline{r}')^2 + \lambda'(\underline{r}-\underline{r}')^2 \right] (\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}'}) \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2 \right]$$

$$= \xi^2 (\underline{\sigma}_1 \cdot \underline{r}' \wedge \underline{r})(\underline{\sigma}_2 \cdot \underline{r}' \wedge \underline{r}) + \xi\{(\underline{\sigma}_1 \cdot \underline{\sigma}_2) r^2 - (\underline{\sigma}_1 \cdot \underline{r})(\underline{\sigma}_2 \cdot \underline{r})\}$$

and so we have

$$\exp\left[\nu(\underline{r}+4\underline{r})^2 + \lambda'(\underline{r}-\underline{r}')^2 \right] D_1 \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2 \right]$$

$$= \xi^2 U_{12} - \xi T_{12}(\underline{r},\underline{r}) \qquad (6.7.15)$$

We now consider the last expression, viz.

$$\exp\left[\nu(\underline{r}+4\underline{r}')^2 + \lambda'(\underline{r}-\underline{r}')^2 \right] (\underline{\sigma}_1 \cdot \underline{r}' \wedge \frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}'}) \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2 \right]$$

$$= -\xi\eta(\underline{\sigma}_1 \cdot \underline{r}' \wedge \underline{r})(\underline{\sigma}_2 \cdot \underline{r}' \wedge \underline{r}) + \xi\{(\underline{\sigma}_1 \cdot \underline{\sigma}_2)(\underline{r} \cdot \underline{r}') - (\underline{\sigma}_1 \cdot \underline{r})(\underline{\sigma}_2 \cdot \underline{r}')\}$$

Thus

$$\exp\left[\nu(\underline{r}+4\underline{r}')^2 + \lambda'(\underline{r}-\underline{r}')^2 \right] D_4 \exp\left[-\nu(\underline{r}+4\underline{r}')^2 - \lambda'(\underline{r}-\underline{r}')^2 \right]$$

$$= -\xi\eta U_{12} - \xi T_{12}(\underline{r},\underline{r}') \qquad (6.7.16)$$

Hence by Green's Theorem we have

$$\tfrac{1}{2}(D_{12}+D_{21}) \rightarrow (\xi+\eta)^2 U_{12} + (\xi+\eta)\left[T_{12}(\underline{r},\underline{r}') - T_{12}(\underline{r},\underline{r}) \right] \qquad (6.7.17)$$

Before we collect terms we need a third step to evaluate the integral

$$IU_{12} = \int r d\underline{r}' d\Omega \exp -[\varkappa(r^2+r'^2)-\lambda_{LL}(\underline{r}\cdot\underline{r}')] Y^*(\Omega)\chi(1) \times$$

$$U_{12}(\underline{r},\underline{r}')\chi(2)Y(\Omega) \frac{1}{r'} f_{\ell J(r')}$$

By simple differentiation we obtain the following identities

$$(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'}) \exp[-\varkappa(r^2+r'^2)-\lambda_{LL}(\underline{r}.\underline{r}')]$$

$$= [\lambda_{LL}^2(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})+\lambda_{LL}(\underline{\sigma}_1\wedge\underline{r}').(\underline{\sigma}_2\wedge\underline{r})] \times$$

$$\exp[-\varkappa^2(r^2+r'^2)-\lambda_{LL}(\underline{r}.\underline{r}')]$$

Hence

$$U_{12} \exp[-\varkappa(r^2+r'^2)-\lambda_{LL}\underline{r}.\underline{r}']$$

$$= \left[\frac{1}{\lambda_{LL}^2}\{(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})+(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'}) \times\right.$$

$$\left.(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial\underline{r}'})\} + \frac{1}{\lambda_{LL}} T_{12}(\underline{r},\underline{r}')\right] \exp[-\varkappa(r^2+r'^2) -$$

$$\lambda_{LL}\ \underline{r}.\underline{r}']$$

We now rearrange the integrand of $IU_{12}(r)$ so that we may apply Green's Theorem.

Thus

$$IU_{12} = r\int d\underline{r}' d\Omega \exp[-\varkappa(r^2+r'^2)-\lambda_{LL}\ \underline{r}.\underline{r}'] Y^*(\Omega)\chi(1) \times$$

$$\left[-\frac{1}{\lambda_{LL}^2} Q_{12}(r^2) + \frac{1}{\lambda_{LL}} T_{12}(\underline{r},\underline{r}')\right] \chi(2)Y(\Omega') \frac{1}{r'} \times$$

$$f_{\ell J(r')}$$

Hence, using $T_{12}(\underline{A},\underline{B}) = \frac{1}{3} S_{12}(\underline{A},\underline{B}) - \frac{2}{3} (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{A}.\underline{B})$

IU_{12} reduces to

$$IU_{12} = r \int d\underline{r}' d\Omega \exp[-\varkappa(r^2+r'^2)-\lambda_{LL}\ \underline{r}.\underline{r}'] Y^*(\Omega)\chi(1) \times$$

$$\left[-\frac{1}{\lambda_{LL}^2} Q_{12}(r'^2)+\frac{1}{3\lambda_{LL}} S_{12}(\underline{r},\underline{r}') - \frac{2}{3}\lambda_{LL}(\underline{\sigma}_1\cdot\underline{\sigma}_2)\right.$$

$$\left.\times (\underline{r}.\underline{r}')\right] \chi(2)Y(\Omega') \frac{1}{r'} f_{\ell J(r')} \qquad (6.7.18)$$

Now consider the expression for $\frac{1}{2}(B_{12}+B_{21})$

$$\int \exp\left[-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2\right] \tfrac{1}{2}(B_{12}+B_{21}) \exp\left[-\nu(4\underline{r}+\underline{r}')^2\right] x$$

$$Y(\theta',\varphi')\, f(r')\, d\underline{r}'$$

$$= \int \exp\left[-\nu(4\underline{r}+\underline{r}')^2\right] Y(\theta',\varphi')\, f(r') \left[-T_{12}(\frac{\partial}{\partial \underline{r}'},\underline{r}') + T_{12}(\underline{r},\frac{\partial}{\partial \underline{r}'}) + 8\nu\{2T_{12}(\underline{r},\underline{r}')-T_{12}(r^2)-T_{12}(r'^2)\} + (40\nu)\tfrac{1}{2}\{\underline{\sigma}_2\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}'},\ (\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})+\underline{\sigma}_1\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}'}\ x\ (\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})\}\right] \exp\left[-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2\right] d\underline{r}'$$

$$= \int \exp\left[-\varkappa(r^2+r'^2)-\lambda_{LL}\,\underline{r}.\underline{r}'\right]\left[-40\nu(\xi+\eta)U_{12}+(32\nu+\eta)\ x\right.$$

$$\left. T_{12}(r^2)-(8\nu+\xi)T_{12}(r'^2)+2(\underline{\sigma}_1\cdot\underline{\sigma}_2)-(24\nu-\xi+\eta)T_{12}(\underline{r},\underline{r}')\right] x$$

$$Y(\theta',\varphi')f(r')\, d\underline{r}' \qquad (6.7.19)$$

Further consider

$$\int \exp\left[-\nu(\underline{r}+4\underline{r}')-\lambda'(\underline{r}-\underline{r}')^2\right] \tfrac{1}{2}\left[C_{12}+C_{21}\right] \exp\left[-\nu(4\underline{r}+\underline{r}')^2\right] x$$

$$Y(\theta',\varphi')f(r')\, d\underline{r}'$$

$$= \int \exp\left[-\nu(4\underline{r}+\underline{r}')^2\right] Y(\theta'\varphi')f(r') \left[40\nu\{T_{12}(\underline{r},\underline{r}') - T_{12}(r^2)\} -(40\nu)\tfrac{1}{2}\{(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}})+(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})\ x\ (\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})-(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})-(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})\}\right.$$

$$-(40\nu)\tfrac{1}{2}\{(\underline{\sigma}_1\wedge\underline{r}').(-\underline{\sigma}_2\wedge\underline{r})+(\underline{\sigma}_2\wedge\underline{r}').(-\underline{\sigma}_1\wedge\underline{r})-(\underline{\sigma}_1\wedge\underline{r}).$$

$$\left.(-\underline{\sigma}_2\wedge\underline{r})-(\underline{\sigma}_2\wedge\underline{r}).(-\underline{\sigma}_1\wedge\underline{r})\}\right] \exp\left[-\nu(\underline{r}+4\underline{r}')^2-\lambda'(\underline{r}-\underline{r}')^2\right]$$

$$x\ d\underline{r}'$$

$$= \int \exp\left[-\varkappa(r^2+r'^2)-\lambda_{LL}\,\underline{r}.\underline{r}'\right] Y(\theta',\varphi')\, f(r')\, d\underline{r}' \times$$

$$\{-40\nu(\xi+\eta)U_{12}\} \qquad (6.7.20)$$

On collecting terms we obtain the indirect term of Q_{12}, viz.

$$^{LL}_{I}Q_{12} = -\left(\frac{16}{15}\right)^3 N_S^2\, \frac{8M}{5\hbar^2}\, \left(\frac{3}{2}\right)^4 \left(\frac{\pi}{2\alpha}\right)^{3/2} \left(\frac{\pi}{6\alpha}\right)^{3/2} \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \times$$

$$\frac{^{LL}U_\varkappa^\nu}{1+c^2} \int \exp\left[-{}^{8}/_{75}\,(17\alpha+6\,{}^{LL}\mu_\varkappa^\nu)(r^2+r'^2)-\lambda_{LL}\underline{r}.\underline{r}'\right] \times$$

$$Y^*(\Omega)\chi(1)\,\left[\{(40\nu)^2-80\nu(\xi+\eta)+(\xi+\eta)^2\}\, U_{12}+2(\underline{\sigma}_1.\underline{\sigma}_2)\,+\right.$$

$$\{(32\nu+\eta)-(\xi+\eta)\}\, T_{12}(r^2)-2(32\nu-\xi)\, T_{12}(\underline{r},\underline{r}')+(32\nu-\xi) \times$$

$$\left. T_{12}(r'^2)\right] \sum_{J,\ell} Y(\Omega')\chi(2)\, f_{\ell J(r')}\, rr'\, dr'd\Omega d\Omega'$$

$$= -\left(\frac{16}{15}\right)^3 \left(\frac{3}{2}\right)^4 \frac{8M}{5\hbar^2} \left(\frac{\pi}{2\alpha}\right)^{3/2} \left(\frac{\pi}{6\alpha}\right)^{3/2} N_S^2 \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \times$$

$$\frac{^{LL}U_\varkappa^\nu}{1+c^2} \int \exp\left[-\varkappa(r^2+r'^2)-\lambda_{LL}\,\underline{r}.\underline{r}'\right] Y(\Omega)\chi(1) \times$$

$$\left[\left(\frac{64}{15}\right)^2 (\alpha_i+\alpha_j)^3\, U_{12} + \frac{32}{75}\,(8\alpha_i+8\alpha_j+3\,{}^{LL}\mu_\varkappa^\nu)(T_{12}(r^2)\,-\right.$$

$$\left. 2T_{12}(\underline{r},\underline{r}') + T_{12}(r'^2))+6\right] \sum_{J,\ell} Y(\Omega')\chi(2) f_{\ell Jm(r')} \times$$

$$rr'dr'd\Omega d\Omega' \qquad (6.7.21)$$

The above integrand reduces to the following expression on using the result:

$$U_{12} \exp\left[-\varkappa(r^2+r'^2)-\lambda_{LL}\,\underline{r}.\underline{r}'\right]$$

$$= \left[-\frac{1}{\lambda_{LL}^2}\, Q_{12}(r'^2) + \frac{1}{3\lambda_{LL}}\, S_{12}(\underline{r},\underline{r}') - \frac{2}{3\lambda_{LL}}\,(\underline{\sigma}_1.\underline{\sigma}_2) \times\right.$$

$$\left.(\underline{r}.\underline{r}')\right] \exp\left[-\varkappa(r^2+r'^2)-\lambda_{LL}(\underline{r}.\underline{r}')\right]$$

Thus

$$LL_{IQ_{12}} = -\left(\frac{16}{15}\right)^3 \left(\frac{3}{2}\right)^4 \frac{8M}{5\hbar^2} \left(\frac{4\alpha}{3\pi}\right)^{3/2} \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \frac{LL_{U}{}^{\nu}_{\varkappa}}{1+c^2} \times$$

$$\int \exp\left[-\varkappa_{LL}(r^2+r'^2)-\lambda_{LL}(\underline{r}.\underline{r}')\right] Y(\Omega)\chi(1) \left[\ \right]_Q \times$$

$$\sum_{J,\ell} Y(\Omega')\chi(2)\, f_{\ell JM(r')}\, rr'\, dr'\, d\Omega d\Omega' \qquad (6.7.22)$$

where $\left[\ \right]_Q = -\frac{\omega^2}{\lambda_{LL}^2} Q_{12}(r'^2) + \frac{1}{3}\zeta \{S_{12}(r^2)+S_{12}(r'^2)\}$

$$+ \frac{1}{3}\left(\frac{\omega^2}{\lambda_{LL}} - 2\zeta\right) S_{12}(\underline{r},\underline{r}') - 2\zeta(r^2+r'^2)$$

$$- 2\left(\frac{\omega^2}{\lambda_{LL}} - 2\zeta\right)\underline{r}.\underline{r}' + 6. \qquad (6.7.23)$$

§6.8 (iii) INTEGRATION OVER SPHERICAL HARMONICS

Using the relations given in §6.1 and in §6.6, the indirect integral of the operator Q_{12} becomes finally

$$LL_{I^{Q_{12}}_{s-s(r)}} = \left(\frac{16}{15}\right)\left(\frac{3}{2}\right)^3 \frac{8M}{5\hbar^2}\, 4\left(\frac{\alpha}{3\pi}\right)^{3/2} \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \times$$

$$\frac{4\pi}{\lambda_{LL}} \frac{LL_{U}{}^{\nu}_{\varkappa}}{1+c^2} \int dr' \exp\left[-\varkappa_{LL}(r^2+r'^2)\right]\Big[\{6-2\zeta(r^2+r'^2) -$$

$$\left(\frac{\omega}{\lambda_{LL}}\right)^2 \ell(\ell-1)-4\zeta\frac{\ell}{\lambda_{LL}} \} \vartheta_{\ell+\frac{1}{2}}(\lambda_{LL}\, rr') +$$

$$2\left(2\zeta - \frac{\omega^2}{\lambda_{LL}}\right) rr'\, \vartheta_{\ell+3/2}(\lambda_{LL}\, rr')\Big] f_{\ell J(r')} \qquad (6.8.1)$$

§6.9 (iv) FINAL RESULTS

The indirect term of $L_{12} \equiv (\underline{\sigma}_1.\underline{\sigma}_2)L^2 - Q_{12}$ is

$$Qs_{I^{12}_{s-s(r)}} = \left(\frac{16}{15}\right)^3 \left(\frac{3}{2}\right)^3 \left(\frac{\alpha}{3\pi}\right)^{3/2} \frac{8M}{5\hbar^2} \sum_{\varkappa=1}^{2} \sum_{\nu=1}^{4} 2(w-2h)_\nu \times$$

$$\frac{{}^{LL}U_{\kappa}^{\nu}}{1+c^2}\ \frac{75\pi}{4\alpha-3\,{}^{LL}\mu_{\kappa}^{\nu}}\ \int \exp\left[-\kappa_{LL}(r^2+r'^2)\right]\Big[\{6-2\zeta(r^2+r'^2)\ -$$

$$\left(\frac{\omega}{\lambda_{LL}}\right)^2\ \ell(\ell-1)-\ 4\zeta\ \frac{\ell}{\lambda_{LL}}\ \}\ \vartheta_{\ell+\frac{1}{2}}(\lambda_{LL}rr')+2(2\zeta-\ \frac{\omega^2}{\lambda_{LL}})rr'\ x$$

$$\vartheta_{\ell+3/2}(\lambda_{LL}rr')\Big]\ f_{\ell J}(r')\ dr' \qquad (6.9.1)$$

where $\kappa_{LL}(\kappa)\ \equiv\ \frac{8}{75}\ (17\alpha\ +\ 6\,{}^{LL}\mu_{\kappa}^{\nu})$ (6.9.2)

CHAPTER VII

THE ENERGY TERMS (S-S INTERACTION

§7.1 THE N-KERNEL

This kernel is given by the following expression:

$$N_{ss(r)} = -2\left(\frac{16}{15}\right)^3 r\varkappa^2 \int d\underline{r}'\, d\Omega Y^*(\Omega)\chi^*(-1)\ \varphi^*(\underline{s}',\underline{\rho},\underline{\rho}')\ x$$

$$\varphi(\underline{s},\underline{\rho},\underline{\rho}')\chi(-2)Y(\Omega')\ \frac{1}{r'}\ f_{\ell J(r')}$$

where

$$\varkappa^2 = \frac{8M}{5\hbar^2}\ (E_n+E_\alpha)$$

$$\underline{s} = \frac{4}{15}\ (4\underline{r}+\underline{r}'); \qquad \underline{s}' = \frac{4}{15}\ (\underline{r}+4\underline{r}') \quad \text{and}$$

$$\chi^*(-1)\chi(-2) = -\tfrac{1}{2}.$$

The above kernel is easily evaluated and the final result is given by

$$N_{s-s(r)} = \frac{1}{1+c^2}\ \frac{128}{15}\ \left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}}\ \varkappa^2 \int \exp\left[-\frac{136\alpha}{75}\ (r^2+r'^2)\right] x$$

$$\vartheta_{\ell+\frac{1}{2}}\ (\varepsilon rr')\ f_{\ell J(r')}\ dr'$$

Thus

$$N(r,r') = \frac{1}{1+c^2}\ \frac{128}{15}\ \left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}}\ \varkappa^2 \int \exp\left[-\frac{136\alpha}{75}\ (r^2+r'^2)\right] x$$

$$\vartheta_{\ell+\frac{1}{2}}(\varepsilon rr')\ f_{\ell J(r')}\ dr' \qquad (7.1.1)$$

§7.2 THE KINETIC ENERGY KERNELS

These kernels are given by the following expression:

$$S_{s-s(r)} = -2r \int \varphi^*(-1)\left[\ \nabla^2_{1-2345} + \frac{16}{15}\ \nabla^2_{2-345} + \frac{6}{5}\ \nabla^2_{3-45} +\right.$$

$$\frac{8}{5}\nabla^2_{45}\Big]\varphi(-2)\frac{1}{r'}f_{\ell J(r')}\,d\underline{r}'$$

Consider ∇^2_{1-2345} and ∇^2_{2-345}.

Since the above kernel is symmetrical in the spatial coordinates of the particles 1 and 2 as shown by the T operator identities in Chapter I, we have

$$\nabla^2_{1-2345}+\nabla^2_{2-345}=\nabla^2_{2-1345}+\nabla^2_{1-345}$$

$$=\tfrac{1}{2}\left[\nabla^2_{1-2345}+\nabla^2_{2-1345}\right]+\tfrac{1}{2}\left[\nabla^2_{1-345}+\nabla^2_{2-345}\right] \qquad (7.2.1)$$

Consider

$$\int\varphi^*(-1)\varphi(-2)\nabla^2\underline{r}F(r')\,d\tau_{-1}$$

$$=\iiint\varphi^*(\underline{s}',\underline{\rho},\underline{\rho}')\,\varphi(\underline{s},\underline{\rho},\underline{\rho}')\,\nabla^2\underline{r}F(r')\,d\underline{s}'\,d\underline{\rho}\,d\underline{\rho}'$$

$$=\left(\frac{16}{15}\right)^3\iiint\varphi^*(\underline{s}',\underline{\rho},\underline{\rho}')\varphi(\underline{s},\underline{\rho},\underline{\rho}')\,\nabla^2\underline{r}\,F(r')\,d\underline{r}'\,d\underline{\rho}\,d\underline{\rho}' \qquad (7.2.2)$$

Using Green's Theorem, the above integral becomes

$$\left(\frac{16}{15}\right)^3\iiint F(r')\,\nabla^2\underline{r}\left\{\varphi\left(\frac{16\underline{r}'}{15}+\frac{4}{15}\underline{r},\underline{\rho},\underline{\rho}'\right)\varphi\left(\frac{16}{15}\underline{r}+\frac{4}{15}\underline{r}',\underline{\rho},\underline{\rho}\right)\right\}$$

$$\times\,d\underline{r}'\,d\underline{\rho}\,d\underline{\rho}'$$

$$=\left(\frac{16}{15}\right)^3\iiint F(r')\left[\left(\frac{16}{15}\right)^2\nabla^2\underline{s}'\varphi(\underline{s}',\underline{\rho},\underline{\rho}')\,\varphi(\underline{s},\underline{\rho},\underline{\rho}')+\right.$$

$$\frac{1}{16}\left(\frac{16}{15}\right)^2\nabla^2\underline{s}\,\varphi(\underline{s},\underline{\rho},\underline{\rho}')\,\varphi(\underline{s}',\underline{\rho},\underline{\rho}')+\frac{1}{2}\left(\frac{16}{15}\right)^2\nabla_{\underline{s}}\varphi(\underline{s}',\underline{\rho},\underline{\rho}')$$

$$\left.\cdot\,\nabla_{\underline{s}}\,\varphi(\underline{s},\underline{\rho},\underline{\rho}')\right]d\underline{r}'\,d\underline{\rho}\,d\underline{\rho}' \qquad (7.2.3)$$

Similarly

$$-r\left(\frac{16}{15}\right)^4\int\varphi^*(\underline{s}',\underline{\rho},\underline{\rho}')\,\nabla^2_{1-345}\,\varphi(\underline{s},\underline{\rho},\underline{\rho}')\,d\underline{r}'\,d\underline{\rho}\,d\underline{\rho}'$$

$$=-r\left(\frac{16}{15}\right)^4\int\varphi^*(\underline{s}',\underline{\rho},\underline{\rho}')\,\nabla^2\underline{s}\,\varphi(\underline{s},\underline{\rho},\underline{\rho}')\,d\underline{r}'\,d\underline{\rho}\,d\underline{\rho}' \qquad (7.2.4)$$

Thus $- \int [\, \varphi^*(-1)\varphi(-2)\ \nabla^2_{\underline{r}} + \frac{16}{15}\, \varphi^*(-1)\varphi(2)\ \nabla^2_{\underline{s}}\,]\, d\tau_{-1}$

$= -(\frac{16}{15})^5 \iiint F(r')\, [\nabla^2_{\underline{s}'} \varphi(\underline{s}', \underline{\rho}, \underline{\rho}')\varphi(\underline{s}, \underline{\rho}, \underline{\rho}') +$

$\nabla^2_{\underline{s}}\, \varphi(\underline{s}, \underline{\rho}, \underline{\rho}')\ \varphi(\underline{s}', \underline{\rho}, \underline{\rho}') + \frac{1}{2}\nabla_{\underline{s}'}\ \varphi(\underline{s}', \underline{\rho}, \underline{\rho}')\ .$

$\nabla_{\underline{s}}\ \varphi(\underline{s}, \underline{\rho}, \underline{\rho}')]\ d\underline{r}'\ d\underline{\rho}\ d\underline{\rho}'$

$= -\frac{1}{1+c^2}\ \frac{1}{2}(\frac{16}{15})^5\ (\frac{3\alpha}{\pi})^{3/2}\ (3\alpha)^2 \int \int \exp\Big[-\frac{3\alpha}{2}\ (s^2+s'^2)\Big]$

$x\, [\, s^2+s'^2+ \tfrac{1}{2}\underline{s}.\underline{s}' - 2/\alpha]\ f_{\ell J(r')}\ rr'\ dr' \qquad (7.2.5)$

$s^2+s'^2+ \tfrac{1}{2}\underline{s}.\underline{s}' = (\frac{4}{15})^2\, [19(r^2+r'^2) + \frac{49}{2}\ \underline{r}.\underline{r}'\,] \qquad (7.2.6)$

Thus equation (7.2.5) becomes

$-\frac{1}{1+c^2}\ \frac{1}{2}\ (\frac{16}{15})^5\ (\frac{3\alpha}{\pi})^{3/2}\ (3\alpha)^2 \int \Big[(\frac{4}{15})^2 \{19(r^2+r'^2) + \frac{49}{2}\ \underline{r}.\underline{r}'\}$

$- \frac{2}{\alpha}\ \Big] \exp\Big[-\frac{136\alpha}{75}\ (r^2+r'^2) - \frac{128\alpha}{75}\ \underline{r}.\underline{r}'\Big]\ x$

$f_{\ell J(r')}\ rr'\ dr' \qquad (7.2.7)$

$= \frac{1}{1+c^2}\ \frac{16}{15}\ (\frac{3\alpha}{\pi})^{\frac{1}{2}}\ \varepsilon^2 \int [\{19(r^2+r'^2) - \frac{1}{\varepsilon}\ (\frac{49\ell}{2} + 48)\}$

$x\ \vartheta_{\ell+\frac{1}{2}}\ (\varepsilon rr') + \frac{49}{2}\ rr'\ \vartheta_{\ell+3/2}\ (\varepsilon rr')\,]\, f_{\ell J(r')}\ dr'$

$(7.2.8)$

Similarly

$-r \int \varphi^*(-1)\ [\nabla^2_{2-1345} + \nabla^2_{2-345}]\ \varphi(-2)\ F(r')\ d\tau_{-1}$

$= \frac{1}{1+c^2}\ (\frac{16}{15})(\frac{3\alpha}{\pi})^{\frac{1}{2}}\ \varepsilon^2 \int \Big[\{19(r^2+r'^2) - \frac{1}{\varepsilon}\ (\frac{49\ell}{2} + 48)\}$

$x\ \vartheta_{\ell+\frac{1}{2}}\ (\varepsilon rr') + \frac{49rr'}{2}\ \vartheta_{\ell+3/2}\ (\varepsilon rr')\Big]\ f_{\ell J(r')}\ dr'$

$(7.2.9)$

Hence

$$-2r \int \varphi^*(-1)\ \tfrac{1}{2}\left[\left(\nabla^2_{1-2345} + \nabla^2_{2-1345}\right) + \left(\tfrac{16}{15}\right)\left(\nabla^2_{1-345} + \nabla^2_{2-345}\right)\right] \times$$

$$\varphi(-2)\ F(r')\ d\tau_{-1}$$

$$= \frac{1}{1+c^2}\left(\frac{16}{15}\right)\left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}} \varepsilon^2 \int \left[\left\{38(r^2+r'^2) - \frac{1}{\varepsilon}(49\ell + 96)\right\} \times \right.$$

$$\left. \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') + 49rr'\ \vartheta_{\ell+3/2}(\varepsilon rr')\right] f_{\ell J(r')}\ dr' \qquad (7.2.10)$$

We consider finally the last expression which is given by

$$-2r \int \varphi^*(-1)\left[\frac{6}{5}\ \nabla^2_{3-45} + \frac{8}{5}\ \nabla^2_{45}\right] \varphi(-2) F(r') d\tau_{-1} \qquad (7.2.11)$$

The above integral (7.2.11) can easily be evaluated and the result is

$$-\frac{1}{1+c^2}\left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}} 48\varepsilon \int \exp\left[-\frac{136\alpha}{75}(r^2+r'^2)\right] \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') \times$$

$$f_{\ell J(r')}\ dr' \qquad (7.2.12)$$

Thus the S(r,r') kernel is given by

$$S(r,r') = \frac{1}{1+c^2}\left(\frac{16}{15}\right)\left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}} \varepsilon^2 \exp\left[-\frac{136\alpha}{75}(r^2+r'^2)\right] \times$$

$$\left[\left\{38(r^2+r'^2) - \frac{1}{\varepsilon}(49\ell + 141)\right\} \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr') + \right.$$

$$\left. 49rr'\ \vartheta_{\ell+3/2}(\varepsilon rr')\right] \qquad (7.2.13)$$

where

$$\varepsilon \equiv \frac{128\alpha}{75} \qquad (7.2.14)$$

CHAPTER VIII (A)

THE TENSOR FORCE TERMS: (S-D INTERACTION)

§ 8.1 FORMULATION

Several workers including Dancoff (1940), Feingold (1956), Sugie et al. (1957), S. Nagata et al. (1959), and H Kanada et al. (1963) have investigated the effect of the tensor force on the doublet splitting of N-He^4. Dancoff (1940) estimated the splitting using second order perturbation theory and thereby treating He^5 as a bound system. His results showed that the two P-states form a close normal doublet which is in disagreement with experiment. Feingold (1956) included the tensor force in a variational perturbational manner. He too treated He^5 as a bound system. He found that the splitting was dependent on the parameters in the wave function. In these calculations besides the shortcomings of the perturbational approach there exists the unsatisfactory feature in that the values of the splitting and even its sign depend seriously on the parameters of the wave function. (They treated He^5 as a bound system.)

In view of the uncertainty of the conclusion a more detailed attempt to calculate the tensor splitting was made by Sugie et al. Their method of approach is similar to that of Hochberg et al. (1954, 1955). They assume the nuclear interaction with central and tensor components of the form

$$V_{ij} = (w + mM_{ij} + bB_{ij} + hH_{ij})V^c(rij) + (w + mM_{ij}) x \; S_{ij} \; V^T(rij) \qquad (8.1.1)$$

where S_{ij} is the tensor operator given by

$$S_{ij} = \{3(\underline{\sigma}_i \cdot \underline{r}_{ij})(\underline{\sigma}_j \cdot \underline{r}_{ij}) - (\underline{\sigma}_i \cdot \underline{\sigma}_j) r_{ij}^2\} / r_{ij}^2 \qquad (8.1.2)$$

We note that the tensor part of the potential has only two components. This is because the tensor force contributes only in the triplet state of the two particles.

The He^4 ground state is no longer wholly a ^1S_o state. Due to the tensor force it has a small admixture of ^5D_o and ^3P_o states (Gerjuoy and Schwinger, 1942; Irving, 1953; and Abraham et al., 1955). Sugie et al. considered only the most important amongst these, that is, the symmetric ^5D_o state.

In this chapter we shall follow closely the method of Sugie et al. As a first approximation, we shall neglect the ^3P_o-state probability. It is well known that the He^4 ground state comprises about 96% S-state and 4% D-state. In our extension of the preceding calculations to include the D-states, we shall assume that the contribution of the D-D interaction is negligible.

§8.2 THE D-STATE OPERATOR

In the previous chapters we have been using the He^4 ground state wave function given by

$$\varphi(-1)\chi(-1) = \frac{N_S}{(1+c^2)^{\frac{1}{2}}} \exp\left\{-\frac{\alpha}{2} \sum_{i>j=2}^{5} r_{ij}^2\right\} \chi(-1)$$

$$\equiv \psi(-1) \qquad (8.2.1)$$

and N_S is the normalization constant.

We now write down the symmetrical D-state operator (given by Gerjuoy and Schwinger, 1942) for the internal He^4 wave function. Then the extended wave function

$$\psi(-1) = \{g_S\chi(-1)+Cg_D w_D\chi(-1)\}\Big/(1+c^2)^{\frac{1}{2}} \qquad (8.2.2)$$

represents the He^4 ground state which contains a mixture of S and D states. The symmetric D-state w_D is given by

$$w_D = \sum_{i>j=2}^{5} r_{ij}^2 S_{ij}$$

$$= 3(\underline{\sigma}_2\cdot\underline{r}_{23})(\underline{\sigma}_4\cdot\underline{r}_{45}) + 3(\underline{\sigma}_2\cdot\underline{r}_{45})(\underline{\sigma}_4\cdot\underline{r}_{23}) -$$

$$2(\underline{\sigma}_2\cdot\underline{\sigma}_4)(\underline{r}_{23}\cdot\underline{r}_{45}) \qquad (8.2.3)$$

In equation (8.2.2) g_S and g_D represent the normalized spatial parts of the wave functions for the principal ^1S_o- and ^5D_o-state respectively.

$$\left.\begin{aligned} g_S &= N_S \exp\left\{-\frac{\alpha}{2}\sum_{i>j=2}^{5} r_{ij}^2\right\} \\ g_D &= N_D \exp\left\{-\frac{\beta}{2}\sum_{i>j=2} r_{ij}^2\right\} \end{aligned}\right) \qquad (8.2.4)$$

N_S and N_D are the normalization constants.

The nucleon-nucleon interaction shape is chosen to be of double Gaussian and is of the form

$$V(r_{ij}) = r_{ij}^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} {}^{T}U_{\kappa}^{\nu} \exp\{-{}^{T}\mu_{\kappa}^{\nu} r_{ij}^2\} \qquad (8.2.5)$$

This enables the integration to be performed analytically and this avoids the procedure of equation (26) in Sugie

et al. The parameters in equation (8.2.5) are determined by the Least Squares fit in such a way that the potential fits to the recent Hamada and Johnston's potential.

§8.3 (i) THE SPIN SUMMATION

Using §6.2 we found that all the direct terms vanish after the spin summation. This is because each of the four operators $S_{ij}w_D$ (j = 2,3,4,5) contains $\underline{\sigma}_2$ or $\underline{\sigma}_4$ only once and it was shown in Chapter VI that the expectation values of $\underline{\sigma}_2$ or $\underline{\sigma}_4$ between two similar spin functions is zero. It therefore follows that the only non-vanishing contribution comes from the indirect integrals. Of the ten pairs of the exchange indirect terms S_{12}, S_{13} and S_{23} vanish because each operator contains $\underline{\sigma}_4$ only once. S_{45} vanishes also for there is a singlet state in the S-state wave function. We note that the terms containing $\underline{\sigma}_2$ do not vanish because of the exchange nature of the function for $\underline{\sigma}_2\chi = -\underline{\sigma}_3\chi$ and the terms containing $\underline{\sigma}_3$ produce the splitting of the P-phases while those without it do not. Of the non-vanishing terms only three are independent since $S_{14} = S_{15}$, $S_{24} = S_{25}$ and $S_{34} = S_{35}$.

§8.4 THE INDIRECT INTEGRATION

The indirect integration due to the tensor force term is given by

$$T_{I_{S-D(r)}} = \frac{8M}{5\hbar^2}\, 2\int \bar{\psi}(-1)\bar{\chi}_{\ell J}{}^{m}(1) \sum_{i>j} S_{ij}\, T_{U_{ij}}\, \psi(-2)\, x$$

$$\chi_{\ell J}{}^{m}(2)\, \{f_{\ell J(r')}/r'\}\, d\tau_{-1}\, r\, d\Omega$$

$$= \frac{8M}{5\hbar^2}\, 4 \int \bar{\Psi}(-1)\bar{\chi}_{\ell J}{}^{m}(1)\ (S_{14}\ T_{U_{14}} + S_{24}\ T_{U_{24}} +$$

$$S_{34}\ T_{U_{34}})\ \Psi(-2)\chi_{\ell J}{}^{m}(2)\ \{f_{\ell J(r')}/r'\}\ d\tau_{-1} r d\Omega \quad (8.4.1)$$

(ii) INTEGRATION OVER COMPLETE VECTORS

Consider the following integral

$$(1)\quad T_{I^{14}_{S-D(r)}} = \frac{8M}{5\hbar^2}\, 4 \int \bar{\Psi}(-1)\bar{\chi}_{\ell J}{}^{m}(1)\ S_{14}\ T_{U_{14}}\ \Psi(-2)\chi_{\ell J}{}^{m}(2)$$

$$x\ \{f_{\ell J(r')}/r'\}\ d\tau_{-1}\ r\ d\Omega$$

$$= \left(\frac{16}{15}\right)^{3} \frac{8M}{5\hbar^2}\, N_S N_D\, r \sum_{\mu=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_{\nu} \frac{T_{U_{\mu}{}^{\nu}}\ c}{1+c^2}\ x$$

$$\int Y^*_{J\ell M}(\Omega)\ \exp\left[-\frac{\alpha}{2}\,(3s'^2 + 8\rho^2/3 + 2\rho'^2) -\right.$$

$$\left. T_{\mu_{\nu}}{}^{\nu}\ (\underline{s} + \tfrac{1}{3}\,\underline{\rho} - \tfrac{1}{2}\underline{\rho}')^2\right] \bar{\chi}(-1)\chi_{\ell J}{}^{m}(1)\ \left[18(\underline{r}_{13}\cdot\underline{r}_{14})\ x\right.$$

$$(\underline{r}_{14}\cdot\underline{r}_{45}) - 6r_{14}{}^{2}(\underline{r}_{13}\cdot\underline{r}_{45}) + 9i\underline{\sigma}_3\cdot(\underline{r}_{13}\wedge\underline{r}_{14})(\underline{r}_{14}\cdot\underline{r}_{45})$$

$$\left. - 9i\underline{\sigma}_3\cdot(\underline{r}_{14}\wedge\underline{r}_{45})(\underline{r}_{13}\cdot\underline{r}_{14})\right] \chi(-2)\chi_{\ell J}{}^{m}(2)\ x$$

$$\sum_{J,\ell} Y_{J\ell M}(\Omega')\ \exp\left[-\beta/2(s^2 + 8\rho^2/3 + 2\rho'^2)\right] x$$

$$f_{\ell J(r')}/r'\ d\underline{r}'d\underline{\rho}d\rho'd\Omega \quad (8.4.2)$$

We first of all deal with the following integral

$$(a)\quad \int \bar{\chi}(-1)\chi_{\ell J}{}^{m}(1)\left[18(\underline{r}_{13}\cdot\underline{r}_{14})(\underline{r}_{14}\cdot\underline{r}_{45}) - 6r_{14}{}^{2}\ x\right.$$

$$\left.(\underline{r}_{13}\cdot\underline{r}_{45})\right] \exp\left[-\ {}^{3}/2(\alpha s'^2 + \beta s^2) - (3\alpha + 3\beta +\right.$$

$$\left. T_{\mu_{\nu}}{}^{\nu})abs^2\right] \exp\left[-\gamma^{(1)}\ (\underline{\rho}-\eta\underline{r})^2 - \lambda^{(1)}(\underline{\rho}'-\delta\underline{s})^2\right] x$$

$$\chi(-2)\chi_{\ell J}{}^{m}(2)\ d\underline{r}'d\underline{\rho}d\underline{\rho}' \quad (8.4.3)$$

where $\underline{r} = \frac{1}{2}\underline{\rho}' - \underline{s}$; $\underline{r}_{13} = \underline{s} - {}^{2}/_{3}\underline{\rho}$; $\underline{r}_{14} = \underline{s} + \frac{1}{2}\underline{\rho} - \frac{1}{2}\underline{\rho}'$.

Using the transformation

$$\underline{t} = \underline{\rho} - \eta\underline{r} \quad \text{and} \quad \underline{t}' = \underline{\rho}' - \delta\underline{s} \ , \tag{8.4.4}$$

the above integral becomes

$$\left(\frac{\pi}{\alpha+\beta}\right)^{3/2} \left(\frac{3}{2}\right)^{4} \int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1) \exp\left[-\gamma^{(1)}r^{2} - \delta^{(1)}r'^{2}\right] \times$$

$$\left(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu_{\nu}^{\nu}}\right)^{3/2} \left[\frac{45}{2}\left(\frac{1}{3\alpha+3\beta+{}^{T}\mu_{\nu}^{\nu}}\right)^{2} - \frac{30}{3\alpha+3\beta+{}^{T}\mu_{\nu}^{\nu}}\, b(1+a)s^{2}\right.$$

$$\left. + 6ab^{2}(2+a)s^{4}\right] \exp\left[-\lambda\underline{r}.\underline{r}'\right] \chi(-2)\chi_{\ell J}{}^{m}(2)\, d\underline{r}' \tag{8.4.5}$$

Now consider the following terms

$$\text{(b)} \quad 9\int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\, i\underline{\sigma}_{3}.(\underline{r}_{13}\wedge\underline{r}_{14})(\underline{r}_{14}.\underline{r}_{45}) \exp\left[-\gamma^{(1)} \times\right.$$

$$\left.(\underline{\rho}-\eta\underline{r})^{2} - \lambda^{(1)}(\underline{\rho}'-\delta\underline{s})^{2}\right] \exp\left[-{}^{3}/_{2}(\alpha s'^{2}+\beta s^{2}) -\right.$$

$$\left.(3\alpha+3\beta+{}^{T}\mu_{\nu}^{\nu})abs^{2}\right] \chi(-2)\chi_{\ell J}{}^{m}(2)\, d\underline{r}'\, d\underline{\rho}\, d\underline{\rho}'.$$

On using equation (8.4.4), it is found that the above integral (b) $\overset{*}{\rightarrow}$ 0 on performing the integration over $\underline{\rho}$ and $\underline{\rho}'$.

We now consider the last expression in equation (8.4.2), namely the following integral

$$\text{(c)} \quad -9\int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\, i\underline{\sigma}_{3}.(\underline{r}_{14}\wedge\underline{r}_{45})(\underline{r}_{13}.\underline{r}_{14}) \exp\left[-\gamma^{(1)} \times\right.$$

$$\left.(\underline{\rho}-\eta\underline{r})^{2} - \lambda^{(1)}(\underline{\rho}'-\delta\underline{s})^{2}\right] \exp -\left[{}^{3}/_{2}(\alpha s'^{2}+\beta s^{2}) -\right.$$

$$\left.(3\alpha+3\beta+{}^{T}\mu_{\nu}^{\nu})abs^{2}\right] \chi(-2)\chi_{\ell J}{}^{m}(2)\, d\underline{r}'\, d\underline{\rho}\, d\underline{\rho}'.$$

Using equation (8.4.4), it is also found that (c) $\rightarrow$ 0 on integration over $\underline{\rho}$ and $\underline{\rho}'$. Hence we conclude that the splitting S-D terms give no contribution.

* $\Longrightarrow$ 0 (reduces to Zero)

Hence

$$T_{I^{14}_{S-D(r)}} = \frac{3}{2}\left(\frac{16}{15}\right)^3\left(\frac{3}{2}\right)^3 \frac{8M}{5\hbar^2}\left(\frac{\pi}{\alpha+\beta}\right)^{3/2}\frac{c}{1+c^2} N_S N_D \times$$

$$\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_\nu \, T_{U_\kappa^\nu} \exp\left[-(\gamma^{(1)}r^2+\delta^{(1)}r'^2)\right]\times$$

$$\left(\frac{\pi}{3\alpha+3\beta+T_{\mu_\kappa^\nu}}\right)^{3/2}\int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1) \times \left[\frac{45}{2}\frac{1}{(3\alpha+3\beta+T_{\mu_\kappa^\nu})^2} - \right.$$

$$\left.\frac{30}{3\alpha+3\beta+T_{\mu_\kappa^\nu}} b(1+a)s^2 + 6ab^2(2+a)s^4\right] \times$$

$$\exp\left[-\lambda \underline{r}\cdot\underline{r}'\right] \sum_{M} Y_L^M(\Omega)\, \overline{Y}_L^M(\Omega')\, \chi_{\ell J}{}^{m}(2)\chi(-2) \times$$

$$f_{\ell J(r')}\, rr'\, dr'\, d\Omega\, d\Omega' \qquad (8.4.6)$$

(2) The indirect term due to the tensor force $T_{U(24)}$ is given by

$$T_{I^{24}_{S-D(r)}} = \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2} N_S N_D \frac{c}{1+c^2} \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_\nu \times$$

$$T_{U_\kappa^\nu} \int Y^*_{J\ell M}(\Omega) \exp\left[-\frac{\alpha}{2}(3s'^2+8\rho^2/3+2\rho'^2)-\right.$$

$$\left.T_{\mu_\kappa^\nu}\left(\underline{s}'+\tfrac{1}{3}\underline{\rho}-\tfrac{1}{2}\underline{\rho}'\right)^2\right] \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[18(\underline{r}_{13}\cdot\underline{r}_{24})\times\right.$$

$$(\underline{r}_{24}\cdot\underline{r}_{45}) - 6r_{24}{}^2(\underline{r}_{13}\cdot\underline{r}_{45}) - 9i\underline{\sigma}_3\cdot(\underline{r}_{13}\wedge\underline{r}_{24})(\underline{r}_{24}\cdot\underline{r}_{45})$$

$$\left.+ 9i\underline{\sigma}_3\cdot(\underline{r}_{24}\wedge\underline{r}_{45})(\underline{r}_{13}\cdot\underline{r}_{24})\right] \exp\left[-\frac{\beta}{2}(3s^2+8\rho^2/3+\right.$$

$$\left.2\rho'^2)\right] \sum_{J,\ell} Y_{J\ell M}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2)\, f_{\ell J(r')} rr'dr' \times$$

$$d\underline{\rho}d\underline{\rho}'d\Omega d\Omega'$$

We follow the same procedure as for $T_{I^{14}_{S-D(r)}}$. Consider the following integral

$$(d)\quad \int [18(\underline{r}_{13}\cdot\underline{r}_{24})(\underline{r}_{24}\cdot\underline{r}_{45})-6r_{24}^{2}(\underline{r}_{13}\cdot\underline{r}_{45})]\exp[-\gamma^{(2)}\times$$

$$(\rho-\eta\underline{r})^{2}-\lambda^{(2)}(\underline{\rho}'-\delta\underline{s}')^{2}]\exp[-{}^{3}/2(\alpha s'^{2}+\beta s^{2})-$$

$$(3\alpha+3\beta+{}^{T}\mu_{\mu}^{\nu})abs'^{2}]\,d\underline{\rho}d\underline{\rho}' \qquad (8.4.7)$$

where $\underline{r} = \frac{1}{2}\underline{\rho}'-\underline{s}'$; $\underline{r}_{13} = \underline{s}-{}^{2}/3\underline{\rho}$ and $\underline{r}_{24} = \underline{s}'+{}^{1}/3\underline{\rho}-\frac{1}{2}\underline{\rho}'$. Using the transformation

$$\underline{q} = \underline{\rho}-\eta\underline{r} \quad \text{and} \quad \underline{q}' = \underline{\rho}'-\delta\underline{s}', \qquad (8.4.8)$$

the above integral leads to

$$(\tfrac{3}{2})\left[\left(\frac{\pi}{\lambda^{(2)}}\right)\left(\frac{\pi}{\gamma^{(2)}}\right)\right]^{3/2}\left[\frac{45}{2}\,\frac{1}{(3\alpha+3\beta+{}^{T}\mu_{\mu}^{\nu})^{2}}-\frac{30}{3(\alpha+\beta)+{}^{T}\mu_{\mu}^{\nu}}\,abs'^{2}-\right.$$

$$\left.\frac{30}{3(\alpha+\beta)+{}^{T}\mu_{\mu}^{\nu}}\,b(\underline{s}.\underline{s}')+6a^{2}b^{2}s'^{4}+12ab^{2}s'^{2}(\underline{s}.\underline{s}')\right]\times$$

$$\exp[-{}^{3}/2(\alpha s'^{2}+\beta s^{2})-(3\alpha+3\beta+{}^{T}\mu_{\mu}^{\nu})abs'^{2}] \qquad (8.4.9)$$

on integration over $\underline{\rho}$ and $\underline{\rho}'$.

We now consider the integral in the second item, viz.

$$(e)\quad -9i\underline{\sigma}_{3}\cdot\int\{\underline{r}_{13}\wedge\underline{r}_{24})(\underline{r}_{24}\cdot\underline{r}_{45})-(\underline{r}_{24}\wedge\underline{r}_{45})(\underline{r}_{13}\cdot\underline{r}_{24})\}\times$$

$$\exp[-\gamma^{(2)}(\underline{\rho}-\eta\underline{r})^{2}-\lambda^{(2)}(\underline{\rho}'-\delta\underline{s}')^{2}]\exp[-{}^{3}/2(\alpha s'^{2}+$$

$$\beta s^{2})-(3\alpha+3\beta+{}^{T}\mu_{\mu}^{\nu})\,abs'^{2}]\,d\underline{\rho}d\underline{\rho}'.$$

This leads to the following expression (using equation (8.4.8) after performing the integration over $\underline{\rho}$ and $\underline{\rho}'$)

$$(\tfrac{3}{2})\left(\frac{\pi}{\lambda^{(2)}}\right)^{3/2}\left(\frac{\pi}{\gamma^{(2)}}\right)^{3/2}\left[9ab^{2}\,i\underline{\sigma}_{3}\cdot(\underline{s}'\wedge\underline{s})s'^{2}-\frac{45}{2}\times\right.$$

$$\left.\frac{i\underline{\sigma}_{3}\cdot(\underline{s}'\wedge\underline{s})}{(3\alpha+3\beta+{}^{T}\mu_{\mu}^{\nu})}\right]\exp[-{}^{3}/2(\alpha s'^{2}+\beta s^{2})-(3\alpha+3\beta+{}^{T}\mu_{\mu}^{\nu})$$

$$\times\, abs'^{2}] \qquad (8.4.10)$$

Thus the total contribution becomes

$$T^{24}_{S-D(r)} = \left(\frac{\pi}{\alpha+\beta}\right)^{3/2} \left(\frac{3}{2}\right)\left(\frac{16}{15}\right)^3\left(\frac{3}{2}\right)^3 \frac{8M}{5\hbar^2}\frac{c}{1+c^2} N_S N_D \times$$

$$\sum_{\mu=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_\nu \, {}^{T}U_\mu^\nu \exp[-(\gamma^{(2)}r^2+\delta^{(2)}r'^2)] \times$$

$$\left(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu_\mu^\nu}\right)^{3/2} \int \bar{\chi}(-1)\bar{\chi}_{\ell J}{}^{m}(1)\left[\frac{45}{2}\frac{1}{(3\alpha+3\beta+{}^{T}\mu_\mu^\nu)^2} - \right.$$

$$\frac{30\,\mathrm{abs}'^2}{3(\alpha+\beta)+{}^{T}\mu_\mu^\nu} - \frac{30b(\underline{s}\cdot\underline{s}')}{3(\alpha+\beta)+{}^{T}\mu_\mu^\nu} + 6a^2b^2s'^4 + 12ab^2s'^2(\underline{s}'\cdot\underline{s})$$

$$\left. - \frac{45}{2}\frac{b}{3(\alpha+\beta)+{}^{T}\mu_\mu^\nu} i\underline{\sigma}_3\cdot(\underline{s}'\wedge\underline{s}) + 9ab^2 i\underline{\sigma}_3\cdot(\underline{s}'\wedge\underline{s})s^2\right] \times$$

$$\exp[-\lambda\underline{r}\cdot\underline{r}'] \sum_{M} Y_L^M(\Omega)\bar{Y}_L^M(\Omega')\chi(-2)\chi_{\ell J}{}^{m}(2) \times$$

$$f_{\ell J(r')}\, rr'dr'd\Omega d\Omega \qquad (8.4.11)$$

(3) The indirect term due to tensor force ${}^{T}U(34)$ in the S-D is

$${}^{T}I^{34}_{S-D(r)} = \frac{c}{1+c^2}\frac{8M}{5\hbar^2}\left(\frac{16}{15}\right)^3 N_S N_D \sum_{\mu=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_\nu \, {}^{T}U_\mu^\nu \times$$

$$\int Y^*_{J\ell m}(\Omega)\exp\left[-\frac{\alpha}{2}(3s'^2+8\rho^2/3+2\rho'^2) - {}^{T}\mu_\mu^\nu(\underline{\rho}-\tfrac{1}{2}\underline{\rho}')^2\right] \times$$

$$\bar{\chi}(-1)\bar{\chi}_{\ell J}{}^{m}(1)\left[-18(\underline{r}_{34}\cdot\underline{r}_{45})(\underline{r}_{34}\cdot\underline{r}_{13}) + 6r_{34}{}^2(\underline{r}_{13}\cdot\underline{r}_{45}) + \right.$$

$$\left. 9i\underline{\sigma}_3\cdot(\underline{r}_{13}\wedge\underline{r}_{34})(\underline{r}_{34}\cdot\underline{r}_{45}) + 9i\underline{\sigma}_3\cdot(\underline{r}_{34}\wedge\underline{r}_{45})(\underline{r}_{13}\cdot\underline{r}_{34})\right]\times$$

$$\exp[-\beta/2(3s^2+8\rho^2/3+2\rho'^2)] \sum_{J\ell M} Y_{J,\ell}(\Omega')\,\chi_{\ell J}{}^{M}(2) \times$$

$$\chi(-2)f_{\ell J(r')}\, rr'dr'd\underline{\rho}d\underline{\rho}'d\Omega d\Omega' \qquad (8.4.12)$$

We divide the above integral into two separate items, as follows

(i) $\int \{-18(\underline{r}_{34}\cdot\underline{r}_{45})(\underline{r}_{34}\cdot\underline{r}_{13})+6r_{34}^{2}(\underline{r}_{13}\cdot\underline{r}_{45})\} \exp[-\xi(\underline{\rho}-\bar{\varepsilon}\underline{\rho}')^2$

$- \tau\rho'^2] \exp[-3/2(\alpha s'^2+\beta s^2)]\, d\underline{\rho}\, d\underline{\rho}'$ (8.4.13)

where

$$\left.\begin{aligned} \xi &\equiv {}^1/3(4\alpha + 4\beta + 3\,{}^T\mu_\varkappa^\nu) \\ \bar{\varepsilon} &\equiv \frac{3\,{}^T\mu_\varkappa^\nu}{2(4\alpha+4\beta+3\,{}^T\mu_\varkappa^\nu)} \\ \tau &\equiv \frac{4(\alpha+\beta)(\alpha+\beta+{}^T\mu_\varkappa^\nu)}{(4\alpha+4\beta+3\,{}^T\mu_\varkappa^\nu)} \end{aligned}\right) \qquad (8.4.14)$$

We shall make use of the following results due to Newman (1959).

$$\left.\begin{aligned}
&(a)\quad (\tfrac{\lambda}{\pi})^{3/2} \int e^{-\lambda r^2}\, dr = 1 \\
&(b)\quad (\tfrac{\lambda}{\pi})^{3/2} \int r^\alpha e^{-\lambda r^2}\, dr = 0 \\
&(c)\quad (\tfrac{\lambda}{\pi})^{3/2} \int r^\alpha r^\beta e^{-\lambda r^2}\, dr = (\tfrac{1}{2\lambda})\, |\alpha\beta| \\
&(d)\quad (\tfrac{\lambda}{\pi})^{3/2} \int r^\alpha r^\beta r^\gamma e^{-\lambda r^2}\, dr = 0 \\
&(e)\quad (\tfrac{\lambda}{\pi})^{3/2} \int r^\alpha r^\beta r^\gamma r^\delta e^{-\lambda r^2}\, dr = (\tfrac{1}{2\lambda})^2\, \overline{|\alpha\beta\gamma\delta|} \\
&\qquad\qquad \text{etc.} \\
&\text{where} \\
&\qquad |\alpha\alpha| = 3; \quad \overline{|\gamma\gamma\nu\rho|} = 5|\nu\rho| \\
&\qquad \overline{|\alpha\beta\gamma\delta|} = |\alpha\beta\gamma\delta| + |\alpha\gamma\beta\delta| + |\alpha\delta\beta\gamma| \\
&\text{and if } \alpha = \beta = \gamma = \delta, \text{ then } \overline{|\alpha\beta\gamma\delta|} = 15
\end{aligned}\right) \qquad (8.4.15)$$

Using the above results, equation (8.4.13) leads to

$$- {}^3/2\, (\tfrac{3}{2})^3 \left(\frac{\pi}{3(\alpha+\beta)}\right)^{3/2} \left(\frac{\pi}{\alpha+\beta+{}^T\mu_\varkappa^\nu}\right)^{3/2} \frac{15}{2(\alpha+\beta+{}^T\mu_\varkappa^\nu)^2} \times$$

$$\exp[-\,{}^3/2(\alpha s'^2+\beta s^2)] \qquad (8.4.16)$$

We shall now consider the last integrals in equation (8.4.13)

(ii) viz. $9\int\{i\underline{\sigma}_3\cdot(\underline{r}_{13}\wedge\underline{r}_{34})(\underline{r}_{34}\cdot\underline{r}_{45})+i\underline{\sigma}_3\cdot(\underline{r}_{34}\wedge\underline{r}_{45})(\underline{r}_{13}\cdot\underline{r}_{34})\}$

$$x\ \exp[-\xi(\underline{\rho}-\overline{\varepsilon}\underline{\rho}')^2-\tau\rho'^2]\exp[-3/2(\alpha s'^2+\beta s^2)]\,d\underline{\rho}d\underline{\rho}'$$

It can be shown that the above integrals reduce to zero after integration over $\underline{\rho}$ and $\underline{\rho}'$.

Thus

$$T_{I^{34}_{S-D(r)}} = -\frac{3}{2}\left(\frac{16}{15}\right)^3\left(\frac{3}{2}\right)^3\left(\frac{\pi}{3(\alpha+\beta)}\right)^{3/2}\frac{8M}{5\hbar^2}\frac{c\,N_S N_D}{1+c^2}\ x$$

$$\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}4(w+m)_\nu\ {}^{T}U_\kappa^\nu\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[\left(\frac{\pi}{\alpha+\beta+{}^{T}\mu_\kappa^\nu}\right)^{3/2}x\right.$$

$$\left.\frac{15}{2(\alpha+\beta+{}^{T}\mu_\kappa^\nu)^2}\exp[-3/2(\alpha s'^2+\beta s^2)]\right]\sum_{M}Y_L^M(\Omega)\overline{Y}_L^M(\Omega')\ x$$

$$\chi_{\ell J}{}^{m}(2)\chi(-2)f_{\ell J(r')}rr'dr'd\Omega d\Omega'. \qquad (8.4.17)$$

Comment. We note that the splitting S-D terms give no contribution. This is because $\underline{r}_{13}+\underline{r}_{23}$ is the only variable involving $\underline{s}$ and $\underline{s}'$ and $\underline{r}\wedge\underline{r}'$ cannot be formed from this alone.

§8.5 (iii) INTEGRATION OVER SPHERICAL HARMONICS

We shall consider the complete expression for the tensor S-D exchange integral separately, taking the angular integrations into consideration. We start from the contribution due to ${}^{T}U(14)$.

The expression for the tensor S-D exchange integral for ${}^{T}U(14)$ is given by

$$
{}^{T}I^{14}_{S\text{-}D(r)} = \frac{3}{2}\left(\frac{16}{15}\right)^{3}\left(\frac{3}{2}\right)^{3}\frac{8M}{5\hbar^{2}}\left(\frac{\pi}{\alpha+\beta}\right)^{3/2}\frac{2^{7}\alpha^{9/4}\beta^{13/4}}{3\sqrt{5}\,\pi^{9/2}}\,x
$$

$$
\frac{c}{1+c^{2}}\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}4(w+m)_{\nu}\,{}^{T}U^{\nu}_{\kappa}\exp\left[-(\gamma^{(1)}r^{2}+\delta^{(1)}r'^{2})\right]x
$$

$$
\left(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa}}\right)^{3/2}\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[\frac{45}{2}\frac{1}{(3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa})^{2}}-\right.
$$

$$
\left.\frac{30}{3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa}}\,b(1+a)s^{2}+6ab^{2}(2+a)s^{4}\right]\exp\left[-\lambda\underline{r}.\underline{r}'\right]x
$$

$$
\sum_{M}Y^{M}_{L}(\Omega)\overline{Y}^{M}_{L}(\Omega')\,\chi_{\ell J}{}^{m}(2)\chi(-2)f_{\ell J(r')}rr'dr'd\Omega d\Omega' \qquad (8.5.1)
$$

where

$$
\left.\begin{aligned}
\gamma^{(1)} &\equiv \frac{24}{225}(\alpha+16\beta)+3\left(\frac{16}{15}\right)^{2}(\alpha+\beta)a\\
\delta^{(1)} &\equiv \frac{24}{225}(16\alpha+\beta)+\frac{3}{16}\left(\frac{16}{15}\right)^{2}(\alpha+\beta)a\\
\lambda &\equiv 3\left(\frac{8}{15}\right)^{2}(1+2a)(\alpha+\beta)\\
a &\equiv \frac{{}^{T}\mu^{\nu}_{\kappa}}{3(\alpha+\beta)+{}^{T}\mu^{\nu}_{\kappa}}\;;\quad b \equiv \frac{3(\alpha+\beta)}{3(\alpha+\beta)+{}^{T}\mu^{\nu}_{\kappa}}
\end{aligned}\right\} \qquad (8.5.2)
$$

Thus using our previous results given in § 6.6, equation (8.5.1) leads to

$$
{}^{T}I^{14}_{S\text{-}D(r)} = -\frac{16}{15}\left(\frac{3}{5\pi}\right)^{\frac{1}{2}}\frac{2^{6}\alpha^{9/4}\beta^{13/4}}{(\alpha+\beta)^{6}}\,b^{\frac{1}{2}}d\,\frac{c}{1+c^{2}}\,\frac{8M}{5\hbar^{2}}\,x
$$

$$
\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}4(w+m)_{\nu}\,{}^{T}U^{\nu}_{\kappa}\int\exp\left[-(\gamma^{(1)}r^{2}+\delta^{(1)}r'^{2})\right]x
$$

$$
\left[\left\{S^{(1)}_{\ell}-3\left(\frac{16}{15}\right)^{2}(\alpha+\beta)(T^{(1)}_{\ell}r^{2}+T'^{(1)}_{\ell}r'^{2})+9\left(\frac{16}{15}\right)^{4}x\right.\right.
$$

$$
\left.\left.(\alpha+\beta)^{2}(U^{(1)}r^{4}+2U'^{(1)}\,r^{2}r'^{2}+U''^{(1)}\,r'^{4})\right\}\vartheta_{\ell+\frac{1}{2}}(\lambda rr')
$$

$$+ \; 3\left(\frac{16}{15}\right)^2(\alpha+\beta)rr'\{-V^{(1)} + 3\left(\frac{16}{15}\right)^2(\alpha+\beta)(W^{(1)}r^2+W'^{(1)}r'^2)\} \times$$

$$\mathcal{J}_{\ell+3/2}(\lambda rr')\Big] dr' \qquad (8.5.3)$$

where

$$\left.\begin{aligned}
S_\ell^{(1)} &\equiv {}^5/_{2b^2} + {}^{20}/_3\,\ell bd(2a+b) + 8\ell(\ell-1)ad^2(a+{}^2/_{3b}) \\
T_\ell^{(1)} &\equiv \frac{10}{3}\,b^2\,(2a+b) + 8\ell abd(a+{}^2/_{3b}) \\
T'^{(1)}_\ell &\equiv {}^5/_{24b^2}\,(2a+b) + \tfrac{1}{2}\ell abd(a+{}^2/_{3b}) \\
U^{(1)} &\equiv 2ab^2(a+{}^2/_{3b}) \\
U'^{(1)} &= {}^3/_{16}\,U^{(1)} \\
U''^{(1)} &= \frac{1}{256}\,U^{(1)} \\
V^{(1)} &\equiv {}^5/_{3b^2}(2a+b) - 4abd(a+{}^2/_{3b}) \\
W^{(1)} &= U^{(1)} \\
W'^{(1)} &= \frac{1}{16}\,U^{(1)} \\
d &\equiv \frac{\alpha+\beta}{\alpha+\beta+{}^T\mu_\nu^\kappa}
\end{aligned}\right\} \qquad (8.5.4)$$

The expression for the tensor S-D exchange integral for ${}^TU(24)$ will be discussed in the next section.

We now consider the expression for the tensor S-D exchange integral for ${}^TU(34)$ which is given by

$${}^TI^{34}_{S\text{-}D(r)} = -\frac{3}{2}\left(\frac{16}{15}\right)^3\left(\frac{3}{2}\right)^3\left(\frac{\pi}{3(\alpha+\beta)}\right)^{3/2}\frac{8M}{5\hbar^2}\,\frac{c}{1+c^2}\,N_SN_D \times$$

$$\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_\nu\,{}^TU_\kappa^\nu\left(\frac{\pi}{\alpha+\beta+{}^T\mu_\kappa^\nu}\right)^{3/2}\frac{15}{2(\alpha+\beta+{}^T\mu_\kappa^\nu)^2} \times$$

$$\int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\exp\left[-{}^{3}/2(\alpha s'^{2}+\beta s^{2})\right] \sum_{M} Y_{L}^{M}(\Omega)\overline{Y}_{L}^{M}(\Omega)\chi_{\ell J}{}^{m}(2)\chi(-2)\ x$$

$$f_{\ell J(r')}rr'dr'd\Omega d\Omega'. \tag{8.5.5}$$

Using the results given in § 6.6 to perform the angular integration of equation (8.5.5), we see that equation (8.5.5) leads to

$$T_{I}{}^{34}_{S\text{-}D(r)} = 16\left(\frac{3}{5\pi}\right)^{\frac{1}{2}} d^{7/2}\ \frac{2^{6}\alpha^{9/4}\beta^{13/4}}{(\alpha+\beta)^{6}}\ \frac{c}{1+c^{2}}\ \frac{8M}{5\hbar^{2}}\ x$$

$$\sum_{\varkappa=1}^{2}\ \sum_{\nu=3}^{4} 4(w+m)_{\nu}\ T_{U}{}^{\nu}_{\varkappa} \int \exp\left[-\eta^{(1)}r^{2}-\xi^{(1)}r'^{2}\right] \vartheta_{\ell+\frac{1}{2}}(\tau rr')dr' \tag{8.5.6}$$

where

$$\left.\begin{aligned} \tau &\equiv {}^{3}/4\ \left(\frac{16}{15}\right)^{2}(\alpha+\beta) \\ \eta^{(1)} &\equiv \frac{24}{225}\ (\alpha+16\beta) \\ \xi^{(1)} &\equiv \frac{24}{225}\ (16\alpha+\beta) \end{aligned}\right\} \tag{8.5.7}$$

Comment. As already seen above we have not given every step of the calculations of the integrals considered in this chapter explicitly owing to the large amount of analysis involved in some parts of the calculations.

CHAPTER VIII (B)

THE TENSOR FORCE TERMS (D-S INTERACTION)

The formulation of the D-S terms is similar to that of the S-D terms but in the integrands the factors containing the tensor operator of the He^4 D-state wave function are in the reverse order. The results have exactly the same form with the suffices i and j interchanged and in addition, r and r' in the kernels of the indirect interactions interchanged.

§8.6 THE INDIRECT INTEGRATION

The indirect integration due to the tensor force term in the D-S is similar to that given in equation (8.4.1). We shall now consider the integration over complete vectors.

(ii) INTEGRATION OVER COMPLETE VECTORS

Consider the following integrals

$$(1)\quad T_{I_{D-S(r)}}^{14} = \frac{8M}{5\hbar^2}\, 4\int \bar{\Psi}(-1)\bar{\chi}_{\ell J}{}^{m}(1) S_{14}\, T_{U_{14}}\, \Psi(-2)\, x$$

$$\chi_{\ell J}{}^{m}(2)\, \{f_{\ell J(r')}/r'\}\, d_{\tau-1}\, r\, d\Omega$$

$$= \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2}\, N_S N_D \sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_\nu\, T_{U_\kappa^\nu}\, \frac{c}{1+c^2}\, x$$

$$\int Y^*_{J\ell M}(\Omega)\, \exp\left[-\beta/2(3s'^2+8\rho^2/3+2\rho'^2) - \right.$$

$$\left. T_{\mu_\kappa^\nu}(\underline{s}+{}^1/_3\underline{\rho}-\tfrac{1}{2}\underline{\rho}')^2\right]\bar{\chi}(-1)\chi_{\ell J}{}^{m}(1)\, \left[18(\underline{r}_{23}\cdot\underline{r}_{14})\, x\right.$$

$$(\underline{r}_{14}\cdot\underline{r}_{45}) - 6r_{14}^2(\underline{r}_{23}\cdot\underline{r}_{45}) + 9i\underline{\sigma}_3\cdot(\underline{r}_{23}\wedge\underline{r}_{14})(\underline{r}_{14}\cdot\underline{r}_{45}) -$$

$$\left. 9i\underline{\sigma}_3\cdot(\underline{r}_{14}\wedge\underline{r}_{45})(\underline{r}_{23}\cdot\underline{r}_{14})\right]\, \exp\left[-\frac{\alpha}{2}(3s^2+3\rho^2/3+2\rho'^2)\right]\, x$$

$$\sum_{J,\ell} Y_{J\ell M}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2)\{f_{\ell J(r')}/r'\}\ r\ d\underline{r}'d\Omega \qquad (8.6.1)$$

We shall not give the detailed calculations of equation (8.6.1) as they are similar to those of the S-D interaction. Consider the following integral

$$\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\ [18(\underline{r}_{23}\cdot\underline{r}_{14})(\underline{r}_{14}\cdot\underline{r}_{45})-6r_{14}{}^{2}(\underline{r}_{23}\cdot\underline{r}_{45})]\ x$$

$$\exp\ [-{}^{3}/2(\alpha s^{2}+\beta s'^{2})-(3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu})abs^{2}]\exp[-\gamma^{(2)}\ x$$

$$(\underline{\rho}-\eta\underline{r})^{2}-\lambda^{(2)}(\underline{\rho}'-\delta\underline{s})^{2}]\ \chi(-2)\chi_{\ell J}{}^{m}(2)d\underline{\rho}d\underline{\rho}'d\underline{r}'$$

$$= (\frac{\pi}{\alpha+\beta})^{3/2}(\frac{3}{2})^{4}\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\ \exp[-\gamma^{(2)}r^{2}-\delta^{(2)}r'^{2}]\ x$$

$$(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu}})^{3/2}\left[\frac{45}{2}\ \frac{1}{(3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu})^{2}}\ -\ \frac{30abs^{2}}{3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu}}\ -\right.$$

$$\left.\frac{30b(\underline{s}.\underline{s}')}{3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu}}\ +\ 6a^{2}b^{2}s^{4}\ +\ 12ab^{2}s^{2}(\underline{s}.\underline{s}')\right]\ x$$

$$\exp[-\lambda\underline{r}.\underline{r}']\ \chi(-2)\chi_{\ell J}{}^{m}(2)\ d\underline{r}'. \qquad (8.6.2)$$

The following terms are due to the D-S indirect tensor forces

$$\int\ \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)9i\underline{\sigma}_{3}\cdot\ [(\underline{r}_{23}\wedge\underline{r}_{14})(\underline{r}_{14}\cdot\underline{r}_{45})-(\underline{r}_{14}\wedge\underline{r}_{45})(\underline{r}_{23}\cdot\underline{r}_{14})]$$

$$x\ \exp[-{}^{3}/2(\alpha s^{2}+\beta s'^{2})-(3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu})abs^{2}]\ \exp[-\gamma^{(2)}\ x$$

$$(\underline{\rho}-\underline{\eta r})^{2}-\lambda^{(2)}(\underline{\rho}'-\delta\underline{s})^{2}]\ \chi(-2)\chi_{\ell J}{}^{m}(2)d\underline{r}'d\underline{\rho}d\underline{\rho}'$$

$$= (\frac{\pi}{\alpha+\beta})^{3/2}(\frac{3}{2})^{4}\int\ \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\ \exp[-\gamma^{(2)}r^{2}-\delta^{(2)}r'^{2}]\ x$$

$$(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu}})^{3/2}\left[\frac{45}{2}\ \frac{b}{3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu}}\ i\underline{\sigma}_{3}.(\underline{s}\wedge\underline{s}')\ -\right.$$

$$\left.9ab^{2}i\underline{\sigma}_{3}.(\underline{s}\wedge\underline{s}')s^{2}\right]\exp[-\lambda\underline{r}.\underline{r}']\ \chi(-2)\chi_{\ell J}{}^{m}(2)d\underline{r}' \qquad (8.6.3)$$

Hence, the expression for the tensor D-S indirect integral for $^{T}U(14)$ is

$$
{}^{T}I^{14}_{D-S(r)} = \left(\frac{16}{15}\right)^3\left(\frac{3}{2}\right)^4\left(\frac{\pi}{\alpha+\beta}\right)^{3/2}\frac{c}{1+c^2}\;\frac{2^7\alpha^{9/4}\beta^{13/4}}{3\sqrt{5}\,\pi^{9/2}}\;\frac{8M}{5\hbar^2}\;x
$$

$$
\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_{\nu}\;{}^{T}U^{\nu}_{\kappa}\left(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa}}\right)^{3/2}\exp\left[-(\gamma^{(2)}r^2+\delta^{(2)}x\right.
$$

$$
\left.r'^2)\right]\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[\frac{45}{2}\;\frac{1}{(3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa})^2}-\frac{30abs^2}{3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa}}-\right.
$$

$$
\frac{30b(\underline{s}'.\underline{s})}{3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa}}+6a^2b^2s^4+12ab^2s^2(\underline{s}.\underline{s}')+\frac{45}{2}\;x
$$

$$
\left.\frac{b}{(3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa})}\;i\underline{\sigma}_3.(\underline{s}\wedge\underline{s}')-9ab^2i\underline{\sigma}_3.(\underline{s}\wedge\underline{s}')s^2\right]\;x
$$

$$
\exp\left[-\lambda\underline{r}.\underline{r}'\right]\sum_{M}Y^{M}_{L}(\Omega)\overline{Y}^{M}_{L}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2)f_{\ell J(r')}rr'dr'\;x
$$

$$
d\Omega d\Omega' \qquad (8.6.4)
$$

The indirect term due to tensor force $^{T}U(24)$ in the D-S term is given by

$$
{}^{T}I^{24}_{D-S(r)} = \left(\frac{16}{15}\right)^3\frac{8M}{5\hbar^2}\;N_SN_D\;\frac{c}{1+c^2}\sum_{\kappa=1}\sum_{\nu=3}4(w+m)_{\nu}\;x
$$

$$
{}^{T}U^{\nu}_{\kappa}\int Y^{*}_{J\ell m}(\Omega)\exp\left[-\beta/2(3s'^2+8\rho^2/3+2\rho'^2)-{}^{T}\mu^{\nu}_{\kappa}(\underline{s}'+\right.
$$

$$
\left.{}^{1}/3\underline{\rho}-\tfrac{1}{2}\underline{\rho}')^2\right]\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[18(\underline{r}_{23}.\underline{r}_{24})(\underline{r}_{24}.\underline{r}_{45})-6r_{24}{}^{2}\right.
$$

$$
x(\underline{r}_{23}.\underline{r}_{45})-9i\underline{\sigma}_3.(\underline{r}_{23}\wedge\underline{r}_{45})(\underline{r}_{24}.\underline{r}_{45})+9i\underline{\sigma}_3.(\underline{r}_{23}\wedge\underline{r}_{45})\;x
$$

$$
\left.(\underline{r}_{23}.\underline{r}_{45})\right]\exp\left[-\alpha/2(3s^2+8\rho^2/3+2\rho'^2)\right]\sum_{J,\ell}Y_{J\ell M}(\Omega')\;x
$$

$$
\chi_{\ell J}{}^{m}(2)\chi(-2)\{f_{\ell J(r')}/r'\}r\;d\underline{r}'d\underline{\rho}d\underline{\rho}'d\Omega \qquad (8.6.5)
$$

We shall separate the above integral into two parts, viz.

$$(a)\quad \int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\,[18(\underline{r}_{23}\cdot\underline{r}_{24})(\underline{r}_{24}\cdot\underline{r}_{45})-6r_{24}{}^{2}(\underline{r}_{23}\cdot\underline{r}_{45})]\ x$$

$$\exp\,[-\gamma^{(2)}(\underline{\rho}-\eta\underline{r})^{2}-\lambda^{(2)}(\underline{\rho}'-\delta\underline{s})^{2}]\exp\,[-{}^{3}/_{2}(\alpha s^{2}+\beta s'^{2})-$$

$$(3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu})abs'^{2}\,]\,\chi_{\ell J}{}^{m}(2)\chi(-2)d\underline{r}'d\underline{\rho}d\underline{\rho}' \qquad (8.6.6)$$

and

$$(b)\quad \int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)9i\underline{\sigma}_{3}\cdot\,[\,(\underline{r}_{24}\wedge\underline{r}_{45})(\underline{r}_{23}\cdot\underline{r}_{45})-(\underline{r}_{23}\wedge\underline{r}_{24})\ x$$

$$(\underline{r}_{24}\cdot\underline{r}_{45})\,]\,\exp\,[-\gamma^{(2)}(\underline{\rho}-\eta\underline{r})^{2}-\lambda^{(2)}(\underline{\rho}'-\delta\underline{s})^{2}\,]\,x$$

$$\exp\,[-{}^{3}/_{2}(\alpha s^{2}+\beta s'^{2})-(3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu})abs'^{2}\,]\,\chi_{\ell J}{}^{m}(2)\chi(-2)\ x$$

$$d\underline{r}'d\underline{\rho}d\underline{\rho}' \qquad (8.6.7)$$

Consider (a). This is the same as the integral we obtained for a similar term of the above in ${}^{T}I_{S-D}^{14}$ with $\underline{s}\rightleftharpoons\underline{s}'$. After the integration over $\underline{\rho}$ and $\underline{\rho}'$ the result of the integral in equation (8.6.6) is

$$({}^{3}/_{2})^{4}\left(\frac{\pi}{\alpha+\beta}\right)^{3/2}\int\,\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\exp\,[-{}^{3}/_{2}(\alpha s^{2}+\beta s'^{2}]\ x$$

$$\left(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu}}\right)^{3/2}\left[\frac{45}{2}\,\frac{1}{(3\alpha+3\beta+{}^{T}\mu_{\mathcal{H}}^{\nu})^{2}}-\frac{30}{3(\alpha+\beta)+{}^{T}\mu_{\mathcal{H}}^{\nu}}\ x\right.$$

$$\left.b(1+a)s'^{2}+6ab^{2}(2+a)s'^{4}\right]\exp\,[-\{3(\alpha+\beta)+{}^{T}\mu_{\mathcal{H}}^{\nu}\}abs'^{2}]\ x$$

$$\chi_{\ell J}{}^{m}(2)\chi(-2)\,d\underline{r}' \qquad (8.6.8)$$

Consider the integral in item (b), i.e.

$$\int\,\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)9i\underline{\sigma}_{3}\cdot\,[\,(\underline{r}_{24}\wedge\underline{r}_{45})(\underline{r}_{23}\cdot\underline{r}_{24})-(\underline{r}_{23}\wedge\underline{r}_{24})\ x$$

$$(\underline{r}_{24}\cdot\underline{r}_{45})\,]\,\exp\,[-\gamma^{(2)}(\underline{\rho}-\eta\underline{r})^{2}-\lambda^{(2)}(\underline{\rho}'-\delta\underline{s})^{2}]x$$

$$\exp\,[-{}^{3}/_{2}(\alpha s^{2}+\beta s'^{2})-\{3(\alpha+\beta)+{}^{T}\mu_{\mathcal{H}}^{\nu}\}abs'^{2}\,]\,\chi_{\ell J}{}^{m}(2)\ x$$

$\chi(-2)d\underline{r}'d\underline{\rho}d\underline{\rho}'$

This is the same as the integral of the same expression obtained in ${}^{T}I^{14}_{S-D(r)}$ with $(\underline{r}_{23} \rightleftharpoons \underline{r}_{13})$ $\underline{s} \rightleftharpoons \underline{s}'$ and $\underline{\sigma}_3 \rightleftharpoons -\underline{\sigma}_3$. This reduces to zero after the integration over $\underline{\rho}$ and $\underline{\rho}'$. Hence the splitting term gives no contribution in D-S.

Thus, the total contribution of the indirect term due to tensor force ${}^{T}U(24)$ in the D-S term is given by the following expression:

$$
{}^{T}I^{24}_{D-S(r)} = \left(\frac{16}{15}\right)^3 \left(\frac{3}{2}\right)^4 \frac{c}{1+c^2} \frac{2^7\alpha^{9/4}\beta^{13/4}}{3\sqrt{5}\,\pi^{9/2}} \frac{8M}{5\hbar^2} \left(\frac{\pi}{\alpha+\beta}\right)^{3/2} x
$$

$$
\sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_\nu \, {}^{T}U^{\nu}_{\kappa} \left(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa}}\right)^{3/2} \exp\left[-(\gamma^{(2)}r'^2+\delta^{(2)}r^2)\right]
$$

$$
\int \overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1) \left[\frac{45}{2} \frac{1}{(3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa})^2} - \frac{30}{3(\alpha+\beta)+{}^{T}\mu^{\nu}_{\kappa}} b(1+a)s'^2 + 6ab^2(2+a)s'^4\right] \exp\left[-\lambda\underline{r}\cdot\underline{r}'\right] \sum_{M} Y^{M}_{L}(\Omega)\overline{Y}^{M}_{L}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2) \; x
$$

$$
f_{\ell J(r')} \, rr'dr'd\Omega d\Omega' \qquad (8.6.9)
$$

(3) The indirect term due to tensor force ${}^{T}U(34)$ in the D-S is given by the following expression:

$$
{}^{T}I^{34}_{D-S(r)} = \left(\frac{16}{15}\right)^3 \frac{8M}{5\hbar^2} N_S N_D \sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_\nu \, {}^{T}U^{\nu}_{\kappa} \frac{c}{1+c^2} \; x
$$

$$
\int Y^{*}_{J\ell M}(\Omega) \exp\left[-\beta/2(3s'^2+8\rho^2/3+2\rho'^2)-{}^{T}\mu^{\nu}_{\kappa}(\underline{\rho}-\tfrac{1}{2}\rho')^2\right] x
$$

$$
\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1) \left[18(\underline{r}_{34}\cdot\underline{r}_{45})(\underline{r}_{34}\cdot\underline{r}_{23})+6r_{34}{}^{2}(\underline{r}_{23}\cdot\underline{r}_{45})\right.
$$

$$
\left.+9i\underline{\sigma}_3\cdot(\underline{r}_{23}\wedge\underline{r}_{34})(\underline{r}_{34}\cdot\underline{r}_{45})+9i\underline{\sigma}_3\cdot(\underline{r}_{34}\wedge\underline{r}_{45})(\underline{r}_{23}\cdot\underline{r}_{34})\right] x
$$

$$\exp\left[-\alpha/2(3s^2+8\rho^2/3+2\rho'^2)\right]\sum_{J,\ell} Y_{J\ell M}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2)\ x$$

$$\{f_{\ell J(r')}/r'\}r\ d\underline{r}'d\underline{\rho}d\underline{\rho}'d\Omega \qquad (8.6.10)$$

We separate the above integral into two main items, namely.

$$\text{(i)}\quad \int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[-18(\underline{r}_{34}\cdot\underline{r}_{45})(\underline{r}_{34}\cdot\underline{r}_{23})+6r_{34}{}^{2}(\underline{r}_{23}\cdot\underline{r}_{45})\right]$$

$$x\ \exp\left[-\xi(\underline{\rho}-\overline{\varepsilon}\underline{\rho}')^2-\tau\rho'^2\right]\exp\left[-3/2(\alpha s^2+\beta s'^2)\right]x$$

$$\chi_{\ell J}{}^{m}(2)\chi(-2)\ d\underline{\rho}d\underline{\rho}' \qquad (8.6.11)$$

$$\text{(ii)}\quad \int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)9i\underline{\sigma}_3\cdot\left[(\underline{r}_{23}\wedge\underline{r}_{34})(\underline{r}_{34}\cdot\underline{r}_{45})+(\underline{r}_{34}\wedge\underline{r}_{45})\ x\right.$$

$$\left.(\underline{r}_{23}\cdot\underline{r}_{34})\right]\exp\left[-\xi(\underline{\rho}-\overline{\varepsilon}\underline{\rho}')^2-\tau\rho'^2\right]\exp\left[-3/2(\alpha s^2+\right.$$

$$\left.\beta s'^2)\right]\chi_{\ell J}{}^{m}(2)\chi(-2)\ d\underline{\rho}d\underline{\rho}' \qquad (8.6.12)$$

Note that we have omitted the following terms in the above two integrals which appeared in equation (8.6.10) (a) $\{f_{\ell J(r')}/r'\}\ r\ dr'd\Omega$ and (b) $Y_{\ell,m}$ (the tesseral harmonics).

Using the results given in equation (8.4.15), the result of equation (8.6.11) after the integration over $\underline{\rho}$ and $\underline{\rho}'$ has been performed is quoted below

$$-(3/2)^4\left(\frac{\pi}{3(\alpha+\beta)}\right)^{3/2}\left(\frac{\pi}{\alpha+\beta+{}^{T}\mu_{\nu}}\right)^{3/2}\frac{15}{2(\alpha+\beta+{}^{T}\mu_{\nu})^2}\ x$$

$$\exp\left[-\frac{3}{2}(\alpha s^2+\beta s'^2)\right] \qquad (8.6.13)$$

Consider the integral in (ii) above. This is the same as the one we obtained when considering the S-D terms for the tensor force ${}^{T}U(34)$ after the interchange $\underline{s}\rightleftharpoons\underline{s}'$. This reduces to zero after the integration over $\underline{\rho}$ and $\underline{\rho}'$

has been performed as already shown. Thus the total indirect term due to the tensor force ${}^{T}U(34)$ in the D-S is given below:

$$
{}^{T}I^{34}_{D\text{-}S(r)} = -\left(\frac{3}{2}\right)^{4}\left(\frac{16}{15}\right)^{3}\frac{c}{1+c^{2}}\;\frac{2^{7}\alpha^{9/4}\beta^{13/4}}{3\sqrt{5}\;\pi^{9/2}}\;\frac{8M}{5\hbar^{2}}\;x
$$

$$
\left(\frac{\pi}{3(\alpha+\beta)}\right)^{3/2}\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}4(m+m)_{\nu}\;{}^{T}U^{\nu}_{\kappa}\;\left(\frac{\pi}{\alpha+\beta+{}^{T}U^{\nu}_{\kappa}}\right)^{3/2}x
$$

$$
\frac{15}{2(\alpha+\beta+{}^{T}\mu^{\nu}_{\kappa})^{2}}\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\;\exp\left[-\,{}^{3}/_{2}(\alpha s^{2}+\beta s'^{2})\right]x
$$

$$
\sum_{M}Y^{M}_{L}(\Omega)\overline{Y}^{M}_{L}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2)f_{\ell J(r')}rr'dr'd\Omega d\Omega' \qquad (8.6.14)
$$

§ 8.7 (iii) INTEGRATION OVER SPHERICAL HARMONICS

The expression for the tensor D-S exchange integral for ${}^{T}U(14)$ is given by

$$
{}^{T}I^{14}_{D\text{-}S(r)} = \left(\frac{16}{15}\right)^{3}\left(\frac{3}{2}\right)^{4}\left(\frac{\pi}{\alpha+\beta}\right)^{3/2}\frac{c}{1+c^{2}}\;\frac{2^{7}\alpha^{9/4}\beta^{13/4}}{3\sqrt{5}\;\pi^{9/2}}\;\frac{8M}{5\hbar^{2}}\;x
$$

$$
\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}4(w+m)_{\nu}\;{}^{T}U^{\nu}_{\kappa}\left(\frac{\pi}{3\alpha+3\beta+{}^{T}\mu_{\kappa}{}^{\nu}}\right)^{3/2}\exp\left[-(\gamma^{(2)}r^{2}+\delta^{(2)}r'^{2})\right]x
$$

$$
\int\overline{\chi}(-1)\overline{\chi}_{\ell J}{}^{m}(1)\left[\frac{45}{2}\;\frac{1}{(3\alpha+3\beta+{}^{T}\mu^{\nu}_{\kappa})^{2}}-\frac{30abs^{2}}{3(\alpha+\beta)+{}^{T}\mu^{\nu}_{\kappa}}-\right.
$$

$$
\frac{30b(\underline{s}'.\underline{s})}{3(\alpha+\beta)+{}^{T}\mu^{\nu}_{\kappa}}+6a^{2}b^{2}s^{4}+12ab^{2}s^{2}(\underline{s}'.\underline{s})+\frac{45}{2}\;\frac{b}{3(\alpha+\beta)+{}^{T}\mu^{\nu}_{\kappa}}\;x
$$

$$
\left.i\underline{\sigma}_{3}.(\underline{s}\wedge\underline{s}')-9ab^{2}i\underline{\sigma}_{3}.(\underline{s}\wedge\underline{s}')s^{2}\right]\;\exp\left[-\lambda\underline{r}.\underline{r}'\right]\sum_{M}Y^{M}_{L}(\Omega)\;x
$$

$$
\overline{Y}^{M}_{L}(\Omega')\chi_{\ell J}{}^{m}(2)\chi(-2)f_{\ell J(r')}rr'dr'd\Omega d\Omega' \qquad (8.7.1)
$$

We shall use the previous results to perform the integration over spherical harmonics. In addition to this, we shall use equation (5.5.4) to integrate the terms in $i\underline{\sigma}_3.(\underline{r}\wedge\underline{r}')$. This avoids the method of equation (29) in Sugie et al. Similarly we replace equation (30) in Sugie et al. by equation (5.6.2), the proof of which is given in equation (5.5.1).

Thus, we may write the total expression for the tensor D-S exchange integral for ${}^{T}U(14)$ as

$$
\begin{aligned}
{}^{T}I^{14}_{D\text{-}S(r)} = & -\frac{16}{15}\left(\frac{3}{5\pi}\right)^{\frac{1}{2}}\frac{2^{6}\alpha^{9/4}\beta^{13/4}}{(\alpha+\beta)^{6}}\,b^{\frac{1}{2}}d\,\frac{c}{1+c^{2}}\,\frac{8M}{5\hbar^{2}}\;x \\
& \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_{\nu}\;{}^{T}U^{\nu}_{\kappa}\int\exp\left[-(\gamma^{(2)}r^{2}+\delta^{(2)}r'^{2})\right]\;x \\
& \Big[\{S^{(2)}_{\ell}-3\left(\tfrac{16}{15}\right)^{2}(\alpha+\beta)(T^{(2)}_{\ell}+r^{2}+T'^{(2)}_{\ell}r'^{2})+9\left(\tfrac{16}{15}\right)^{4}(\alpha+\beta)^{2}\;x \\
& (U^{(2)}r^{4}+2U'^{(2)}r^{2}r'^{2}+U''^{(2)}r'^{4})\}\mathcal{J}_{\ell+\frac{1}{2}}(\lambda rr') + 3\left(\tfrac{16}{15}\right)^{2}\;x \\
& (\alpha+\beta)rr'\{-V^{(2)}+3\left(\tfrac{16}{15}\right)^{2}(\alpha+\beta)(W^{(2)}r^{2}+W'^{(2)}r'^{2})\}\;x \\
& \mathcal{J}_{\ell+3/2}(\lambda rr')\Big]\,dr' + k^{\ell J}_{sp}(r,r') \qquad (8.7.2)
\end{aligned}
$$

where

$$
\begin{aligned}
k^{\ell J}_{sp}(r,r') = & \frac{15}{4}\left(\frac{3}{5\pi}\right)^{\frac{1}{2}}\frac{2^{6}\alpha^{9/4}\beta^{13/4}}{(\alpha+\beta)^{6}}\,b^{\frac{1}{2}}d^{2}\;||\;\underline{\sigma}\;\underline{\ell}\;||\;x \\
& \frac{c}{1+c^{2}}\,\frac{8M}{5\hbar^{2}}\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} 4(w+m)_{\nu}\;{}^{T}U^{\nu}_{\kappa}\int\exp\left[-(\gamma^{(2)}r^{2}+\delta^{(2)}r'^{2})\right] \\
& x\;\Big[\{X_{\ell}-3\left(\tfrac{16}{15}\right)^{2}(\alpha+\beta)(Yr^{2}+Y'r'^{2})\}\mathcal{J}_{\ell+\frac{1}{2}}(\lambda rr')-3\left(\tfrac{16}{15}\right)^{2}\;x \\
& (\alpha+\beta)rr'z\;\mathcal{J}_{\ell+3/2}(\lambda rr')\Big]\;dr' \qquad (8.7.3)
\end{aligned}
$$

where

$$
\begin{aligned}
\gamma^{(2)} &\equiv \frac{24}{225}\,(16\alpha+\beta) + 3\left(\frac{16}{15}\right)^2 (\alpha+\beta)a \\
\delta^{(2)} &\equiv \frac{24}{225}\,(\alpha+16\beta) + \frac{3}{16}\left(\frac{16}{15}\right)^2 (\alpha+\beta)a \\
S_{\ell}^{(2)} &\equiv \frac{5}{2}\,b^2 + \frac{5}{6}\,\ell bd\,(25a+17b)+2\ell(\ell-1)\ x \\
&\qquad ad^2\left(7a + \frac{17}{3}\,b\right) \\
T_{\ell}^{(2)} &\equiv \frac{5}{6}\,b^2\,(5a+b) + \ell abd\left(9a+ \frac{19}{3}\,b\right) \\
T_{\ell}'^{(2)} &\equiv \frac{5}{24}\,b^2(5a+4b)+ \frac{1}{16}\,\ell abd\left(19a+ \frac{49}{3}\,b\right) \\
U^{(2)} &\equiv ab^2(a+ {}^{1}/_{3}b) \\
U'^{(2)} &\equiv \frac{1}{32}\,ab^2\,(21a+17b) \\
U''^{(2)} &\equiv \frac{1}{128}\,ab^2\,\left(3a + \frac{8b}{3}\right) \\
V^{(2)} &\equiv \frac{5}{24}\,b^2\,(25a+17b) - abd\left(7a + \frac{17b}{3}\right) \\
W^{(2)} &\equiv \frac{1}{4}\,ab^2\,\left(9a+ \frac{19b}{3}\right) \\
W'^{(2)} &\equiv \frac{1}{64}\,ab^2\,\left(19a+ \frac{49b}{3}\right) \\
X_{\ell} &\equiv \frac{8b}{3} + \frac{32}{15}\,\ell ad \\
Y^{(2)} &\equiv \frac{16}{15}\,ab \\
Y'^{(2)} &= \frac{1}{16}\,Y^{(2)} \\
Z &= \tfrac{1}{2}Y^{(2)}
\end{aligned}
\qquad (8.7.4)
$$

$|| \underline{\sigma}\ \underline{\ell} ||$ is defined in equation (5.6.2).

We shall not consider the integration over spherical harmonics for S_{24} ($^{T}I^{24}_{S\text{-}D(r)}$ and $^{T}I^{24}_{D\text{-}S(r)}$) since S_{24} becomes the same as S_{14} ($^{T}I^{14}_{S\text{-}D(r)}$ and $^{T}I^{14}_{D\text{-}S(r)}$) after the interchange $1 \rightleftharpoons 2$ and hence kernel S_{24} is obtained from

S_{14} by exchanging coordinates $\underline{r}$ and $\underline{r}'$.

Similarly we obtain from the total tensor S-D exchange integral ${}^{T}U(34)$ the corresponding total tensor D-S integral by interchanging the coordinates $\underline{r}$ and $\underline{r}'$. Thus

$$
{}^{T}I^{34}_{D\text{-}S(r)} = 16\left(\frac{3}{5\pi}\right)^{\frac{1}{2}} d^{7/2} \frac{2^{6}\alpha^{9/4}\beta^{13/4}}{(\alpha+\beta)^{6}} \frac{c}{1+c^{2}} \frac{8M}{5\hbar^{2}} \times
$$

$$
\sum_{\varkappa=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_{\nu} \, {}^{T}U^{\nu}_{\varkappa} \int \exp\left[-(\eta^{(2)}r^{2}+\xi^{(2)}r'^{2})\right] \times
$$

$$
\vartheta_{\ell+\frac{1}{2}}(\tau rr') \, dr' \qquad (8.7.5)
$$

where

$$
\left.\begin{aligned} \eta^{(2)} &\equiv \frac{24}{225}(16\alpha+\beta) \\ \xi^{(2)} &\equiv \frac{24}{225}(\alpha+16\beta) \end{aligned}\right\} \qquad (8.7.6)
$$

and τ is defined in equation (8.5.7).

§8.8 (iv) FINAL RESULTS

The complete expression for the tensor SD and DS exchange integrals consist of four similar parts, interchangeable by means of the transformation $\underline{r} \rightleftharpoons \underline{r}'$. The indirect term is given by

$$
\begin{aligned} I &= I_{14}(r,r') + I_{24}(r,r') + I_{34}(r,r') + I_{14}k^{\ell J}_{sp}(r,r') + \\ &\quad I_{24}k^{\ell J}_{sp}(r,r') \\ &\equiv I'(r,r') + I'k^{\ell J}_{sp}(r,r'). \end{aligned} \qquad (8.8.1)
$$

where

$$
I'(r,r') = -\frac{16}{15}\left(\frac{3}{5\pi}\right)^{\frac{1}{2}} \frac{2^{6}\alpha^{9/4}\beta^{13/4}}{(\alpha+\beta)^{6}} b^{\frac{1}{2}} d \frac{c}{1+c^{2}} \frac{8M}{5\hbar^{2}} \times
$$

$$
\sum_{i=1}^{2} \sum_{\varkappa=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_{\nu} \, {}^{T}U^{\nu}_{\varkappa} \int \exp\left[-(\gamma^{(i)}r^{2}+\delta^{(i)}r'^{2})\right] \times
$$

$$\Big[\{S_\ell^{(i)} - 3(\tfrac{16}{15})^2 (\alpha+\beta)(T_\ell^{(i)} r^2 + T_\ell'^{(i)} r'^2) + 9(\tfrac{16}{15})^4 (\alpha+\beta)^2 \times$$

$$(U^{(i)} r^4 + 2U'^{(i)} r^2 r'^2 + U''^{(i)} r'^4)\} \mathcal{J}_{\ell+\frac{1}{2}}(\lambda rr') + 3(\tfrac{16}{15})^2 \times$$

$$(\alpha+\beta) rr' \{-V^{(i)} + 3(\tfrac{16}{15})^2 (\alpha+\beta)(W^{(i)} r^2 + W'^{(i)} r'^2)\} \times$$

$$\mathcal{J}_{\ell+3/2}(\lambda rr')\Big] dr'$$

+ a similar term with $r \rightleftharpoons r'$

$$+ 16(\tfrac{3}{5\pi})^{\frac{1}{2}} \frac{2^6 \alpha^{9/4} \beta^{13/4}}{(\alpha+\beta)^6} d^{7/2} \frac{c}{1+c^2} \frac{8M}{5\hbar^2} \sum_{i=1}^{2} \sum_{\varkappa=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_\nu$$

$$\times T_{U_\varkappa^\nu} \int \exp\left[-(\eta^{(i)} r^2 + \xi^{(i)} r'^2)\right] \mathcal{J}_{\ell+\frac{1}{2}}(\tau rr') dr' \qquad (8.8.2)$$

and

$$I'k_{sp}^{\ell J}(r,r') = \frac{15}{4} (\tfrac{3}{5\pi})^{\frac{1}{2}} \frac{2^6 \alpha^{9/4} \beta^{13/4}}{(\alpha+\beta)^6} b^{\frac{1}{2}} d^2 \; ||\underline{\sigma}\; \underline{\ell}\;|| \times$$

$$\frac{c}{1+c^2} \frac{8M}{5\hbar^2} \sum_{i=1}^{2} \sum_{\varkappa=1}^{2} \sum_{\nu=3}^{4} 4(w+m)_\nu T_{U_\varkappa^\nu} \int \exp\left[-(\gamma^{(i)} r^2 + \right.$$

$$\left. \delta^{(i)} r'^2)\right] \Big[\{X_\ell - 3(\tfrac{16}{15})^2 (\alpha+\beta)(Y^{(i)} r^2 + Y'^{(i)} r'^2)\} \times$$

$$\mathcal{J}_{\ell+\frac{1}{2}}(\lambda rr') - 3(\tfrac{16}{15})^2 (\alpha+\beta) rr' Z \mathcal{J}_{\ell+3/2}(\lambda rr')\Big] dr' \qquad (8.8.3)$$

where

$$Y'^{(1)} \equiv \frac{16}{15} ab, \qquad Y^{(1)} = \frac{1}{16} Y'^{(1)} \qquad (8.8.4)$$

PART III

THE BINDING ENERGY OF He^4

CHAPTER IX

THE BINDING ENERGY OF THE ALPHA-PARTICLE (B.E.(He^4))

The problem of the alpha-particle S and D states binding energy is formulated in coordinate space and is followed by a variational calculation of the principal ^1S_o-state and the principal ^5D_o-state contribution to the B.E.(He^4) using a radial wave function of the form $\exp(-\mu \sum_{i>j=2}^{5} r_{ij}^2)$. The calculation is based on the nuclear forces given in Chapter II taking into account the effect of a "hard core" on B.E(He^4). The results obtained are compared with those of other authors.

§9.1 INTRODUCTION

Many authors have described variational calculations of the binding energies of the triton and the alpha-particle, using the phenomenological potentials which satisfied current two-body data (Abraham et al. (1955); Irving (1951, 1952, 1953); Clark (1954); Kikuta et al. (1956); Blatt et al. (1958); Nagata et al. (1959); and H. Kanada et al. (1963)). The introduction of a "hard core" into the two-body potentials reopens interest in further calculations of this kind. Several approaches have been made in the problems of three- and four-particle nuclei and in this thesis we describe the direct variational calculations for the alpha-particle.

The way we treat our contribution of the hard core to the B.E(He^4) is very similar to that of Brueckner (1958) for a two-particle problem. (Ref. § 2.5).

§9.2 THE BINDING ENERGY CALCULATION

Let H be the complete Hamiltonian of the internal He^4 system. Then the total binding energy, inclusive of the D-state, is given by the following form:

$$E = \int \psi^* H \psi \, d\tau \tag{9.2.1}$$

where the Hamiltonian is given by

$$H = -(\hbar^2/2M) \sum_{j=2}^{5} \nabla_j^2 + \sum_{i>j=2}^{5} V(r_{ij}) \tag{9.2.2}$$

∇_j^2 is the Laplacian operator acting on the coordinates of the particle whose position vector is $\underline{r}_i$. ψ and $V(r_{ij})$ have already been defined.

Thus we may write equation (9.2.1) in the form:

$$\begin{aligned} E = \int \psi^* H \psi \, d\tau = \frac{1}{1+c^2} \Big[& \int \psi^*_{s(-1)} \{ -\frac{\hbar^2}{2M} \sum_{j=2}^{5} \nabla_j^2 \} \psi_{s(-1)} d\tau + \\ & c^2 \int \psi^*_{D(-1)} \{ -\hbar^2/2M \sum_{j=2}^{5} \nabla_j^2 \} \psi_{D(-1)} \, d\tau + \\ & \sum_{i>j=2}^{5} \{ \int \psi^*_{s(-1)} Vc(r_{ij}) \psi_{s(-1)} d\tau + c^2 \int \psi^*_{D(-1)} \, Vc(r_{ij}) \psi_{D(-1)} \, d\tau \\ & + c^2 \int \psi^*_{D(-1)} \, V_{Ls}(r_{ij}) \psi_{D(-1)} \, d\tau + 2c \int \psi^*_{s(-1)} V_T(r_{ij}) \psi_{D(-1)} \\ & x \, d\tau + c^2 \int \psi^*_{D(-1)} V_T(r_{ij}) \psi_{D(-1)} d\tau + c^2 \int \psi^*_{D(-1)} \, V_{LL}(r_{ij}) \, x \\ & \psi_{D(-1)} \, d\tau \} \Big] \end{aligned} \tag{9.2.3}$$

where $V_c(r_{ij})$, $V_{Ls}(r_{ij})$, $V_T(r_{ij})$ and $V_{LL}(r_{ij})$ are the central, linear spin-orbit, tensor and quadratic spin-orbit parts respectively of the two-particle interaction of the form given in equation (4.1.2).

The coulomb energy of He^4 is given by

$$E_{coulomb} = \frac{e^2}{1+c^2} \{\int \psi^*_{s(-1)} \left(\frac{1}{r_{45}}\right) \psi_{s(-1)} \, d\tau + c^2 \int \psi^*_{D(-1)} \left(\frac{1}{r_{45}}\right) \psi_{D(-1)} \, d\tau\} \qquad (9.2.4)$$

where e is the electronic charge.

The above expressions have to be minimized in the variational calculation of the binding energy which includes the D-states.

§ 9.3 THE CONTRIBUTION OF THE KINETIC ENERGY TO THE B.E. (He^4)

We consider first the contribution of the S-S terms to the B·E. (He^4). The energy operator of He^4 is given by

$$T_{2345} = T_{2-345} + T_{3-45} + T_{45}$$

$$= -\hbar^2/2M(^4/_3 \nabla^2_{2-345} + {}^3/_2 \nabla^2_{3-45} + \frac{2}{1} \nabla^2_{45}) \qquad (9.3.1)$$

Also we have

$$\psi_{s(-1)} = N_s \exp\{-\frac{\alpha}{2} \sum_{i>j=2}^{5} r_{ij}^2\} \chi(-1)$$

$$= N_s \exp\{-\frac{\alpha}{2} (3s'^2 + 8\rho^2/3 + 2\rho'^2)\} \chi(-1) \qquad (9.3.2)$$

N_s and $\chi(-1)$ have already been defined.

Thus

$$\langle \psi^*_{s(-1)} | T_{2345} | \psi_{s(-1)} \rangle = N_s^2 \frac{\hbar^2}{M} 2\alpha(9+\alpha \frac{\partial}{\partial \alpha}) \, x$$

$$\int \exp\{-\alpha(3s'^2 + 8\rho^2/3 + 2\rho'^2)\} \, d\tau \qquad (9.3.3)$$

where $N_s^2 = 2^6\alpha^{9/2}/\pi^{9/2}$ (9.3.4)

Expression (9.3.3) can easily be evaluated and the result is

$$\frac{\hbar^2}{2M} \quad (18\alpha).$$

Hence

$$\frac{1}{1+c^2} \int \psi_s^* \{ - \frac{\hbar^2}{2M} \sum_{j=2}^{5} \nabla_j^2 \} \psi_s \, d\tau$$

$$= \frac{1}{1+c^2} \frac{\hbar^2}{2M} (18\alpha) \qquad (9.3.5)$$

We now consider the contribution from the D-D terms. It should be noted that the S-D terms give no contribution (S-D = D-S) to the B.E. (He^4). This is because of the spin properties of the D-state operator.

We define $\psi_D(-1)$ as

$$\psi_D(-1) = N_D \exp\{-\beta/2(3s'^2+8\rho^2/3+2\rho'^2)\}[\,3(\underline{\sigma}_2\cdot\underline{r}_{23})(\underline{\sigma}_4\cdot\underline{r}_{45})$$

$$+ 3(\underline{\sigma}_2\cdot\underline{r}_{45})(\underline{\sigma}_4\cdot\underline{r}_{23})-2(\underline{\sigma}_2\cdot\underline{\sigma}_4)(\underline{r}_{23}\cdot\underline{r}_{45})]\ \chi(-1) \qquad (9.3.6)$$

where $\underline{r}_{23} = \underline{s}' - {}^2/_3\underline{\rho}$ and $\underline{r}_{45} = \underline{\rho}'$.

Thus

$$\langle \psi^*_{D(-1)} \,|T_{2345}|\, \psi_{D(-1)} \rangle = -N_D^2 \frac{\hbar^2}{2M} \int \exp\{-\beta(3s'^2+8\rho^2/3+$$

$$2\rho'^2)\}\ (4\beta^2\rho'^2-10\beta)\ [18(\underline{s}'-{}^2/_3\underline{\rho})^2\rho'^2 +$$

$$6\{(\underline{s}'-{}^2/_3\underline{\rho}).\underline{\rho}'\}^2]x\ d\underline{s}'d\underline{\rho}d\underline{\rho}' \qquad (9.3.7)$$

$$= N_D^2 \left(\frac{\pi^3}{16\beta^3}\right)^{3/2} \frac{\hbar^2}{2M} \left(\frac{585}{2\beta}\right) \qquad (9.3.8)$$

But $N_D^2 = \frac{4\beta^2}{45} \left(\frac{16\beta^3}{\pi^3}\right)^{3/2}$ (9.3.9)

Hence

$$\Sigma^{\sigma}_{(-1)} \int d\tau_{-1} \chi_{\alpha}(-1) \varphi^{*}_{D(-1)} \; (T_{2345}) \varphi_{D(-1)} \chi_{\alpha}(-1)$$

$$= \frac{c^2}{1+c^2} \; \frac{\hbar^2}{2M} \; (26\beta) \qquad (9.3.10)$$

Thus

$$\Sigma^{\sigma}_{(-1)} \int d\tau_{-1} \chi^{*}_{\alpha}(-1) \; [\varphi^{*}_{s(-1)} \; (T_{2345}) \varphi_{s(-1)} + \varphi^{*}_{D(-1)} (T_{2345}) \; x$$

$$\varphi_{D(-1)}] \; \chi_{\alpha}(-1)$$

$$= \frac{1}{1+c^2} \; \Big[\int \psi^{*}_{s(-1)} \{-\hbar^2/2M \sum_{j=2}^{5} \nabla^2_j \} \; \psi_{s(-1)} \; d\tau \; +$$

$$c^2 \int \psi^{*}_{D(-1)} \; \{-\hbar^2/2M \sum_{j=2}^{5} \nabla^2_j \; \} \; \psi_{D(-1)} \; d\tau \Big]$$

$$= \frac{1}{1+c^2} \; \frac{\hbar^2}{2M} \; (18\alpha + 26\beta c^2) \qquad (9.3.11)$$

§9.4 THE CONTRIBUTION OF THE CENTRAL FORCE TO THE B.E.(He^4)

POTENTIAL (S-S TERMS)

We consider the following expression:

$$\Sigma^{\sigma}_{(-1)} \int d\tau_{-1} \; \chi^{*}_{\alpha}(-1) \varphi^{*}_{s(-1)} \; (\Sigma(2345) V_{c(ij)}) \chi_{\alpha}(-1) \varphi_{s}(-1) \qquad (9.4.1)$$

where $V_{c(ij)} = (w + mM_{ij} + b\beta_{ij} + hH_{ij}) \; V_{c(ij)}$ (9.4.2)

M, B and H have their usual meanings. The N-N potential shape will be chosen to be of the double Gaussian type, that is, of the form

$$V(r_{ij}) = \sum_{\mu=1}^{2} U_{\mu} \; \exp \{- \mu_{\mu} r_{ij}^{2}\} \qquad (9.4.3)$$

Using equations (9.4.2) and (9.4.3), expression (9.4.1) becomes

$$\frac{6N_s^2}{1+c^2} \sum_{\mu=1}^{2} \sum_{\nu=1}^{4} (w+m)_\nu \, {}^cU_\mu^\nu \int \exp\{-\lambda(\underline{s}'-\gamma\underline{\rho})^2 - 2\alpha\rho'^2 - \eta\rho'^2\} \times d\underline{s}'\,d\underline{\rho}\,d\underline{\rho}' \qquad (9.4.4)$$

where

$$\left.\begin{aligned} \lambda &= 3\alpha + {}^c\mu_\mu^\nu \\ \eta &= \frac{4\alpha(2\alpha+{}^c\mu_\mu^\nu)}{3\alpha+{}^c\mu_\mu^\nu} \end{aligned}\right) \qquad (9.4.5)$$

On performing the integration over $\underline{s}'$, $\underline{\rho}$ and $\underline{\rho}'$ in equation (9.4.4) we obtain

$$6 \sum_{\mu=1}^{2} \sum_{\nu=1}^{4} (w+m)_\nu \, {}^cU_\mu^\nu \left(\frac{2\alpha}{2\alpha+{}^c\mu_\mu^\nu}\right)^{3/2} \qquad (9.4.6)$$

POTENTIAL ($\Sigma(2345)V_{ij}$) (D-D TERMS)

Consider the potential with the ~~ordering~~ ordinary Wigner term, that is

$$w\langle {}^5D_o^* | V_{ij} | {}^5D_o \rangle = 2w\int d\tau_{-1}\chi_\alpha^*(-1)\varphi_D^*(-1)V_{23}\varphi_D(-1)\chi_\alpha(-1) + 4w\int d\tau_{-1}\chi_\alpha^*(-1)\varphi_D^*(-1)V_{24}\varphi_D(-1)\chi_\alpha(-1) \qquad (9.4.7)$$

Consider the first term on the R.H.S. of equation (9.4.7), i.e.

$$2w\int d\tau_{-1}\chi_\alpha^*(-1)\varphi_D^*(-1)V_{23}\varphi_D(-1)\chi_\alpha(-1)$$

$$= \frac{c^2}{1+c^2} N_D^2 \sum_{\mu=1}^{2} \sum_{\nu=1}^{4} w_\nu \, {}^cU_\mu^\nu \exp\{-\lambda(\underline{s}'-\gamma\underline{\rho})^2 - \delta\rho^2 - \eta\rho'^2\} \times [18\rho'^2(\underline{s}'-{}^2/_3\underline{\rho})^2 + 6(\underline{s}'.\underline{\rho}'-{}^2/_3\underline{\rho}.\underline{\rho}')^2]\, d\underline{s}'\,d\underline{\rho}\,d\underline{\rho}' \qquad (9.4.8)$$

where

$$\left.\begin{aligned} \lambda &= (3\beta+{}^{c}\mu_{\kappa}^{\nu}) \;;\quad \gamma = 2{}^{c}\mu_{\kappa}^{\nu}/3\lambda \;; \\ \delta &= 4\beta(2\beta+{}^{c}\mu_{\kappa}^{\nu})/(3\beta+{}^{c}\mu_{\kappa}^{\nu}); \quad \eta = 2\beta \end{aligned}\right\} \qquad (9.4.9)$$

On performing the integration with respect to $\underline{s}'$, $\underline{\rho}$ and $\underline{\rho}'$, the R.H.S. in equation (9.4.8) reduces to

$$2\,\frac{c^2}{1+c^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} w_{\nu}\,{}^{c}U_{\kappa}^{\nu}\,\left(\frac{2\beta}{2\beta+{}^{c}\mu_{\kappa}^{\nu}}\right)^{5/2} \qquad (9.4.10)$$

Consider the second expression on the R.H.S. of equation (9.4.7), that is,

$$4w\int d\tau_{-1}\chi_{\alpha}^{*}(-1)\varphi_{D(-1)}^{*}V_{24}\varphi_{D(-1)}\chi_{\alpha}(-1)$$

$$= 4\,\frac{c^2}{1+c^2}\,N_D{}^2\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} w_{\nu}\,{}^{c}U_{\kappa}^{\nu}\int\exp\{-\lambda(\underline{s}'-\xi\underline{r})^2-\omega(\underline{\rho}-\varepsilon\underline{\rho}')^2 -$$

$$\varkappa\rho'^2\}\,[18\rho'^2(\underline{s}'-{}^{2}/_{3}\underline{\rho})^2+6(\underline{s}'.\underline{\rho}'-{}^{2}/_{3}\underline{\rho}.\underline{\rho}')^2]\,d\underline{s}'d\underline{\rho}d\underline{\rho}' \qquad (9.4.11)$$

where $\lambda = 3\beta+{}^{c}\mu_{\kappa}^{\nu}$; $\xi = {}^{c}\mu_{\kappa}^{\nu}/3\lambda$; $\underline{r} = {}^{3}/_{2}\underline{\rho}'-\underline{\rho}$;

$$\omega = \beta(8\beta+3{}^{c}\mu_{\kappa}^{\nu})/(3\beta+{}^{c}\mu_{\kappa}^{\nu}); \quad \varepsilon = {}^{c}\mu_{\kappa}^{\nu}/2(8\beta+3{}^{c}\mu_{\kappa}^{\nu});$$

$$\varkappa = 8\beta(2\beta+{}^{c}\mu_{\kappa}^{\nu})/(8\beta+3{}^{c}\mu_{\kappa}^{\nu}) \qquad (9.4.12)$$

On using the following transformation

$\underline{s}'-\xi\underline{r} = \underline{t}$, $\underline{\rho}-\varepsilon\underline{\rho}' = \underline{t}'$, and $\underline{\rho}' = \underline{\rho}'$, equation (9.4.11) leads to

$$\frac{c^2}{1+c^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} w_{\nu}\,{}^{c}U_{\kappa}^{\nu}\left[\frac{5}{2}\left(\frac{2\beta}{2\beta+{}^{c}\mu_{\kappa}^{\nu}}\right)^{3/2}+\left(\frac{2\beta}{2\beta+{}^{c}\mu_{\kappa}^{\nu}}\right)^{5/2}+\right.$$

$$\left.\tfrac{1}{2}\left(\frac{2\beta}{2\beta+{}^{c}\mu_{\kappa}^{\nu}}\right)^{7/2}\right] \qquad (9.4.13)$$

Thus equation (9.4.7) reduces to

$$\frac{c^2}{1+c^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} w_\nu\, {}^cU_\kappa^\nu \left[5/2\left(\frac{2\beta}{2\beta+{}^c\mu_\kappa^\nu}\right)^{3/2} + 3\left(\frac{2\beta}{2\beta+{}^c\mu_\kappa^\nu}\right)^{5/2} + \frac{1}{2}\left(\frac{2\beta}{2\beta+{}^c\mu_\kappa^\nu}\right)^{7/2}\right] \qquad (9.4.14)$$

We now consider the potential with the Majorana exchange operator. The matrix element of the D-state is given by

$$\langle {}^5D_o^* | V_{ij} m_\nu P^M(ij) | {}^5D_o \rangle$$

$$= 2m_\nu \int d\tau_{-1} \chi_\alpha^*(-1) \varphi_{D(-1)}^* V_{23} P^M(23) \varphi_{D(-1)} \chi_\alpha(-1) +$$

$$4m_\nu \int d\tau_{-1} \chi_\alpha^*(-1) \varphi_{D(-1)}^* V_{24} P^M(24) \varphi_{D(-1)} \chi_\alpha(-1) \qquad (9.4.15)$$

The above expression is easily evaluated and the final result is

$$\frac{c^2}{1+c^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} m_\nu\, {}^cU_\kappa^\nu \left[\frac{5}{2}\left(\frac{2\beta}{2\beta+{}^c\mu_\kappa^\nu}\right)^{3/2} - 3\left(\frac{2\beta}{2\beta+{}^c\mu_\kappa^\nu}\right)^{5/2} + \frac{1}{2}\left(\frac{2\beta}{2\beta+{}^c\mu_\kappa^\nu}\right)^{7/2}\right] \qquad (9.4.16)$$

By the same procedure, it can be shown that the following results hold:

(a) $\langle {}^5D_o^* | V_{ij} P^B(ij) | {}^5D_o \rangle = \langle {}^5D_o^* | V_{ij} | {}^5D_o \rangle$

(b) $\langle {}^5D_o^* | V_{ij} P^H(ij) | {}^5D_o \rangle = \langle {}^5D_o^* | V_{ij} P^M(ij) | {}^5D_o \rangle$

Thus $\langle {}^5D_o^* | (w_\nu + m_\nu M_{ij} + b_\nu B_{ij} + h_\nu H_{ij}) | {}^5D_o \rangle$

$$= \frac{c^2}{1+c^2} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} {}^{c}U_{\kappa}^{\nu} \left[\frac{5}{2}(w+m+b+h)_{\nu} \left(\frac{2\beta}{2\beta+{}^{c}\mu_{\kappa}^{\nu}}\right)^{3/2} + \right.$$

$$\left. 3(w-m+b-h)_{\nu} \left(\frac{2\beta}{2\beta+{}^{c}\mu_{\kappa}^{\nu}}\right)^{5/2} + \frac{1}{2}(w+m+b+h)_{\nu} \left(\frac{2\beta}{2\beta+{}^{c}\mu_{\kappa}^{\nu}}\right)^{7/2} \right]$$

(9.4.17)

§9.5 THE CONTRIBUTION OF THE COULOMB ENERGY TO THE B.E.(He^4)

From equation (9.2.4), the contribution of the coulomb energy to the B.E.(He^4) is as follows:

$$E_{coul.} = \frac{e^2}{1+c^2} \{ \int \psi^*_{s(-1)} \left(\frac{1}{\underline{r}_{45}}\right) \psi_{s(-1)} d\tau_{-1} + c^2 \int \psi^*_{D(-1)} \left(\frac{1}{\underline{r}_{45}}\right) \times$$

$$\psi_{D(-1)} d\tau_{-1} \} \qquad (9.5.1)$$

e being the electronic charge.

Thus we obtain

$$E_{coul.} = \frac{N_s^2}{1+c^2} e^2 \int \exp\{-\alpha(3s'^2+8\rho^2/3+2\rho'^2\} \frac{1}{\underline{\rho}}, \, d\underline{s}' d\underline{\rho} d\underline{\rho}'$$

$$+ N_D^2 \frac{c^2}{1+c^2} e^2 \int \exp\{-\beta(3s'^2+8\rho^2/3+2\rho'^2)\} \times$$

$$[18\underline{\rho}'^2(\underline{s}'-{}^{2}/3\underline{\rho})^2+6(\underline{s}', \underline{\rho}'-{}^{2}/3\underline{\rho}, \underline{\rho}')^2] \frac{1}{\underline{\rho}}, \, d\underline{s} d\underline{\rho} d\underline{\rho}'$$

$$= \frac{2}{1+c^2} e^2 \left(\frac{2}{\pi}\right)^{\frac{1}{2}} [\sqrt{\alpha} + \frac{2}{3} c^2 \sqrt{\beta}] \qquad (9.5.2)$$

§9.6 THE CONTRIBUTION OF THE TENSOR FORCE TO THE B.E.(He^4)

The tensor component of the potential U_{ij} is given by

$${}^{T}U_{ij}(r_{ij}) = (w+mM)\,{}^{T}U(r_{ij}) \qquad (9.6.1)$$

Since the tensor force contributes to the B.E.(He^4) only in the triplet state. Neither does the tensor force give any contribution to the B.E.(He^4) in S-S states. The only contributions come from both the S-D (= D-S) and the D-D terms. We consider first the contribution from the S-D terms. This is given by the following expression

$$(a)\quad {}^{T}I_{S-D(r)} = \langle {}^{1}S_o^* | S_{ij} | {}^{5}D_o \rangle$$

$$= \frac{4cN_S N_D}{1+c^2} \int d\tau_{-1} \chi_\alpha^*(-1) \left[18(\underline{r}_{23}\cdot\underline{r}_{24})(\underline{r}_{24}\cdot\underline{r}_{45}) - 6r_{24}^2(\underline{r}_{23}\cdot\underline{r}_{45})\right] \exp\{-\lambda(\underline{s}'-\xi\underline{r})^2 - \omega(\underline{\rho}-\varepsilon\underline{\rho}')^2 - \varkappa\rho'^2\} \times \chi_\alpha(-1) \qquad (9.6.2)$$

It can easily be shown that equation (9.6.2) leads to

$${}^{T}I_{S-D(r)} = -3\sqrt{5}\,\frac{c}{1+c^2}\left(\frac{2\alpha}{\alpha+\beta}\right)\left(\frac{2\beta}{\alpha+\beta}\right)^2 \sum_{\varkappa=1}^{2}\sum_{\nu=3}^{4}\left(\frac{2\sqrt{\alpha\beta}}{\alpha+\beta+{}^{T}\mu_{\varkappa}^{\nu}}\right)^{5/2} \times \frac{{}^{T}U_{\varkappa}^{\nu}}{\alpha+\beta+{}^{T}\mu_{\varkappa}^{\nu}} \qquad (9.6.3)$$

Thus the total contribution from S-D and D-S terms is given by

$${}^{T}I_{S-D(r)} + {}^{T}I_{D-S(r)} = -6\sqrt{5}\,\frac{c}{1+c^2}\left(\frac{2\alpha}{\alpha+\beta}\right)\left(\frac{2\beta}{\alpha+\beta}\right)^2 \times \sum_{\varkappa=1}^{2}\sum_{\nu=3}^{4} {}^{T}U_{\varkappa}^{\nu}\left(\frac{2\sqrt{\alpha\beta}}{\alpha+\beta+{}^{T}\mu_{\varkappa}^{\nu}}\right)^{5/2} \frac{1}{\alpha+\beta+{}^{T}\mu_{\varkappa}^{\nu}} \qquad (9.6.4)$$

Hence we obtain

$$2\langle {}^{1}S_o^* | S_{ij}(w+mM_{ij})_\nu | {}^{5}D_o \rangle = -6\sqrt{5}\,\frac{c}{1+c^2}\left(\frac{2\alpha}{\alpha+\beta}\right)\left(\frac{2\beta}{\alpha+\beta}\right)^2 \sum_{\varkappa=1}^{2}\sum_{\nu=3}^{4}(w+m)_\nu\, {}^{T}U_{\varkappa}^{\nu} \times$$

$$\left(\frac{2\sqrt{\alpha\beta}}{\alpha+\beta+{}^{T}\mu_{\nu}}\right)^{5/2} \frac{1}{\alpha+\beta+{}^{T}\mu_{\nu}} \qquad (9.6.5)$$

Note that we have no contributions from S_{23} and S_{24}. This is because each contains $\underline{\sigma}_2$ or $\underline{\sigma}_4$ only once and the expectation values of $\underline{\sigma}_2$ or $\underline{\sigma}_4$ between two similar spin functions is zero as shown previously.

We now consider the contribution from the D-D terms. This is given by the following expression:

$$\text{(b)} \quad \langle {}^5D_o^* | S_{ij} | {}^5D_o \rangle = 2\langle {}^5D_o^* | S_{23} | {}^5D_o \rangle + 4\langle {}^5D_o^* | S_{34} | {}^5D_o \rangle$$

$$= -2\frac{c^2}{1+c^2} N_D^2 \sum_{\nu=1}^{2} {}^{T}U_{\nu} \int \exp\{-\lambda(\underline{s}'-\gamma\underline{\rho})^2-\delta\rho^2-\eta\rho'^2\}$$

$$\times \left[18r_{23}r_{24}^2+30r_{23}^2(\underline{r}_{23}\cdot\underline{r}_{45})^2\right] d\underline{s}'d\underline{\rho}d\underline{\rho}' +$$

$$\frac{4c^2}{1+c^2} N_D^2 \int \exp\{-\lambda s'^2-w(\underline{\rho}-\varepsilon\underline{\rho}')-\nu\rho'^2\} \left[\{42(\underline{r}_{23}\cdot\underline{r}_{45})^2-\right.$$

$$18r_{23}^2r_{45}^2\}r_{24}^2-72(\underline{r}_{34}\cdot\underline{r}_{23})(\underline{r}_{34}\cdot\underline{r}_{45})(\underline{r}_{23}\cdot\underline{r}_{45}) +$$

$$\left.54\,[\,\underline{r}_{23},\underline{r}_{34},\underline{r}_{45}\,]^2\right] d\underline{s}'d\underline{\rho}d\underline{\rho}'. \qquad (9.6.6)$$

Equation (9.6.6) leads to

$$-\frac{c^2}{1+c^2} \sum_{\nu=1}^{2} {}^{T}U_{\nu} \left[\frac{21}{2}\left(\frac{2\beta}{2\beta+{}^{T}\mu_{\nu}}\right)^{5/2} + \frac{7}{2}\left(\frac{2\beta}{2\beta+{}^{T}\mu_{\nu}}\right)^{7/2}\right] \frac{1}{2\beta+{}^{T}\mu_{\nu}} \qquad (9.6.7)$$

Thus $w_\nu \langle {}^5D_o^* | S_{ij} | {}^5D_o \rangle$

$$= -\frac{c^2}{1+c^2} \sum_{\nu=1}^{2} \sum_{\nu=3}^{4} w_\nu \, {}^{T}U_{\nu} \left[\frac{21}{2}\left(\frac{2\beta}{2\beta+{}^{T}\mu_{\nu}}\right)^{5/2} + \frac{7}{2}\left(\frac{2\beta}{2\beta+{}^{T}\mu_{\nu}}\right)^{7/2}\right]$$

$$\times \frac{1}{2\beta+{}^{T}\mu_{\nu}} \qquad (9.6.8)$$

It can also be shown that

$$m_\nu \left\langle {}^5D_o^* \left| S_{ij} P^M(ij) \right| {}^5D_o \right\rangle$$

$$= 2N_D^2 \frac{c^2}{1+c^2} \sum_{\mu=1}^{2} \sum_{\nu=3}^{4} m_\nu {}^T U_\mu^\nu \int \exp\{-\lambda(\underline{s}'-\gamma\underline{\rho})^2 - \delta\rho^2 - \eta\rho'^2\} \times$$

$$\left[18 r_{23}^4 r_{45}^2 + 30 r_{23}^2 (\underline{r}_{23}\cdot\underline{r}_{45})^2\right] d\underline{s}'\, d\underline{\rho}\, d\underline{\rho}'$$

$$+ 4N_D^2 \frac{c^2}{1+c^2} \sum_{\mu=1}^{2} \sum_{\nu=3}^{4} m_\nu {}^T U_\mu^\nu \int \exp\{-\lambda s'^2 - \omega(\underline{\rho}-\varepsilon\underline{\rho}')^2 - \kappa\rho'^2\}$$

$$\times \left[\{42(\underline{r}_{23}\cdot\underline{r}_{45})^2 - 18 r_{23}^2 r_{45}^2\} r_{34}^2 - 72(\underline{r}_{34}\cdot\underline{r}_{23})(\underline{r}_{34}\cdot\underline{r}_{45}) \times \right.$$

$$\left. (\underline{r}_{23}\cdot\underline{r}_{45}) + 54 [\underline{r}_{23}, \underline{r}_{34}, \underline{r}_{45}]^2 \right] d\underline{s}\, d\underline{\rho}\, d\underline{\rho}'$$

$$= \frac{c^2}{1+c^2} \sum_{\mu=1}^{2} \sum_{\nu=3}^{4} m_\nu {}^T U_\mu^\nu \frac{1}{2\beta + {}^T\mu_\mu^\nu} \left[\frac{21}{2} \left(\frac{2\beta}{2\beta + {}^T\mu_\mu^\nu}\right)^{5/2} - \right.$$

$$\left. \frac{7}{2} \left(\frac{2\beta}{2\beta + {}^T\mu_\mu^\nu}\right)^{7/2}\right] \qquad (9.6.9)$$

Thus

$$\left\langle {}^5D_o^* \left| S_{ij} (w + m M_{ij})_\nu \right| {}^5D_o \right\rangle$$

$$= -\frac{c^2}{1+c^2} \sum_{\mu=1}^{2} \sum_{\nu=3}^{4} {}^T U_\mu^\nu \frac{1}{2\beta + {}^T\mu_\mu^\nu} \left[\frac{21}{2} (w-m)_\nu \left(\frac{2\beta}{2\beta + {}^T\mu_\mu^\nu}\right)^{5/2} + \right.$$

$$\left. \frac{7}{2}(w+m)_\nu \left(\frac{2\beta}{2\beta + {}^T\mu_\mu^\nu}\right)^{7/2}\right] \qquad (9.6.10)$$

9.7 THE CONTRIBUTION OF SPIN-ORBIT FORCE ($\underline{L}.\underline{S}$) TO B.E.($He^4$)

The spin-orbit force $\underline{L}.\underline{S}$ between the i^{th} and the j^{th} nucleons may be written in the following form:

$$V_{Ls}(r_{ij}) = \underline{L}.\underline{S}\,(w_{Ls} + m_{Ls} P^M(ij)) V_{Ls}(r_{ij}) \qquad (9.7.1)$$

where

where

$$\underline{L}_{ij}\cdot\underline{S}_{ij} = \frac{\hbar}{2}(\underline{\sigma}_i+\underline{\sigma}_j)\cdot(\underline{r}_i-\underline{r}_j)\wedge(\underline{p}_i-\underline{p}_j) \tag{9.7.2}$$

$$\underline{p}_i = -i\hbar\frac{\partial}{\partial\underline{r}_i} \tag{9.7.3}$$

The spin-orbit potential has only two components. This is because the spin-orbit contributes only in the triplet state of the two particles. It can easily be shown that both the S-S and the S-D or D-S terms give no contribution to the B.E.(He^4). Thus, only the D-D terms give a contribution to the B.E.(He^4). As before the wave functions are of the Gaussian type, that is, of the form

$$g_D = N_D \exp\{-\beta/2 \sum_{i>j=2}^{5} r_{ij}^2\} \tag{9.7.4}$$

where N_D is the D-state normalization factor $(=2^8\ \beta^{13/2}/45\pi^{9/2})^{\frac{1}{2}}$.

The wave function of He^4 is given by

$$\psi(-1) = \frac{c}{(1+c^2)^{\frac{1}{2}}}\ g_D\ w_D\ \chi_\alpha(-1) \tag{9.7.5}$$

where g_D represents the normalized spatial part of the wave function for the principal ^5D_o-state and $\chi_\alpha(-1)$ has been defined previously. w_D is defined by

$$w_D = \sum_{i>j=2}^{5} r_{ij}^2 S_{ij} = 3(\underline{\sigma}_2\cdot\underline{r}_{23})(\underline{\sigma}_4\cdot\underline{r}_{45}) + 3(\underline{\sigma}_2\cdot\underline{r}_{45})$$

$$\times\ (\underline{\sigma}_4\cdot\underline{r}_{23}) - 2(\underline{\sigma}_2\cdot\underline{\sigma}_4)(\underline{r}_{23}\cdot\underline{r}_{45}) \tag{9.7.6}$$

The following coordinate system will be used throughout the calculations in this section.

$\underline{r}_{23} = \underline{v}, \qquad \underline{r}_{45} = \underline{w}$

$\frac{1}{2}(\underline{r}_2+\underline{r}_3-\underline{r}_4-\underline{r}_5) = \underline{u}$

give rise to the following

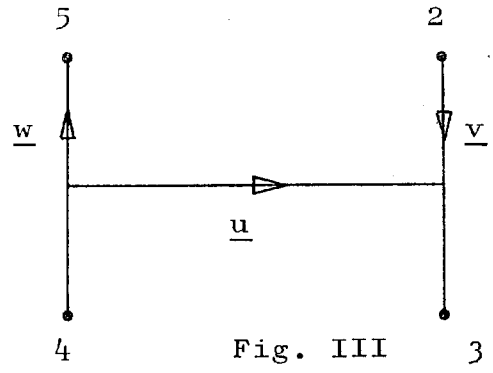


Fig. III

$$\underline{r}_{24} = \underline{u} + \tfrac{1}{2}(\underline{v}-\underline{w})$$

$$\underline{r}_{25} = \underline{u} + \tfrac{1}{2}(\underline{v}+\underline{w})$$

$$\underline{r}_{34} = \underline{u} - \tfrac{1}{2}(\underline{v}+\underline{w})$$

$$\underline{r}_{35} = \underline{u} - \tfrac{1}{2}(\underline{v}-\underline{w}) \qquad (9.7.7)$$

Consider the Ls potential with the ordinary Wigner operator. The expectation value with respect to the D-state is given by

$$\langle {}^*_D | V_{Ls} | D \rangle = \frac{c^2}{1+c^2} \int \chi^*_\alpha(-1)\, w^*_D\, g^*_D \sum_{i>j=2}^{5} V_{Ls}(ij)\, g_D w_D \times$$

$$\chi_\alpha(-1)\, d\tau \qquad (9.7.8)$$

Here $\underline{\sigma}_3\chi(\widetilde{23}) = -\underline{\sigma}_2\chi(\widetilde{23})$ and similar expression for $\chi(45)$. Thus equation (9.7.8) can be rewritten in the following form:

$$\langle {}^*_D | V_{Ls} | D \rangle = \frac{2c^2}{1+c^2} \int \chi^*_\alpha\, w^*_D\, g^*_D\, V_{Ls}(23)\, g_D w_D \chi_\alpha\, d\tau \; +$$

$$\frac{4c^2}{1+c^2} \int \chi^*_\alpha\, w^*_D g^*_D V_{Ls}(24) g_D w_D \chi_\alpha(-1)\, d\tau \qquad (9.7.9)$$

Consider the first expression on the R.H.S. of equation (9.7.9), that is,

$$\frac{2c^2}{1+c^2} \int \chi^*_\alpha w^*_D g^*_D V_{Ls}(23) g_D w_D \chi_\alpha d\tau.$$

Before proceeding with further calculations, some preliminary results are given.

$$
\begin{aligned}
&(a)\langle\chi_\alpha|(\underline{\sigma}_2\cdot\underline{A})|\chi_\alpha\rangle = \langle\chi_\alpha|(\underline{\sigma}_4\cdot\underline{A})|\chi_\alpha\rangle = 0 \\
&(b)\langle\chi_\alpha|(\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_4\cdot\underline{B})|\chi_\alpha\rangle = 0 \\
&(c)\langle\chi_\alpha|(\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_3\cdot\underline{B})|\chi_\alpha\rangle = -(\underline{A}.\underline{B}) \\
&(d)\langle\chi_\alpha|(\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_2\cdot\underline{a})(\underline{\sigma}_4\cdot\underline{b})|\chi_\alpha\rangle = 0
\end{aligned}
\qquad (9.7.10)
$$

where $\underline{A}$, $\underline{B}$, $\underline{a}$, $\underline{b}$ etc. are commuting vectors.

Thus we get

$$
\chi_\alpha^* w_D^* V_{Ls}(23) w_D \chi_\alpha = 18(i\hbar)^2 \left[3v^2w^2 + (\underline{v}.\underline{w})^2\right] \qquad (9.7.11)
$$

Hence
$$
\begin{aligned}
&\frac{2c^2}{1+c^2}\int \chi_\alpha^* w_D^* g_D^* V_{Ls}(23) g_D w_D \chi_\alpha d\tau \\
&= 36\,\frac{c^2}{1+c^2}\,N_D{}^2 V_{Ls}(i\hbar)^2 \int \left[3v^2w^2+(\underline{v}.\underline{w})^2\right] \exp\left\{-4\beta u^2 - (2\beta+{}^{Ls}\mu_\kappa^\nu)v^2 - 2\beta w^2\right\} d\underline{u}d\underline{v}d\underline{w} \\
&= -6\,\frac{c^2}{1+c^2}\,\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} {}^{Ls}U_\kappa^\nu \left(\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\right)^{5/2}
\end{aligned}
\qquad (9.7.12)
$$

We also obtain

$$
\begin{aligned}
&2w_{Ls}\,\frac{c^2}{1+c^2}\int \chi_\alpha^* w_D^* g_D^* V_{Ls}(23) g_D w_D \chi_\alpha d\tau \\
&= -6\,\frac{c^2}{1+c^2}\,\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} w_\nu\, {}^{Ls}U_\kappa^\nu \left(\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\right)^{5/2}
\end{aligned}
\qquad (9.7.13)
$$

It can now easily be shown that

$$
\begin{aligned}
&2\,\frac{c^2}{1+c^2}\,m_{Ls}\int \chi_\alpha^* w_D^* g_D^* V_{Ls}(23)\, P^M(23) g_D w_D \chi_\alpha d\tau \\
&= 6\,\frac{c^2}{1+c^2}\,\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} m_\nu\, {}^{Ls}U_\kappa^\nu \left(\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\right)^{5/2}
\end{aligned}
\qquad (9.7.14)
$$

Consider the second term on the R.H.S. of equation (9.7.9), that is the integral

$$\frac{4c^2}{1+c^2}\int \chi_\alpha w_D^* g_D^* V_{Ls}(24) g_D w_D \chi_\alpha d\tau$$

$$= \frac{36c^2}{1+c^2} N_D^2 \hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} {}^{Ls}U_\kappa^\nu \int d\underline{u}d\underline{v}d\underline{w}\,[3v^2(\underline{r}_{24}\cdot\underline{w})+(\underline{r}_{24}\cdot\underline{v})\times$$

$$(\underline{v}\cdot\underline{w})-3w^2(\underline{r}_{24}\cdot\underline{v})-(\underline{r}_{24}\cdot\underline{w})(\underline{v}\cdot\underline{w})]\exp\{-2\beta(2u^2+v^2+w^2)-$$

$${}^{Ls}\mu_\kappa^\nu\,(\underline{u}+\underline{v}/2-\underline{w}/2)^2\} \qquad (9.7.15)$$

$$= \frac{36c^2}{1+c^2} N_D^2 \hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} {}^{Ls}U_\kappa^\nu \int d\underline{u}d\underline{v}d\underline{w}\,[3v^2(\underline{r}_{24}\cdot\underline{w}) +$$

$$(\underline{r}_{24}\cdot\underline{v})(\underline{v}\cdot\underline{w})-3w^2(\underline{r}_{24}\cdot\underline{v})-(\underline{r}_{24}\cdot\underline{w})(\underline{v}\cdot\underline{w})]\exp\{-\xi(\underline{u}-\gamma(\underline{w}-\underline{v}))^2-$$

$$\delta(\underline{v}\cdot\eta\underline{w})^2-\varkappa w^2\} \qquad (9.7.16)$$

where $\xi = 4\beta+{}^{Ls}\mu_\kappa^\nu$; $\gamma = {}^{Ls}\mu_\kappa^\nu/2\xi$;

$\delta = \beta(8\beta+3{}^{Ls}\mu_\kappa^\nu)/\,4\beta+{}^{Ls}\mu_\kappa^\nu$; $\eta = {}^{Ls}\mu_\kappa^\nu/8\beta+3{}^{Ls}\mu_\kappa^\nu$;

and

$$\varkappa = 8\beta(2\beta+{}^{Ls}\mu_\kappa^\nu)/8\beta+3{}^{Ls}\mu_\kappa^\nu \; . \qquad (9.7.17)$$

Using the transformations

$\underline{s} = \underline{u} - \gamma(\underline{w}-\underline{v})$, $\underline{s}' = \underline{v}-\eta\underline{w}$ and $\underline{\rho} = \underline{w}$, the above integration leads to

$$-2\frac{c^2}{1+c^2}\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}\left(1+\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\right)\left(\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\right)^{5/2} {}^{Ls}U_\kappa^\nu \qquad (9.7.18)$$

Thus $\frac{4c^2}{1+c^2} w_{Ls} \int \chi_\alpha^* w_D^* g_D^* V_{Ls}(24) g_D w_D \chi_\alpha d\tau$

$$= -3\frac{c^2}{1+c^2}\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} w_\nu\, {}^{Ls}U_\kappa^\nu \left(\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\right)^{5/2}\left(1+\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\right) \qquad (9.7.19)$$

Hence $w_{Ls} \frac{c^2}{1+c^2} \int \chi_\alpha^* w_D^* g_D^* \sum_{i>=2}^{5} V_{Ls}(ij)\ g_D w_D \chi_\alpha d\tau$

$$= -\frac{3c^2}{1+c^2} \hbar^2 \sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} w_\nu\ {}^{Ls}U_\kappa^\nu \left(\frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right)^{5/2} x$$

$$\left[3 + \frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right] \qquad (9.7.20)$$

By the same procedure as above it can easily be shown that evaluating the expression

$$\frac{4c^2}{1+c^2} \int \chi_\alpha^* w_D^* g_D^* V_{Ls}(24) P^M(24) g_D w_D \chi_\alpha d\tau$$

leads to the following result

$$3 \frac{c^2}{1+c^2} \hbar^2 \sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} {}^{Ls}U_\kappa^\nu \left(\frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right)^{5/2} \left(1 - \frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right)$$

Thus we obtain

$$\frac{c^2}{1+c^2} m_{Ls} \int \chi_\alpha^* w_D^* g_D^* \sum_{i>j=2}^{5} V_{Ls}(ij)\ P^M(ij)\ g_D w_D \chi_\alpha d\tau$$

$$= 3 \frac{c^2}{1+c^2} \hbar^2 \sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} m_\nu\ {}^{Ls}U_\kappa^\nu \left(\frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right)^{5/2} x$$

$$\left(3 - \frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right) \qquad (9.7.21)$$

and hence finally

$$\left\langle {}^5D_o^{(1)*} \middle| V_{Ls}(ij)(w+mM_{ij})_\nu \middle| {}^5D_o^{(1)} \right\rangle$$

$$= -3 \frac{c^2}{1+c^2} \hbar^2 \sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} {}^{LS}U_\kappa^\nu \left[3(w-m)_\nu \left(\frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right)^{5/2} + \right.$$

$$\left. (w+m)_\nu \left(\frac{2\beta}{2\beta + {}^{Ls}\mu_\kappa^\nu}\right)^{7/2}\right] \qquad (9.7.22)$$

§9.8 THE CONTRIBUTION OF THE QUADRATIC SPIN-ORBIT FORCE TO THE B.E.(He^4)

So far we have been considering the contributions of the central, linear spin-orbit and tensor forces to the B.E.(He^4). No attempts were made in recent years to include the contribution of the quadratic spin-orbit force to the binding energies of light nuclei. H. Kanada et al. (1963) claimed that even in the scattering problem of N-He^4 the contribution of the quadratic spin-orbit force could be neglected because of its very small contribution. In their calculation of the B.E.(He^4) they neglected this effect. In our work the effect is taken into account.

The S-S and the S-D contributions of the quadratic spin-orbit force to the B.E.(He^4) can easily be shown to vanish. Thus, only the D-D terms contribute. In this section we shall not give the detailed analysis of the calculations as the approach is exactly the same as in Chapter VI.

Consider the LL potential with the ordinary Wigner operator. Its expectation value in the D-state is given by

$$w_{LL}\left\langle {}^5D_o^{(1)*}\middle|Q_{LL}(ij)\middle|{}^5D_o^{(1)}\right\rangle$$

$$= \frac{c^2}{1+c^2}\, w_{LL}\int \chi_\alpha^* w_D^* g_D^* \sum_{i>j=2}^{5} Q_{LL}(ij)\, g_D w_D \chi_\alpha \, d\tau \qquad (9.8.1)$$

where

$$Q_{LL}(ij) = V_{LL}(ij)\left[(\underline{\sigma}_i\cdot\underline{\sigma}_j)\underline{L}_{ij}^2 - \tfrac{1}{2}\{(\underline{\sigma}_i\cdot\underline{L}_{ij})(\underline{\sigma}_j\cdot\underline{L}_{ij}) + (\underline{\sigma}_j\cdot\underline{L}_{ij})(\underline{\sigma}_i\cdot\underline{L}_{ij})\}\right]$$

$$= V_{LL}(ij)\left[(\underline{\sigma}_i\cdot\underline{\sigma}_j)\underline{L}_{ij}^2 - Q_{ij}\right] \qquad (9.8.2)$$

$\underline{L}_{ij}$ has previously been defined.

The potential shape is chosen to be of the form:

$$V_{LL}(ij) = \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} {}^{LL}U_{\kappa}^{\nu} \exp\{-{}^{LL}\mu_{\kappa}^{\nu} r_{ij}^{2}\} \qquad (9.8.3)$$

It can be shown that the evaluation of the integration in (9.8.1) leads to

$$\frac{2}{3}\frac{c^2}{1+c^2}\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} w_{\nu}\, {}^{LL}U_{\kappa}^{\nu}\left[2\left(\frac{2\beta}{2\beta+{}^{LL}\mu_{\kappa}^{\nu}}\right)^{5/2} - 9\left(\frac{2\beta}{2\beta+{}^{LL}\mu_{\kappa}^{\nu}}\right)^{7/2}\right] \qquad (9.8.4)$$

Hence we obtain

$$\left\langle {}^{5}D_{o}^{*(1)} \middle| Q_{LL}(ij)(w_{LL}+m_{LL}P^{M}(ij) + b_{LL}P^{B}(ij) + h_{LL}P^{H}(ij)) \middle| {}^{5}D_{o}^{(1)} \right\rangle$$

$$= \frac{2}{3}\frac{c^2}{1+c^2}\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{LL}U_{\kappa}^{\nu}\left[2(w-m+b-h)_{\nu}\left(\frac{2\beta}{2\beta+{}^{LL}\mu_{\kappa}^{\nu}}\right)^{5/2} - 9(w+m+b+h)_{\nu}\left(\frac{2\beta}{2\beta+{}^{LL}\mu_{\kappa}^{\nu}}\right)^{7/2}\right] \qquad (9.8.5)$$

§ 9.9 THE CONTRIBUTION OF THE "HARD CORE" TO THE B.E.(He^4)

We now consider the effect of the "hard core" on the B.E. (He^4). Our method of approach will be the same as the method used for a two-body problem by Brueckner (1958). Since we want our potential to vanish at the core radius and also we want it to be infinitely replusive inside the hard core, we shall assume that

$$\varphi(r)\, rV(r) \rightarrow \delta(|r|-r_c) \qquad (9.9.1)$$

where r_c is the core radius and $\varphi(r)$ is the spatial part of the wave function and r is the distance between two

particles. It therefore follows from equation (9.9.1) that the contribution from the potential terms is zero. Hence the only contribution arises from the energy term and this will be calculated below.

When the effect of the hard core is taken into consideration, the limits of integrations become very complicated and thus care must be taken to see that the correct limits of integrations are used. To avoid prohibitively complex mathematical analysis the small contribution from the D-D terms will be neglected.

The energy operator term is given by

$$T_{2345} = T_{2-345} + T_{3-45} + T_{45}$$

$$= -\frac{\hbar^2}{2M}\left(\frac{4}{3}\nabla^2_{2-345} + 3/2\ \nabla^2_{3-45} + {}^2/_1\nabla^2_{45}\right) \quad (9.9.2)$$

The following co-ordinate system will be considered:

$$\left.\begin{aligned} \underline{s}' &= \underline{r}_2 - \tfrac{1}{2}(\underline{r}_3+\underline{r}_4+\underline{r}_5) \\ \underline{\rho} &= \underline{r}_3 - \tfrac{1}{2}(\underline{r}_4+\underline{r}_5) \\ \underline{\rho}' &= \underline{r}_4 - \underline{r}_5 \end{aligned}\right\} \quad (9.9.3)$$

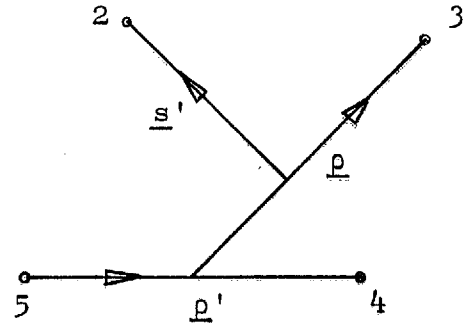


Fig. IV

Consider $\langle {}^1S_o{}^* | T_{2345} | {}^1S_o \rangle$

$$= \frac{N_S^2}{1+c^2} \int \exp\{-\frac{\alpha}{2} \sum_{i>j=2}^{5} r_{ij}^2\}(T_{2345})\exp\{-\frac{\alpha}{2} \sum_{i>j=2}^{5} r_{ij}^2\}d\tau \quad (9.9.4)$$

where

$$\sum_{i>j=2}^{5} r_{ij}^2 = (3s'^2 + 8\rho^2/3 + 2\rho'^2) \quad (9.9.5)$$

Thus we have

$$\exp\{-\frac{\alpha}{2}\sum_{i>j=2}^{5} r_{ij}^2\}(T_{2345})\exp\{-\frac{\alpha}{2}\sum_{i>j=2}^{5} r_{ij}^2\}$$

$$= -2\alpha\frac{\hbar^2}{M}[\alpha(3s'^2+8\rho^2/3+2\rho'^2)-9]\exp\{-\alpha(3s'^2+8\rho^2/3+2\rho'^2)\} \qquad (9.9.6)$$

So equation (9.9.4) becomes

$$I \equiv -2\alpha^2\frac{\hbar^2}{M}\frac{N_S^2}{1+c^2}\iiint(-\frac{\partial}{\partial\alpha})\exp\{-\alpha(3s'^2+8\rho^2/3+2\rho'^2)\}\,x$$

$$d\underline{s}'d\underline{\rho}d\underline{\rho}' + 18\alpha\frac{\hbar^2}{M}\frac{N_S^2}{1+c^2}\iiint\exp\{-\alpha(3s'^2+8\rho^2/3+2\rho'^2)\}$$

$$x\, d\underline{s}'d\underline{\rho}d\underline{\rho}' \qquad (9.9.7)$$

Further, consider the following integral

$$I' \equiv \iiint\exp\{-\alpha(3s'^2+8\rho^2/3+2\rho'^2)\}\,d\underline{s}'d\underline{\rho}d\underline{\rho}' \qquad (9.9.8)$$

THE LIMITS OF INTEGRATIONS

The limits of integrations are

(a) $0 < |\underline{s}'| \leqslant \underline{r}_c$, (b) $0 < |\underline{\rho}| \leqslant \underline{r}_c$, (c) $0 < |\underline{\rho}'| \leqslant \underline{r}_c$

(d) $|\underline{s}'-{}^2/3\underline{\rho}| \leqslant \underline{r}_c$ (e) $|\underline{\rho}\pm\frac{1}{2}\underline{\rho}'| \leqslant \underline{r}_c$ and

(f) $|\underline{s}'+{}^1/3\underline{\rho}\pm\frac{1}{2}\underline{\rho}'| \leqslant \underline{r}_c$ (9.9.9)

For the angular part of the integrations we have the following limits:

(g) $\cos\theta_{34} \leqslant \pm(r_c^2 - \rho^2 - \rho'^2)/\rho\rho'$

(h) $\cos\theta_{23} \leqslant -(r_c^2 - s'^2 - {}^4/9\rho^2)/\frac{4}{3}s'\rho$

$$\text{(i)} \quad \cos\theta_{23} \leqslant (r_c^2 - s'^2 - {}^1/9\rho^2 - {}^1/4\rho'^2)/\tfrac{2}{3}s'\rho \qquad (9.9.10)$$

The integration with respect to $\underline{\rho}'$ is performed over a solid angle. We may write equation (9.9.8) as

$$I' = 2(2\pi)^3 \int_{x_2}^{x_1} \sin\theta_{23}\, d\theta_{23} \int_{x_4}^{x_3} \sin\theta_{34}\, d\theta_{34}\, x \int_0^{r_c}\int_0^{r_c}\int_0^{r_c} \exp\{-\alpha(3s'^2+8\rho^2/3+2\rho'^2)\}s'^2\rho^2\rho'^2\, ds'd\rho d\rho' \qquad (9.9.11)$$

where

$$x_1 \equiv \cos\theta_{23} = \frac{3}{2s'\rho}(r_c^2 - s'^2 - {}^1/9\rho^2 - {}^1/4\rho'^2)$$

$$x_2 \equiv \cos\theta_{23} = -\frac{3}{4s'\rho}(r_c^2 - s'^2 - {}^4/9\rho^2)$$

$$x_3 \equiv \cos\theta_{34} = \frac{1}{\rho\rho'}(r_c^2 - \rho^2 - \rho'^2)$$

and $$x_4 \equiv \cos\theta_{34} = -\frac{1}{\rho\rho'}(r_c^2 - \rho^2 - \rho'^2) \qquad (9.9.12)$$

We have

$$\int_{x_2}^{x_1} \sin\theta_{23}\, d\theta_{23} \int_{x_4}^{x_3} \sin\theta_{34}\, d\theta_{34} = \frac{3}{2s'\rho'\rho^2}(3r_c^2-3s'^2-{}^2/3\rho^2-\tfrac{1}{2}\rho'^2)(r_c^2-\rho^2-\rho'^2)$$

and so equation (9.9.11) becomes

$$I' \equiv 3(2\pi)^3 \int_0^{r_c}\int_0^{r_c}\int_0^{r_c} (3r_c^2-3s'^2-{}^2/3\rho^2-\tfrac{1}{2}\rho'^2)(r_c^2-\rho^2-\rho'^2)\, x\, s'\rho'\exp\{-\alpha(3s'^2+8\rho^2/3+2\rho'^2)\}\, ds'd\rho d\rho' \qquad (9.9.13)$$

Consider the expression

$$D_1 \equiv \int_0^{r_c} (3r_c^2-3s'^2-{}^2/3\rho^2-\tfrac{1}{2}\rho'^2)s'e^{-\lambda s'^2}\, ds' \qquad (\lambda = 3\alpha)$$

$$= \frac{1}{2\lambda}[\,3r_c^2-{}^2/3\rho^2-\tfrac{1}{2}\rho'^2-{}^3/\lambda] + \frac{1}{2\lambda}\left[\frac{2}{3}\rho^2+\tfrac{1}{2}\rho'^2+\frac{3}{\lambda}\right] e^{-\lambda r_c^2}$$

Therefore

$$I' = -3(2\pi)^3 \frac{1}{2\lambda}(1-e^{-\lambda r_c^2}) \int_o^{r_c}\int_o^{r_c} (\frac{2}{3}\rho^2+\tfrac{1}{2}\rho'^2+\frac{3}{\lambda})\ x$$

$$(r_c^2-\rho^2-\rho'^2)\rho' \exp\{-\alpha(8\rho^2/3+2\rho'^2)\}d\rho d\rho' +$$

$$\frac{9r_c^2}{2\lambda}(2\pi)^3 \int_o^{r_c}\int_o^{r_c}(r_c^2-\rho^2-\rho'^2)\rho' \exp[-\alpha(8\rho^2/3$$

$$+ 2\rho'^2)\}\ d\rho d\rho' \qquad (9.9.14)$$

In tackling the evaluation of I' we consider first the following integral

$$D_2 \equiv \int_o^{r_c}\int_o^{r_c}(r_c^2-\rho^2-\rho'^2)\rho' \exp\{-\alpha(8\rho^2/3 + 2\rho'^2)\}d\rho d\rho'$$

$$= \frac{r_c}{8\alpha^2}[2\alpha r_c^2-(1-e^{2\alpha r_c^2})]\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}} \exp(-x^2)dx +$$

$$\frac{r_c^3}{4\alpha}(1-e^{2\alpha r_c^2})(\frac{\partial}{\partial t})\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}} \exp(-x^2)dx \qquad (9.9.15)$$

where $t = \frac{8\alpha}{3} r_c^2$.

Thus we have

$$\frac{9r_c^2}{2\lambda}(2\pi)^3 \int_o^{r_c}\int_o^{r_c}(r_c^2-\rho^2-\rho'^2)\rho' \exp\{-\alpha(8\rho^2/3+2\rho'^2)\}d\rho d\rho'$$

$$= 3/2\ (\frac{\pi r_c}{\alpha})^3[2\alpha r_c^2-(1-e^{-2\alpha r_c^2})]\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}} \exp(-x^2)dx +$$

$$3\alpha r_c^2\ (\frac{\pi r_c}{\alpha})^3(1-e^{-2\alpha r_c^2})(\frac{\partial}{\partial t})\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}}\exp(-x^2)dx$$

$$\equiv I_1 \text{ (say)} \qquad (9.9.16)$$

We now consider the last integral in equation (9.9.14), that is,

$$\int_o^{r_c}\int_o^{r_c}(\frac{2}{3}\rho^2+\tfrac{1}{2}\rho'^2+3/\lambda)(r_c^2-\rho^2-\rho'^2)\rho' \exp[-\alpha(8\rho^2/3 + 2\rho'^2)]$$

$$x\ d\rho d\rho'$$

$$= \frac{r_c}{16\alpha^3}\left[(5\alpha r_c^2-3)+(\alpha r_c^2+3)e^{-2\alpha r_c^2}\right]\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}}\exp(-x^2)dx -$$

$$\frac{r_c^3}{48\alpha^2}\left[(1-e^{-2\alpha r_c^2})(8\alpha r_c^2-19)+14\alpha r_c^2 e^{-2\alpha r_c^2}\right](\frac{\partial}{\partial t})\ x$$

$$\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}}\exp(-x^2)dx - \frac{r_c^5}{6\alpha}(1-e^{-2\alpha r_c^2})(\frac{\partial^2}{\partial t^2})\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}}\exp(-x^2)dx$$

(9.9.17)

Hence we get the result

$$-3(2\pi)^3\frac{1}{2\lambda}(1-e^{-\lambda r_c^2})\int_o^{r_c}\int_o^{r_c}(\frac{2}{3}\rho^2+\frac{1}{2}\rho'^2+\frac{3}{\lambda})(r_c^2-\rho^2-\rho'^2)\rho'\ x$$

$$\exp\{-\alpha(8\rho^2/3+2\rho'^2)\}\,d\rho d\rho'$$

$$= -\frac{r_c}{4\alpha}(\frac{\pi}{\alpha})^3(1-e^{-3\alpha r_c^2})\left[(5\alpha r_c^2-3)+(\alpha r_c^2+3)e^{-2\alpha r_c^2}\right]\frac{1}{\sqrt{t}}\ x$$

$$\int_o^{\sqrt{t}}\exp(-x^2)dx + \frac{2}{3}(\frac{\pi r_c}{\alpha})^3(1-e^{-3\alpha r_c^2})\left[(1-e^{-2\alpha r_c^2})\ x\right.$$

$$\left.(8\alpha r_c^2-19)+14\alpha r_c^2 e^{-2\alpha r_c^2}\right](\frac{\partial}{\partial t})\frac{1}{\sqrt{t}}\int_o^{\sqrt{t}}\exp(-x^2)dx +$$

$$\frac{2}{3}\alpha r_c^2(\frac{\pi r_c}{\alpha})^3(1-e^{-3\alpha r_c^2})(1-e^{-2\alpha r_c^2})(\frac{\partial^2}{\partial t^2})\frac{1}{\sqrt{t}}\ x$$

$$\int_o^{\sqrt{t}}\exp(-x^2)dx$$

$$\equiv I_2 \text{ (say)} \qquad (9.9.18)$$

To simplify the above expressions, that is, I_1 and I_2, we use the following relations:

$$D^2(uv) = vD^2v + 2DuDv + uD^2V \qquad (9.9.19)$$

where $D^2 \equiv \frac{\partial^2}{\partial t^2}$

Thus if $I = \int_o^{U(x)} f(x)\,dx$

Then $\frac{dI}{dx} = \frac{dI}{du}\frac{du}{dx}$ (9.9.20)

Hence $\frac{\partial}{\partial t}\ \frac{1}{\sqrt{t}}\ \int_o^{\sqrt{t}} \exp(-x^2)dx = -\frac{1}{2t\sqrt{t}} \int_o^{\sqrt{t}} \exp(-x^2)dx + \frac{1}{2t}\ e^{-t}$

Also we have

$$\frac{\partial^2}{\partial t^2}\ \frac{1}{\sqrt{t}}\ \int_o^{\sqrt{t}} \exp(-x^2)dx = \frac{3}{4t^2\sqrt{t}}\ \int_o^{\sqrt{t}} \exp(-x^2)dx - \frac{3}{4t^2}\ e^{-t} - \frac{1}{2}e^{-t} \qquad (9.9.21)$$

Thus we obtain

$$I' = \frac{N_S^2}{1+c^2}\ (I_1+I_2) = \frac{2^6\alpha^{9/2}}{(1+c^2)\pi^{9/2}}\ (I_1+I_2)$$

$$= \frac{1}{1+c^2}\ (\frac{\alpha}{\pi})^{3/2}\ \frac{r_c}{2\alpha}\ \Big[\{(1-e^{-2\alpha r_c^2})(1-e^{-3\alpha r_c^2})(409-96\alpha r_c^2)$$

$$+ 24\alpha r_c^2\ [8\{2\alpha r_c^2-(1-e^{-3\alpha r_c^2})\} - 11] +$$

$$8\alpha r_c^2(5+28e^{-3\alpha r_c^2})e^{-2\alpha r_c^2}\}\ \frac{1}{\sqrt{t}}\ \int_o^{\sqrt{t}} \exp(-x^2)dx +$$

$$(1-e^{-2\alpha r_c^2})\{\ [(112\alpha r_c^2-313)(1-e^{-3\alpha r_c^2})+72\alpha r_c^2]+$$

$$224\alpha r_c^2(1-e^{-3\alpha r_c^2})(e^{-2\alpha r_c^2}\}\ e^{-t}\ \Big] \qquad (9.9.22)$$

Hence equation (9.9.7) becomes

$$I = (\frac{\alpha}{\pi})^{3/2}\ r_c\ \frac{\hbar^2}{M}\ (5+\ \alpha\ \frac{\partial}{\partial\alpha})\ \Big[\{(1-e^{-2\alpha r_c^2})(1-e^{-3\alpha r_c^2})\ x$$

$$(409-96\alpha r_c^2)+24\alpha r_c^2\ [8\{2\alpha r_c^2-(1-e^{-3\alpha r_c^2})\} - 11] +$$

$$8\alpha r_c^2(5+28e^{-3\alpha r_c^2})e^{-2\alpha r_c^2}\}\ \frac{1}{\sqrt{t}}\ \int_o^{\sqrt{t}} \exp(-x^2)dx +$$

$$[(1-e^{-2\alpha r_c^2})\{(112\alpha r_c^2-313)(1-e^{-3\alpha r_c^2})+72\alpha r_c^2\} +$$

$$224\alpha r_c^2(1-e^{-3\alpha r_c^2})e^{-2\alpha r_c^2}\ ]\ e^{-t}\ \Big] \qquad (9.9.23)$$

where $t = \frac{8\alpha}{3}\ r_c^2$. (9.9.24)

I is the total contribution of the hard core to the B.E.(He^4).

§9.10 FINAL RESULT FOR B.E.(He^4)

The total contribution of the kinetic energy, central, linear, spin-orbit, tensor and quadratic spin-orbit forces, the coulomb energy and the hard core effect to the B.E.(He^4) is given in the following form:

$$(1+c^2)E_\alpha = \frac{\hbar^2}{2M}(18\alpha+26\beta c^2) + \sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{c}U_\kappa^\nu \Big[6(w+m)_\nu \times$$

$$\Big(\frac{2\alpha}{2\alpha+{}^{c}\mu_\kappa^\nu}\Big)^{3/2} + c^2\Big\{\tfrac{5}{2}(w+m+b+h)_\nu \Big(\frac{2\beta}{2\beta+{}^{c}\mu_\kappa^\nu}\Big)^{3/2} +$$

$$3(w-m+b-h)_\nu \Big(\frac{2\beta}{2\beta+{}^{c}\mu_\kappa^\nu}\Big)^{5/2} + \tfrac{1}{2}(w+m+b+h)_\nu \Big(\frac{2\beta}{2\beta+{}^{c}\mu_\kappa^\nu}\Big)^{7/2}\Big\}\Big]$$

$$- 3c^2\hbar^2 \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} {}^{Ls}U_\kappa^\nu \Big[3(w-m)_\nu \Big(\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\Big)^{5/2} + (w+m)_\nu \times$$

$$\Big(\frac{2\beta}{2\beta+{}^{Ls}\mu_\kappa^\nu}\Big)^{7/2}\Big] - \sum_{\kappa=1}^{2}\sum_{\nu=3}^{4} {}^{T}U_\kappa^\nu \Big[6\sqrt{5}\, c(w+m)_\nu \Big(\frac{2\alpha}{\alpha+\beta}\Big)\Big(\frac{2\beta}{\alpha+\beta}\Big)^2 \times$$

$$\Big(\frac{2\sqrt{\alpha}\beta}{\alpha+\beta+{}^{T}\mu_\kappa^\nu}\Big)^{5/2} \frac{1}{\alpha+\beta+{}^{T}\mu_\kappa^\nu} + c^2\Big\{\frac{21}{2}(w-m)_\nu \Big(\frac{2\beta}{2\beta+{}^{T}\mu_\kappa^\nu}\Big)^{5/2} +$$

$$\frac{7}{2}(w+m)_\nu \Big(\frac{2\beta}{2\beta+{}^{T}\mu_\kappa^\nu}\Big)^{7/2}\Big\} \frac{1}{2\beta+{}^{T}\mu_\kappa^\nu}\Big] + \frac{2}{3}c^2\hbar^2 \times$$

$$\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} {}^{LL}U_\kappa^\nu \Big[2(w-m+b-h)_\nu \Big(\frac{2\beta}{2\beta+{}^{LL}\mu_\kappa^\nu}\Big)^{5/2} - 9(w+m+b+h)_\nu \times$$

$$\Big(\frac{2\beta}{2\beta+{}^{LL}\mu_\kappa^\nu}\Big)^{7/2}\Big] + \frac{2}{3}e^2\Big[3\Big(\frac{2\alpha}{\pi}\Big)^{\frac{1}{2}} + 2c^2\Big(\frac{2\beta}{\pi}\Big)^{\frac{1}{2}}\Big] + \Big(\frac{\alpha}{\pi}\Big)^{3/2} \times$$

$$r_c \frac{\hbar^2}{M}\Big(5+\alpha\frac{\partial}{\partial\alpha}\Big)\Big[\{(1-e^{-2\alpha r_c^2})(1-e^{-3\alpha r_c^2})(409-96\alpha r_c^2)$$

$$+ 24\alpha r_c^2\Big[8\{2\alpha r_c^2-(1-e^{-3\alpha r_c^2})\}-11\Big] + 8\alpha r_c^2 \times$$

$$(5+28e^{-3\alpha r_c^2})e^{-2\alpha r_c^2}\Big\}\frac{1}{\sqrt{t}}\int_0^{\sqrt{t}}\exp(-x^2)dx +$$

$$+ \left[(1-e^{-2\alpha r_c^2})\{(112\alpha r_c^2-313)(1-e^{-3\alpha r_c^2})+72\alpha r_c^2\}\right.$$

$$\left. + 224\alpha r_c^2(1-e^{-3\alpha r_c^2})e^{-2\alpha r_c^2}\right]e^{-t}\Big] \qquad (9.10.1)$$

§9.11 RESULTS OF THE VARIATIONAL CALCULATIONS OF THE BINDING ENERGY OF He^4

The B.E. (He^4) is calculated from equation (9.10.1) using Hamada and Johnston's potentials expressed in double Gaussian forms (Hochberg et al.,1968). The B.E. (He^4) is found to be -58.457 MeV (c.f. -120 MeV obtained by H. Kanada et al.). When α is fixed to be 0.140 fm^{-2} (as is well established from high energy e-He^4 scattering) the B.E.(He^4) is found to be -26.038 MeV (c.f. -23.341 MeV and -33 MeV obtained by H. Kanada et al. and Nagata et al. respectively). Our results in detail are as follows.

TABLE I

B.E.(He^4)

Type	State	Coupled State	Contribution for B.E.(He^4) (MeV)
Kinetic Energy	(	SS	51.1027572
	(		
	(	DD	2.90721623
Coulomb Energy	(	SS	0.845026793
	(		
	(	DD	0.0162066586
Hardcore		SS	- 3.87538170

cont...

TABLE I (cont.)

Type	State	Coupled State	Contribution for B.E.(He^4) (MeV)
Central	$^1V^+$	SS	-47.3475852
		DD	0.0000000
	$^1V^-$	SS	0.0000000
		DD	0.0000000
	$^3V^+$	SS	-22.8152930
		DD	- 0.775156457
	$^3V^-$	SS	0.00000000
		DD	- 0.0646799367
Spin-Orbit	$^3V^+$	SS	0.00000000
		DD	- 0.0142644582
	$^3V^-$	SS	0.00000000
		DD	0.962596191
Tensor	$^3V^+$	SD	- 6.82400751
		DD	0.0597416108
	$^3V^-$	SD	0.00000000
		DD	- 0.189037152

cont..

TABLE I (cont.)

Type	State	Coupled State	Contribution for B.E.(He^4) (MeV)
Quadratic Spin-Orbit	$^1V^+$	SS	0.0000000
		DD	0.0000000
	$^1V^-$	SS	0.0000000
		DD	0.0000000
	$^3V^+$	SS	0.0000000
		DD	-0.0330651863
	$^3V^-$	SS	0.00000000
		DD	0.00653934800
TOTAL ($E_{\alpha(min)}$)			-26.0383865

α = 0.140 fm^{-2}, β = 0.262399998 fm^{-2} and c = -0.144960001 which give the minimum value of the B.E.(He^4).

§9.12 CONCLUSION

The B.E.(He^4) was calculated by the Direct Search Method (R. Hooke and T.A. Jeeves, 1961; and A.F. Kaupe, Jr., 1963) which was modified by the author to avoid any square root of a negative argument during computing processes. The B.E.(He^4) is found to be -26.038 MeV, as compared with the experimental value of -28.2 MeV. When c is fixed to be -0.2, the B.E. (He^4) is found to be

-57.432 MeV with α = 0.432 fm^{-2} and β = 0.473 fm^{-2}. Sugie et al. obtained $E_{\alpha(min)}$ to be -17.8 MeV with α = 0.195 fm^{-2}, β = 0.307 fm^{-2} and c = -0.19 by parabolic interpolation method. If Sugie et al. had assumed α to be 0.140 fm^{-2} as in our case their results would have been $E_{\alpha(min)}$ = -15.7 MeV, β = 0.241 fm^{-2} and c = -0.177.

It should be pointed out that the inclusion of additional D-states in the wave function for the He^4 will definitely increase the B.E. (He^4) (Abraham et al. (1955)), so that a value very close to the experimental value of -28.2 MeV may be obtained. An attempt is being made to include the second most important D-state in the calculation of this kind. Thus from the above results we conclude that the B.E. (He^4) may be calculated using a two-body interaction which accounts for the N-N scattering (up to 300 MeV) and deuteron data.

PART IV

NUMERICAL ANALYSIS AND COMPUTATION

CHAPTER X

THE COMPLETE INTEGRO-DIFFERENTIAL EQUATIONS FOR THE ELASTIC SCATTERING OF NEUTRON BY ALPHA PARTICLES

§ 10.1 As pointed out previously, coupled equations do not arise in the analysis of the scattering of neutron by alpha particles. We shall therefore write down the full integro-differential equations for the uncoupled states for the radial wave functions. We shall collect the results obtained in Chapters IV to VIII and regroup the terms in a way convenient for numerical calculations.

Below are the complete integro-differential equations (for both the S- and D-states alpha wave functions) including the linear spin-orbit interaction, tensor interaction and the quadratic spin-orbit interaction.

$$\mathcal{D}_\ell^2 f_{\ell J}(r) = T_{\ell(r)} \frac{1}{r^2} f_{\ell J}(r) + U_{\ell(r)} f_{\ell J}(r) + V_{\ell(r)} \times \frac{1}{r}\frac{d}{dr} f_{\ell J}(r) + W_{\ell(r)} \frac{d^2}{dr^2} f_{\ell J}(r) + \int_o^\infty \left[N_\ell(r,r') + P_\ell(r,r') + S_\ell(r,r') + K_\ell(r,r') \right] f_{\ell J}(r')dr' \qquad (10.1.1)$$

where $\ell = J+\frac{1}{2}$ and $\ell = J-\frac{1}{2}$.

$$\mathcal{D}_\ell^2 = \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2 \qquad (10.1.2)$$

$$k^2 = \frac{8M}{5\hbar^2} E_n$$

and

$$T_{\ell(r)} = {}^{Q}t_\ell(r)$$

$$U_{\ell(r)} = {}^{C}U(r) + {}^{Ls}U_\ell(r) + {}^{coul}U(r)$$

$$V_{\ell(r)} = {}^{Q}V(r)$$

$$W_{\ell(r)} = {}^{Q}w(r)$$

$$K_{\ell(r,r')} = {}^{C}K_{\ell}(r,r') + {}^{Ls}K_{\ell}(r,r') + {}^{Q}K_{\ell}(r,r') + {}^{coul}K_{\ell}(r,r') + {}^{T}K'_{\ell}(r,r') + {}^{T}K''_{\ell}(r,r')$$

The above terms represent the contributions from the various interactions indicated by the symbols attached. The prime and the double prime symbols denote the S-D and the D-S interactions respectively. In writing down the S-D and the D-S terms we shall omit the indices and the prime symbols when there is no confusion.

THE S-S DIRECT TERMS

(i) THE POTENTIAL TERMS

$$Q_{t_{\ell}}(r) = -\frac{8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4} 2(m-2b)_{\nu}\frac{LL_{U}{}^{\nu}_{\kappa}}{1+c^2}\left(\frac{16}{15}\right)^2\frac{\ell(\ell+1)}{\lambda_{LL}(\kappa)}\ x$$

$$P_{LL}^{3/2}(\kappa)\ \exp\left[-P_{LL}(\kappa)\ {}^{LL}\mu_{\kappa}^{\nu}\ r^2\right]$$

and

$$C_{U(r)} = \frac{8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}(4w+2b-m-2h)_{\nu}\frac{C_{U}{}^{\nu}_{\kappa}}{1+c^2}\ P_{c}^{3/2}(\kappa)\ x$$

$$\exp\left[-P_{c}(\kappa)\ {}^{C}\mu_{\kappa}^{\nu}\ r^2\right]$$

$$Ls_{U_{\ell}}(r) = \frac{8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=3}^{4}(w-\tfrac{1}{2}m)_{\nu}\frac{Ls_{U}{}^{\nu}_{\kappa}}{1+c^2}\ \frac{5}{2}\ ||\underline{\sigma}\ \underline{\ell}||\ P_{Ls}^{5/2}(\kappa)\ x$$

$$\exp\left[-\ P_{Ls}(\kappa).\ {}^{Ls}\mu_{\kappa}^{\nu}\ r^2\right]$$

$$coul_{U(r)} = \frac{16M}{5\hbar^2}\ \frac{e^2}{1+c^2}\ \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}}$$

$$Q_{U_{\ell}}(r) = \frac{8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}2(m-2b)_{\nu}\frac{LL_{U}{}^{\nu}_{\kappa}}{1+c^2}\ P_{LL}^{3/2}(\kappa)\left[\frac{135\alpha}{16\lambda_{LL}}-\right.$$

$$\frac{25}{16}\left(1-\frac{3\gamma_{LL}}{4}\right)^2 \ell(\ell+1) + 2\sigma r^2 + 2\eta\Big]\exp\Big[-P_{LL}(\kappa)\,{}^{LL}\mu_{\kappa}^{\nu}\, r^2\Big]$$

and

$$Q_V(r) = \frac{-8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}(2w-4b)_\nu \frac{{}^{LL}U_{\kappa}^{\nu}}{1+c^2} P_{LL}^{3/2}(\kappa)(2\eta r^2)\, x$$

$$\exp\left[-P_{LL}(\kappa)\,{}^{LL}\mu_{\kappa}^{\nu}\, r^2\right]$$

and

$$Q_W(r) = -\frac{1}{\lambda_{LL}(\kappa)}\left(\frac{16}{15}\right)^2 \frac{8M}{5\hbar^2}\sum_{\kappa=1}^{2}\sum_{\nu=1}^{4}(2w-4b)_\nu \frac{{}^{LL}U_{\kappa}^{\nu}}{1+c^2}\, x$$

$$P_{LL}^{3/2}(\kappa)\exp\left[P_{LL}(\kappa)\,{}^{LL}\mu_{\kappa}^{\nu}\, r^2\right]$$

THE S-S INDIRECT TERMS

(ii) THE ENERGY TERMS

$$N_\ell(r,r') = \frac{128}{15}\frac{1}{1+c^2}\left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}}\frac{8M}{5\hbar^2}(E_n+E_\alpha)\exp\left[-\frac{17}{16}\varepsilon(r^2+r'^2)\right]$$

$$x\ \mathcal{J}_{\ell+\frac{1}{2}}(\varepsilon rr')$$

$$P_\ell(r,r') = -\frac{e^2}{1+c^2}\left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}}\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}}\frac{16M}{\alpha\hbar^2}\varepsilon\exp\left[-\frac{17}{16}\varepsilon(r^2+r'^2)\right]$$

$$x\ \mathcal{J}_{\ell+\frac{1}{2}}(\varepsilon rr')$$

$$S_\ell(r,r') = \frac{1}{1+c^2}\left(\frac{16}{15}\right)\left(\frac{3\alpha}{\pi}\right)^{\frac{1}{2}}\varepsilon^2\exp\left[-\frac{17}{16}\varepsilon(r^2+r'^2)\right]x$$

$$\Big[\{38(r^2+r'^2)-\frac{1}{\varepsilon}(49\ell+141)\}\,\mathcal{J}_{\ell+\frac{1}{2}}(\varepsilon rr') +$$

$$49rr'\,\mathcal{J}_{\ell+3/2}(\varepsilon rr')\Big]$$

(iii) THE POTENTIAL TERMS

$$C_{K_\ell}(r,r') = C_{K_\ell}^{(1)}(r,r') + C_{K_\ell}^{(2)}(r,r') + C_{K_\ell}^{(3)}(r,r')$$

where

$$C_{K_\ell}^{(1)}(r,r') = \left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{M}{\hbar^2} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (4m+2h-w-2b)_\nu \; x$$

$$\frac{C_{U_\kappa^\nu}}{1+c^2} \left(\frac{15\pi}{4\alpha-3\,{}^{C}\mu_\kappa^\nu}\right) \exp\left[-\frac{8}{75}(17\alpha+6\,{}^{C}\mu_\kappa^\nu)(r^2+r'^2)\right] x$$

$$\vartheta_{\ell+\frac{1}{2}}(\lambda_c(\kappa)rr')$$

$$C_{K_\ell}^{(2)}(r,r') = -3\left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{M}{\hbar^2} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (w+m)_\nu \; x$$

$$\frac{C_{U_\kappa^\nu}}{1+c^2} \left(\frac{3\pi}{2(2\alpha+{}^{C}\mu_\kappa^\nu)}\right) \eta^{\frac{1}{2}}(\kappa)\Big[\exp\Big[-\frac{4}{75}\eta(\kappa)\{(34\alpha+7\,{}^{C}\mu_\kappa^\nu)r^2 +$$

$$(34\alpha+27\,{}^{C}\mu_\kappa^\nu)r'^2\}\Big]\Big] \vartheta_{\ell+\frac{1}{2}}(\xi(\kappa)rr') + \text{a similar term with } r \rightleftharpoons r'$$

$$C_{K_\ell}^{(3)}(r,r') = -3\left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{M}{\hbar^2} \sum_{\kappa=1}^{2} \sum_{\nu=1}^{4} (w+m)_\nu \frac{C_{U_\kappa^\nu}}{1+c^2}$$

$$\frac{51\pi}{4\alpha} \left(\frac{2\alpha}{2\alpha+{}^{C}\mu_\kappa^\nu}\right)^{3/2} \exp\left[-\frac{17}{16}\varepsilon(r^2+r'^2)\right] \vartheta_{\ell+\frac{1}{2}}(\varepsilon rr')$$

$$Ls_{K_\ell}(r,r') = -\left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{M}{\hbar^2} \sum_{\kappa=1}^{2} \sum_{\nu=3}^{4} (w-2m)_\nu \; x$$

$$\frac{Ls_{U_\kappa^\nu}}{1+c^2} \left(\frac{20\alpha}{4\alpha-3\,{}^{Ls}\mu_\kappa^\nu}\right) \left(\frac{15\pi}{4\alpha-3\,{}^{Ls}\mu_\kappa^\nu}\right) \| \underline{\sigma}\,\underline{\ell} \| \exp\left[-\frac{8}{75} x\right.$$

$$\left.(17\alpha+6\,{}^{Ls}\mu_\kappa^\nu)(r^2+r'^2)\right] \vartheta_{\ell+\frac{1}{2}}(\lambda_{Ls}(\kappa)rr')$$

$$Q_{K_\ell}(r,r') = \left(\frac{16}{15}\right)^3 \left(\frac{3\alpha}{\pi}\right)^{3/2} \frac{M}{\hbar^2} \sum_{k=1}^{2} \sum_{\nu=1}^{4} (2w-4h)_\nu \frac{LL_{U_\kappa^\nu}}{1+c^2} \; x$$

$$\frac{15\pi}{4\alpha-3^{LL}\mu_{\varkappa}^{\nu}}\ \exp\left[-\frac{8}{75}(17\alpha+6^{LL}\mu_{\varkappa}^{\nu})(r^2+r'^2)\right]\Big[\{6-2\zeta(r^2+r'^2)-$$

$$\left(\frac{\omega}{\lambda_{LL}(\varkappa)}\right)^2\ \ell(\ell-1)-4\zeta\ \frac{\ell}{\lambda_{LL}(\varkappa)}\}\ \mathcal{J}_{\ell+\frac{1}{2}}(\lambda_{LL}(\varkappa)rr')\ +$$

$$2(2\zeta\ -\ \frac{\omega^2}{\lambda_{LL}(\varkappa)})rr'\ \mathcal{J}_{\ell+3/2}(\lambda_{LL}(\varkappa)rr')\Big]$$

THE S-D AND THE D-S INDIRECT TERMS

The energy terms give no contribution.

(iv) **THE POTENTIAL TERMS**

$$T_{K'_\ell}(r,r')\ +\ T_{K''_\ell}(r,r')\ =\ -\ \frac{64}{15}\ \left(\frac{3}{5\pi}\right)^{\frac{1}{2}}\ \frac{2^6\alpha^{9/4}\beta^{13/4}}{(\alpha+\beta)^6}\ b^{\frac{1}{2}}d\ \frac{c}{1+c^2}$$

$$x\ \frac{8M}{5\hbar^2}\ \sum_{i=1}^{2}\ \sum_{\varkappa=1}^{2}\ \sum_{\nu=3}^{4}\ (w+m)_\nu\ T_{U_\varkappa^\nu}\ \exp\left[-(\gamma^{(i)}r^2+\delta^{(i)}r^2)\right]\ x$$

$$\Big[\{S_\ell^{(i)}\ -\ 3\left(\frac{16}{15}\right)^2(\alpha+\beta)(T_\ell^{(i)}r^2+T'^{(i)}_\ell r'^2)+9\left(\frac{16}{15}\right)^4(\alpha+\beta)^2$$

$$x\ (U^{(i)}r^4+2U'^{(i)}\ r^2r'^2+U''^{(i)}r'^4)\}\ \mathcal{J}_{\ell+\frac{1}{2}}(\lambda_T(\varkappa)rr')+$$

$$3\left(\frac{16}{15}\right)^2(\alpha+\beta)rr'\ \{-V^{(i)}+3\left(\frac{16}{15}\right)^2(\alpha+\beta)(W^{(i)}r^2+W'^{(i)}r'^2)\}\ x$$

$$\mathcal{J}_{\ell+3/2}(\lambda_T(\varkappa)rr')\ +\ \text{a similar term with}\ \ r\rightleftharpoons r'\ \ +$$

$$\frac{64}{15}\ \left(\frac{3}{5\pi}\right)^{\frac{1}{2}}\ \frac{2^6\alpha^{9/4}\beta^{13/4}d^{7/2}}{(\alpha+\beta)^6}\ \frac{c}{1+c^2}\ \frac{24M}{\hbar^2}\ \sum_{i=1}^{2}\ \sum_{\varkappa=1}^{2}\ \sum_{\nu=3}^{4}\ (w+m)_\nu$$

$$x\ T_{U_\varkappa^\nu}\ \exp\left[-(\rho^{(i)}r^2+\xi^{(i)}r'^2)\right]\ \mathcal{J}_{\ell+\frac{1}{2}}(\tau rr')\ +\ 24\left(\frac{3}{5\pi}\right)^{\frac{1}{2}}\ x$$

$$\frac{2^6\alpha^{9/4}\beta^{13/4}b^{\frac{1}{2}}d^2}{(\alpha+\beta)^6}\ \ ||\underline{\sigma}\ \underline{\ell}||\ \frac{c}{1+c^2}\ \frac{M}{\hbar^2}\ \sum_{i=1}^{2}\ \sum_{\varkappa=1}^{2}\ \sum_{\nu=3}^{4}\ (w+m)_\nu\ x$$

$$T_{U_{\kappa}^{\nu}} \exp\left[-(\gamma^{(i)}r^2+\delta^{(i)}r'^2)\right]\left[\{X_{\ell}-3\left(\frac{16}{15}\right)^2(\alpha+\beta)(Y^{(i)}r^2 + Y'^{(i)}r'^2)\}\vartheta_{\ell+\frac{1}{2}}(\lambda_T(\kappa)rr')-3\left(\frac{16}{15}\right)^2(\alpha+\beta)rr'Z\vartheta_{\ell+3/2}(\lambda_T(\kappa)rr')\right]$$

The definitions of all the parameters are given in Appendix V.

CHAPTER XI

SOLUTIONS OF THE INTEGRO-DIFFERENTIAL EQUATIONS IN NUCLEON-HELIUM ($N\text{-}He^4$) PROBLEMS

§11.1 FORMULATION

Several workers including Southwell (1940), L. Fox (1949) and S. Hochberg (1953) have used relaxation methods with great success to solve the ordinary differential equations associated with physical problems of considerable current importance. S. Hochberg (1953) applied this method to solve the integro-differential equations for $N\text{-}He^4$ scattering problems. His result in terms of phase-shifts were in quite good agreement with the experimental results.

In solving the system of equations (10.1.1) we have to consider first the limitation imposed on the problem by the storage capacity of the computer to be used. The method we are going to adopt here to solve the system of the integro-differential equations given in (10.1.1) is to convert the system into simultaneous algebraic equations with unknowns at the tabulated points of the wave functions. The algebraic equations are then solved by matrix inversion.

In our case, the kernels are tabulated in an n x n array. The solution requires the inversion of an (n-1) x (n-1) matrix for single uncoupled equations (and an m(n-1) x m(n-1) matrix for m coupled equations). In our problem of $n\text{-}He^4$ scattering, we take $n = 52$, with fourteen digits in the calculation. If $n \geqslant 53$, we get exponent overflow. Thus we need only 130 blocks for compilation purposes and about 60 blocks for execution purposes. It took Atlas I

Computer about fifty-five minutes to compute the phase-shift for one value of incident neutron energy (E_n) and for one value of the angular momentum (ℓ).

Because of the Gaussian dependence of the kernels on r and r' the kernels varied most rapidly near the origin and it was necessary to use a small interval of tabulation. Robertson (1956) and Buckingham (1962) suggested two intervals of tabulation so that r and r' are given by

$$r,r' = 0(h)n_1.h\ (2h)\ n_2.h$$

The order n of the sequence array of the kernels is given by

$$n = (\frac{n_1}{2} + n_2)$$

with $n_1 = 16$ and $n_2 = 32$.

§ 11.2 NUMERICAL METHODS

The equations for the radial wave functions to be solved numerically are simultaneous equations of the form:

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} + \frac{1}{r^2}\ T(r) + U(r) + \frac{1}{r}\ V(r)\ \frac{d}{dr} + W(r)\ \frac{d^2}{dr^2}\right] f_\ell(r) + \int_0^\infty K(r,r')\ f_\ell(r')dr' = 0 \qquad (11.2.1)$$

where T, U, V, W and K are defined in Chapter X. The functions T, U, K, etc. have the following properties:

$$K(r,0) = K(0,r') = 0 \qquad (11.2.2)$$

$\frac{1}{r^2}\ T(r)$, $U(r)$, $\frac{1}{r}\ V(r)$, $W(r)$ and $K(r,r')$ vanish at sufficiently large r and/or r'. The boundary conditions on f(r) are

$$f(0) = 0 \quad \text{and} \quad f(h) = 1 \qquad (11.2.3)$$

where h is the interval of integration chosen to give small error terms.

To solve equation (11.2.1), it is written in terms of finite differences and is reduced to a system of linear equations in unknowns

$$f(2h),\quad f(3h)\ \ldots\quad \ldots,\ f(nh)$$

$$\text{i.e. } f(2)\ ,\quad f(3)\quad \ldots\quad \ldots,\ f(n)\ .$$

We shall now take h as the fundamental interval for all points of tabulation. To express $\frac{d^2}{dr^2} f(r)$ and $\frac{d}{dr} f(r)$ in terms of Central differences we make use of the following central difference formulae for derivatives given by:

$$h^2 \frac{d^2}{dr^2} f(r) = (\delta^2 - \frac{1}{12}\delta^4 + \frac{1}{90}\delta^6 - \frac{1}{560}\delta^8 + \ldots) \times f(r)$$

and

$$h \frac{d}{dr} f(r) = \mu(\delta - \frac{1}{6}\delta^3 + \frac{1}{30}\delta^5 - \frac{1}{140}\delta^7 + \ldots) \times f(r) \qquad (11.2.4)$$

where δ and μ have their usual definitions (c.f. Buckingham, 1962). We can now replace equation (11.2.1) by:

$$(1 + W(r))\ (\delta^2 - \frac{1}{12}\delta^4 + \frac{1}{90}\delta^6 - \frac{1}{560}\delta^8 + \ldots)\ f(r)$$

$$+ h^2 \left[\frac{1}{r^2} T(r) + U(r) + k^2 - \frac{\ell(\ell+1)}{r^2}\right] f(r)$$

$$+ h \frac{1}{r} V(r)\ \mu(\delta - \frac{1}{6}\delta^3 + \frac{1}{30}\delta^5 - \frac{1}{140}\delta^7 + \ldots)\ f(r)$$

$$+ h^2 \int_0^\infty K(r,r')\ f(r')\ dr' = 0 \qquad (11.2.5)$$

The kernel function in equation (11.2.5) dies away sufficiently rapidly to enable us to replace the infinite limit in the integral by some convenient finite R', say.

The range of integration can now be split up into a number of pivotal points r_0, r_1, ... , R' at equal interval h. The integral is then expressed in terms of the function values at the pivotal points by means of a formula for numerical integration written in the Lagrangian form. According to Robertson (1956) we rewrite the kernel function as:

$$\int_0^{\infty} K(r,r')\, f(r')\, dr' \equiv \int_0^{R'} K(r,r')\, f(r')\, dr'$$

At the point $r = r_n$, the integral can be written as:

$$\int_0^{R'} K(r,r')\, f(r')\, dr' = \sum_{m=0}^{N} T_m\, K(r_n,r'_m)\, f(r'm)$$

$$= \sum_{m=0}^{N} T_m K_{nm} f_m \qquad (11.2.6)$$

Thus, equation (11.2.5) now becomes

$$(1 + W(r))(\delta^2 - \tfrac{1}{12}\delta^4 + \tfrac{1}{90}\delta^6 - \tfrac{1}{560}\delta^8 + \ldots)\, f(r)$$

$$+ h\,\tfrac{1}{r}\,V(r)\,\mu(\delta - \tfrac{1}{6}\delta^3 + \tfrac{1}{30}\delta^5 - \tfrac{1}{140}\delta^7 + \ldots)\, f(r)$$

$$+ h^2\,(\tfrac{1}{r^2}\,T(r) + U(r) + k^2 - \tfrac{\ell(\ell+1)}{r^2})\, f(r)$$

$$+ h^2 \sum_{m=0}^{N} T_m K_{nm} f_m = 0 \qquad (11.2.7)$$

where T_m are the integration coefficients.

Since the first derivative is present in our problem, the method of L. Fox et al. (1949) to reduce the error in the difference formulae is not practicable. To keep the errors as small as practicable we shall include the terms in δ^4 and $\mu\delta^3$ and neglect those of higher orders.

Taking r = th for all points of tabulation r and using the following relations due to L.J. Comrie (1942).

$$\mu\delta\, f(r) = \tfrac{1}{2}(f(r+1) - f(r-1))$$

$$\delta^2 f(r) = f(r+1) - 2f(r) + f(r-1)$$

$$\mu\delta^3 f(r) = \tfrac{1}{2}(f(r+2) - 2f(r+1) + 2f(r-1) - f(r-2))$$

$$\delta^4 f(r) = f(r+2) - 4f(r+1) + 6f(r) - 4f(r-1) + f(r+2)$$

and the following notations

$$f(th) = f_t$$

$$1 + W(th) = X(th) = X_t$$

$$T_m K(th, mh) = K_{tm}$$

then, equation (11.2.7) can now be written in the form:

$$X_t(-\tfrac{1}{12} f_{t-2} + {}^4/3\, f_{t-1} - {}^5/2\, f_t + {}^4/3\, f_{t+1} - {}^1/12\, f_{t+2}) + h(\tfrac{1}{th})\, V_t\, ({}^1/12\, f_{t-2} - {}^2/3\, f_{t-1} + {}^2/3\, f_{t+1} - {}^1/12\, f_{t+2}) + h^2\{(\tfrac{1}{th})^2 (T_t - \ell(\ell+1)) + k^2 + U_t\} + h^2 \sum_{m=0}^{N} K_{tm} f_m = 0 \qquad (11.2.8)$$

for t = 2,3 ... n-1.

Equations (11.2.8) are system of (n-2) simultaneous equations for n unknowns. The additional two equations are obtained by applying a forward difference formula to the equations at the point where t = 1 and a backward difference formula where t = n. The formulae are chosen so that they carry errors of the same order as the other formulae used. In our calculations we used the three point difference formulae, as given in Appendix I, which

we found to be even more accurate in practice. By specifying the boundary conditions on f, equations (11.2.8) may be written in the form

$$Af = B \qquad (11.2.9)$$

where A and B are matrices of dimensions (n-1) x (n-1) and (n-1)x1 respectively and f is an (n-1)x1 matrix. Thus equations (11.2.9) are partitioned into:

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots & A_{1n-1} \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ A_{n-11} & A_{n-12} & A_{n-13} & & A_{n-1\,n-1} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n-1} \end{bmatrix} = \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_{n-1} \end{bmatrix} \qquad (11.2.10)$$

Hence it remains to evaluate and combine the contributions of all the terms in equation (3.1.18) to the matrices A and B at each pivotal point, and then the radial wave functions given by f are obtained by matrix inversion.

§ 11.3 THE COMPUTATION OF THE KERNELS AND THE DIRECT TERMS

(i) THE EVALUATION OF THE DIRECT TERMS

There are four types of the direct terms in the equation and are classified as T(r), U(r), V(r) and W(r). These expressions are tabulated at h(h)52h (h = 0.2). The computer programmes were written to evaluate these terms as well as the parameters and constants.

(ii) THE EVALUATION OF THE KERNELS (INDIRECT TERMS)

All the kernels appearing in our problems depend on Bessel function of the first kind. A library programme (Ref. Chelsea College of Science and Technology (CCST) library procedures) which computes

$$K(r,r') = A \sum_{j=1}^{N} A_j \exp(-\gamma_j r^2 - \lambda_j r'^2) \varphi_j(r,r') I_{n_j+\frac{1}{2}}(\varkappa_j rr') \tag{11.3.1}$$

where A is a constant and

$$\varphi_j(r,r') = \sum_{\lambda,\zeta} c^j_{\lambda\zeta} r^{\lambda} r'^{\zeta} \tag{11.3.2}$$

was used. According to the magnitude of x, the Bessel function $I_{n+\frac{1}{2}}(x)$ was calculated by using the power series or the asymptotic form. According to Bateman (1953), we have the following results:

$$I_{n+\frac{1}{2}}(x) = (-1)^n \frac{x^{n+1}}{2^n} \sum_{m=0}^{\infty} \frac{(m+n)!\, x^{2m}}{m!((2m+n)+1)!} \qquad x < \infty \tag{11.3.3}$$

$$I_{n+\frac{1}{2}}(x) \underset{x \to \infty}{=} \frac{(-1)^n}{2} \left\{ e^x \left[\sum_{m=0}^{m-1} (-1)^m \frac{(n+\frac{1}{2},m)}{(2x)^m} + O(|x|^{-m}) \right] + (-1)^{n+1} e^{-x} \left[\sum_{m=0}^{m-1} (-1)^m \frac{(n+\frac{1}{2}),m)}{(2x)^m} + O(|x|^{-m}) \right] \right\} \tag{11.3.4}$$

where

$$(n+\tfrac{1}{2},m) = \frac{\Gamma(n+m+1)}{\Gamma(n-m+1)m!} \quad \text{(Bateman 1953, Vol.II)} \tag{11.3.5}$$

(c.f. Watson, 1944).

The programmes for the evaluation of the direct and indirect terms are given in Appendix I. All the programmes used were tested by the author, and found to be correct up to 8D after some little modifications. The programmes for

solving the complete integro-differential equations were used to solve Robertson's problem (1956) and our results were found to be in good agreement with those obtained by Robertson. Most of the library procedures used were modified by the author and Mr. R.F. Shepherd and tested to suit the n-He^4 scattering problems (Ref. Chelsea College of Science and Technology library procedures).

CHAPTER XII

PHASE-SHIFTS ANALYSIS AND CROSS-SECTIONS

§ 12.1 PHASE-SHIFT ANALYSIS

As pointed out previously, coupled states do not arise in n-He^4 collisions. Thus, the asymptotic form of the wave functions is of the following form:

$$\tilde{f}_\ell(x) = k_\ell \left[\sqrt{x} \cos \delta_\ell \, J_{\ell+\frac{1}{2}}(kx) + \sqrt{x} \sin \delta_\ell \, J_{-\ell-\frac{1}{2}}(kx)\right] \tag{12.1.1}$$

where k_ℓ is the constant amplitude, δ_ℓ is the phase-shift and $J_{\ell+\frac{1}{2}}$, $J_{-\ell-\frac{1}{2}}$ are the Bessel functions of half integral order (angular momentum ℓ), k is the wave number of the incident neutron given by

$$k^2 = \frac{8M}{5\hbar^2} E_n \tag{12.1.2}$$

where M is the mass of a nucleon and E_n is the energy of the incident particle in C.M. units.

Given the above formula for $\tilde{f}_\ell(x)$ at two neighbouring points, say r_1 and r_2, we have

$$\frac{\tilde{f}_\ell(r_2)}{\tilde{f}_\ell(r_1)} = \frac{\sqrt{r}_2[\cos \delta_\ell \, J_{\ell+\frac{1}{2}}(kr_2) + \sin \delta_\ell \, J_{-\ell-\frac{1}{2}}(kr_2)]}{\sqrt{r}_1[\cos \delta_\ell \, J_{\ell+\frac{1}{2}}(kr_1) + \sin \delta_\ell \, J_{-\ell-\frac{1}{2}}(kr_1)]} \tag{12.1.3}$$

which immediately reduces to

$$\tan \delta_\ell = - \frac{\tilde{f}_\ell(r_2) \sqrt{r}_1 \, J_{\ell+\frac{1}{2}}(kr_1) - \tilde{f}_\ell(r_1) \sqrt{r}_2 \, J_{\ell+\frac{1}{2}}(kr_2)}{\tilde{f}_\ell(r_2) \sqrt{r}_1 \, J_{-\ell-\frac{1}{2}}(kr_1) - \tilde{f}_\ell(r_1) \sqrt{r}_2 \, J_{-\ell-\frac{1}{2}}(kr_2)} \tag{12.1.4}$$

The amplitude k_ℓ corresponding to each phase-shift δ_ℓ can now be found by writing

$$k_\ell = \tilde{f}_\ell(r_1) / [\cos \delta_\ell \sqrt{r_1}\, J_{\ell+\frac{1}{2}}(kr_1) + \sin \delta_\ell \sqrt{r_1}\, x$$
$$J_{-\ell-\frac{1}{2}}(kr_1)] \qquad (12.1.5)$$

§12.2 TOTAL AND DIFFERENTIAL CROSS-SECTIONS

The experimental measurements of the total and differential cross-sections include the work done by Hall and Kootz (1947), Bashkin et al. (1951), Adair (1951, 1952), Hubber and Baldinger (1952), Seagrave (1953), Alston et al. (1954), Smith (1954), and Shaw (1955). Faxen and Holtsmark (1927) showed that the differential scattering cross-section can be decomposed into a sum over the possible values of the orbital angular momentum ℓ. They expressed the differential cross-section in the following form.

$$\sigma(\theta) = |f(\theta)|^2 \qquad (12.2.1)$$

where

$$f(\theta) = \frac{1}{2ik} \sum_\ell (2\ell+1) \exp[(2i\,\delta_\ell)-1]\, P_\ell(\cos\theta) \qquad (12.2.2)$$

where k has been defined previously, P_ℓ is a Legendre polynomial and θ is the scattering angle of the incident energy in the centre of mass system.

Wheeler and Barschall (1940) found that the observed (Barschall and Kanner, 1940) differential scattering cross-section for n-He^4 collision cannot be fitted by the first two terms of equation (12.2.2), that is, by the S- and P-waves, which are the only ones expected to contribute significantly at the energies concerned.

The possible scattering states are $S_{\frac{1}{2}}$, $P_{\frac{1}{2}}$, $P_{3/2}$, $D_{3/2}$, $D_{5/2}$, $F_{5/2}$, $F_{7/2}$, etc. and the corresponding phase-shifts are designated by δ_0, δ_1^-, δ_1^+, δ_2^-, δ_2^+, δ_3^-, δ_3^+, etc.

The formula for the differential cross-section given by Mott (1932) and Bloch (1940) is

$$r(\theta) = |A|^2 + |B|^2 \qquad (12.2.3)$$

where

$$A = \frac{1}{2ik} \sum_{\ell} \{(\ell+1)\,[\exp(2i\delta_\ell^{+})-1] + \ell \exp[(2i\,\delta_\ell^{-})-1]\} \times P_\ell(\cos\theta)$$

$$B = \frac{1}{2ik} \sum_{\ell} [\exp(2i\,\delta_\ell^{+}) - \exp(2i\,\delta_\ell^{-})]\, P'_\ell(\cos\theta) \qquad (12.2.4)$$

(c.f. Critchfield et al., 1949; P.G. Burke, 1960; and Rosenfeld, p.100). P'_ℓ is an associated Legendre polynomial.

The total cross-section is given by

$$\sigma_T = \frac{4\pi}{k^2} \sum_{\ell} \{(\ell+1)\sin^2\delta_\ell^{+} + \ell \sin^2\delta_\ell^{-}\} \qquad (12.2.5)$$

(c.f. Rosenfeld, p. 100).

Wheeler and Barschall found that it is possible to fit the observed n-He^4 data with the above equations using only $S_{\frac{1}{2}}$, $P_{\frac{1}{2}}$ and $P_{3/2}$ waves. Thus the large value of $(\delta_1^{+}-\delta_1^{-})$ indicated the presence of a strong spin-orbit force between the He^4 and the scattered neutron. For the calculations of phase-shifts, differential cross-sections and total cross-sections we shall be using equations (12.1.4), (12.2.3) and (12.2.5) respectively.

§12.3 PHASE-SHIFTS CALCULATIONS

We shall now calculate the phases using the values of the wave function at the last three pairs of points in the range, that is, (f_{n-3}, f_{n-2}), (f_{n-2}, f_{n-1}) and (f_{n-1}, f_n).

This gives three values of the phase δ_{n-2}, δ_{n-1} and δ_n using equation (12.1.4) which are identical if the kernels are sufficiently negligible at the end of the range of integration. If, however, the kernels have not completely died away an estimate of the asymptotic phase "δ_{lim}" can be obtained by a formula due to Aitken (1937).

Thus

$$\delta_{lim} = \frac{\delta_n\delta_{n-2} - \delta^2_{n-1}}{\delta_{n-2} - 2\delta_{n-1} + \delta_n} \qquad (12.3.1)$$

This assumes that the approximate phases δ_r are the successive partial sums of a geometric progression.

In all our phase-shifts calculations we shall be using equation (12.3.1) whenever the last three phases calculated are not identical. The result obtained will then be compared with the result of the last phase-shift obtained by direct calculation using equation (12.1.4).

TABLE II THE δ_o-PHASES (IN RADIANS)

Author	Energy in MeV	$k^2 = {}^{8M}/_{5\hbar^2}$	k	Phases	δ_o-Phases
Our Results	5	0.193184	0.43954	δ_n δ_{lim}	-1.364258 -1.364205
Seagrave (1953)	5				-1.117
Our Results	10	0.386368	0.62159	δ_n δ_{lim}	-1.368472 -1.369347
Seagrave (1953)	10				-1.379
Our Results	15	0.579552	0.76140	δ_n δ_{lim}	-1.377067 -1.379198

The phase δ_n together with the Aitken asymptotic phase δ_{lim} calculated for the interval $h = 0.2f_m$ and for $\ell = 0$. The phases are given in radians between the range

$$-{}^{\pi}/_{2} \leqslant \delta \leqslant {}^{\pi}/_{2}.$$

TABLE III THE δ_1^+-PHASES (IN RADIANS)

Author	Energy in MeV	$k^2 = 8M/5\hbar^2$	k	Phases	δ_1^+-Phases
Our Results	5	0.193184	0.43954	δ_n δ_{lim}	-1.017591 -1.017582
Seagrave (1953)	5				-1.082
Our Results	10	0.386368	0.62159	δ_n δ_{lim}	-1.368856 -1.368857
Seagrave (1953)	10				-1.396
Our Results	15	0.579552	0.76140	δ_n δ_{lim}	-1.024864 -1.024881

The phase δ_n together with the Aitken asymptotic phase δ_{lim} calculated for the interval of integration $h = 0.2f_m$ and for $\ell = 1$. The phases are given in radians between the range

$$-\pi/2 \leq \delta \leq \pi/2.$$

TABLE IV THE δ_1^--PHASES (IN RADIANS)

Author	Energy in MeV	$k^2 = 8M/5\hbar^2$	k	Phases	δ_1^--Phases
Our Results	5	0.193184	0.43954	δ_n δ_{lim}	0.6165900 0.61658455
Seagrave (1953)	5				0.785
Our Results	10	0.386368	0.62159	δ_n δ_{lim}	1.367405 1.367406
Seagrave (1953)	10				0.873
Our Results	15	0.579552	0.76140	δ_n δ_{lim}	1.014272 1.014816

The phase δ_n together with the Aitken asymptotic phase δ_{lim} calculated for the interval of integration $h = 0.2f_m$ and for $\ell = 1$. The phases are given in radians between the range

$$-\pi/2 \leqslant \delta \leqslant \pi/2.$$

FIG. V

P-PHASE SHIFT IN n-He^4 COLLISIONS

I SEAGRAVE (1953)

II OURS

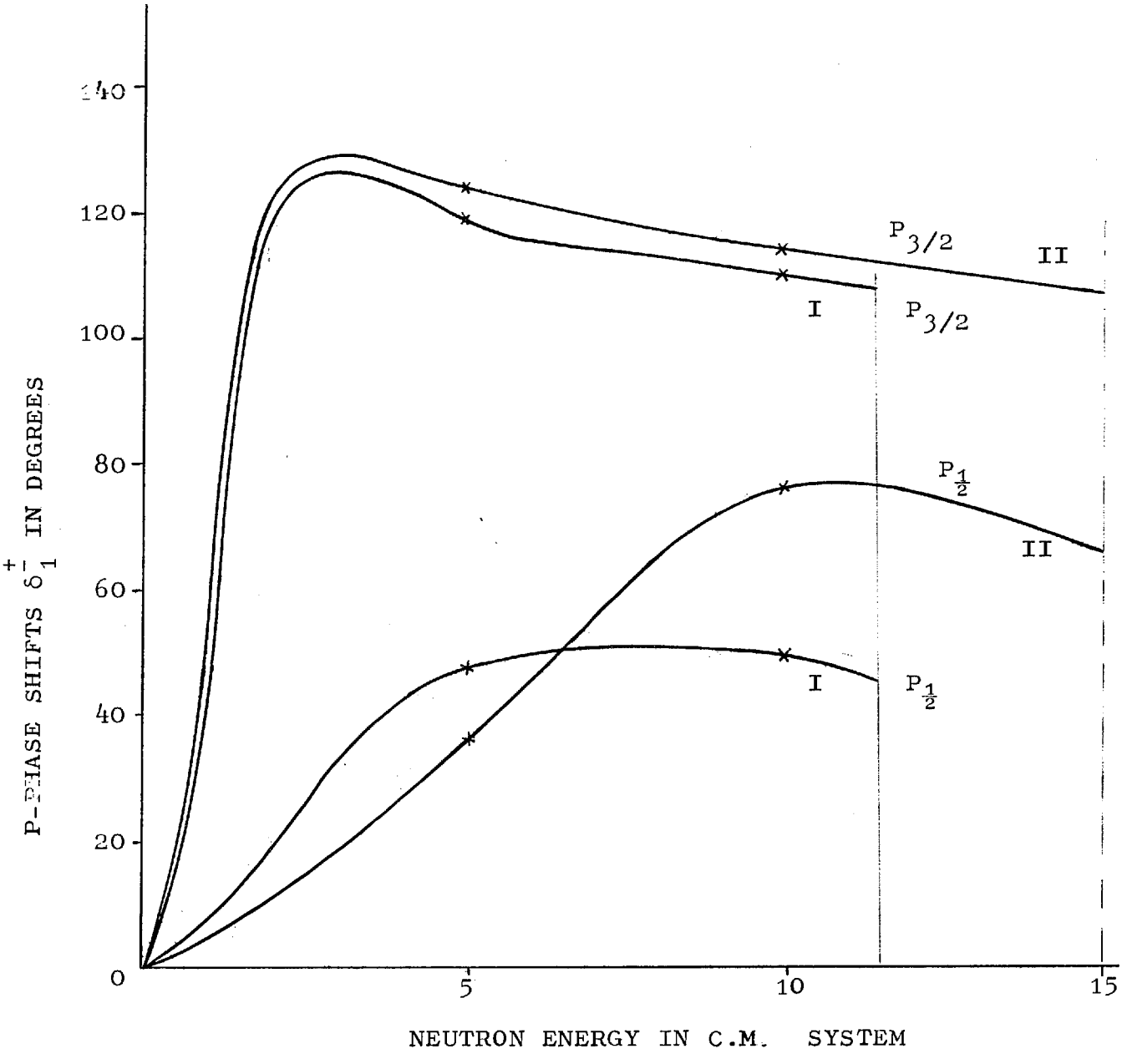
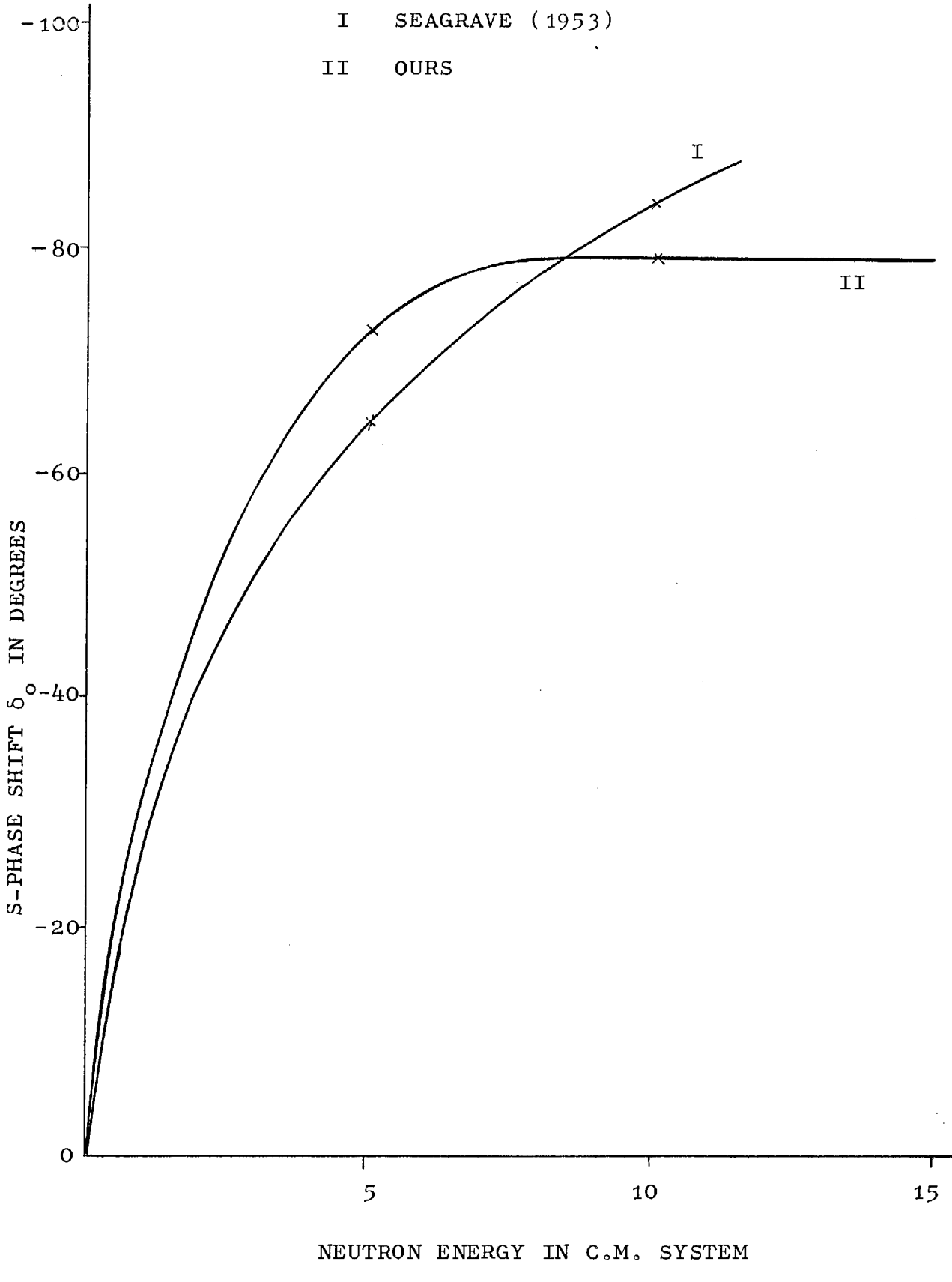


FIG. VI

S-PHASE SHIFT IN n-He^4 COLLISIONS



§12.4 CONCLUSION

The phase-shifts for the elastic scattering of neutron by alpha-particles were calculated for 5, 10 and 15 MeV incident neutron energies (C.M. System) and for the values of the angular momentum $0 \leqslant \ell \leqslant 1$.

Our phase-shifts were compared with the experimental phase shifts obtained by Seagrave (1953) and found to be in good agreement apart from the δ_1^--phases.

As shown in Chapter IX, the nuclear interaction used gives a binding energy of -26.038 MeV for the alpha-particles as compared with the experimental value of -28.2 MeV.

APPENDICES AND REFERENCES

APPENDIX I

PROGRAMMES FOR THE DIRECT AND INDIRECT (KERNELS) TERMS

§AI.1 THE STRUCTURE OF THE PARTITIONED MATRIX

Using the three point difference formulae equation (11.2.8) becomes

$$\sum_{t=1}^{m} X_t(f_{t+1} - 2f_t + f_{t-1}) + \frac{h}{2} \sum_{t=1}^{m} \left(\frac{1}{th}\right) V_t \, (f_{t+1} - t_{t-1}) + h^2 \sum_{t=1}^{m} \left[\left(\frac{1}{th}\right)^2 \{-\ell(\ell+1) + T_t\} + k^2 - U_t\right] f_t$$

$$= h^2 \sum_{t=0}^{m} \sum_{s=0}^{n+1} T_s \, K_{ts} \, f_s \qquad \text{(AI.1.1)}$$

Note that the method suggested by Robertson (1956) to improve the accuracy of the results is not applicable to our problem since our problem contains a first order derivative term. We shall therefore use the method suggested by L. Fox et al. (1949) to solve equation (AI.1.1).

Define

$$\lambda_m \equiv X_t + h/2 \; V_t/(th)$$

$$\mu_m \equiv X_t - h/2 \; V_t/(th)$$

and

$$\nu_m \equiv \left[h^2 \{k^2 - \ell(\ell+1)/(th)^2 + \left(\frac{1}{th}\right)^2 T_t - U_t\} - 2X_t\right] \qquad \text{(AI.1.2)}$$

Using equation (AI.1.2), equation (AI.1.1) becomes

$$\sum_{m=0}^{N} \left[(\delta_{n+1,m})\ \lambda_m + (\delta_{n,m})\ \mu_m + (\delta_{n-1,m})\ \nu_m - a_{n,m} \right] f_m = 0 \qquad \text{(AI 1.3)}$$

where $a_{n,m} \equiv h^2 T_m K_{n,m} = h^2 T_m K(r_n, r'_m)$ (AI.1.4)

and the coefficients T_m are the numerical factors of the integration formula.

Using the boundary conditions:

$$f(0) = 0 \quad \text{and} \quad f(1) = 1$$

we can write equation (AI.1.3) in the following form:

$$\sum_{i=1}^{N-1} \left[(\delta_{n+1,i+1})\lambda_{i+1} + (\delta_{n,i+1})\ \mu_{i+1} + (\delta_{n-1,i+1})\ \nu_{i+1} - a_{n,i+1} \right] f_{i+1}$$

$$= \left[a_{n,1} - \{ (\delta_{n+1,1})\ \lambda_1 + (\delta_{n,1})\ \mu_1 + (\delta_{n-1,1})\ \nu_1 \} \right] \qquad \text{(AI.1.5)}$$

Hence we have

$$A[i,j] : = \left[(\delta_{i+1,j+1})\ \lambda_{j+1} + (\delta_{i,j+1})\ \mu_{j+1} + (\delta_{i-1,j+1})\ \nu_{j+1} - a_{i,j+1} \right] \qquad \text{(AI.1.6)}$$

$i,j = 1,2,3, \ldots \quad \ldots\ n-1$

Also, we have

$$B[i,n] : = \left[a_{i,1} - \{ (\delta_{i+1,1})\ \lambda_1 + (\delta_{i,1})\ \mu_1 + (\delta_{i-1,1})\ \nu_1 \} \right] \qquad \text{(AI.1.7)}$$

Define $f_{i+1} \equiv x_j$, $X_t \equiv 1 + W_t$ and $h^2 \equiv$ hsq.

Consider the following real procedures:

(i)
```
real procedure lambda(h,i);
value h,i;  real h;  integer i;
lambda:  = (1+W(i*h) + h/2*V(i*h)/(i*h));
```

(ii)
```
real procedure  mu(h,i);
value  h,i;  real h;  integer i;
mu:  =  (1+W(i*h)-h/2*V(i*h)/(i*h));
```

(iii)
```
real procedure  nu(h,i,ℓ,k);
value  h,i,ℓ,k;  real h,k;  integer i,ℓ;
nu:  =  (h exp 2*(k exp 2 - ℓ*(ℓ+1)/(i*h) exp 2
     + T(i*h)/(i*h) exp 2 - U(i*h))-2*(1+W(i*h)));
```

Comment

The above procedures form the matrix elements of the integro-differential equations which are solved using Ilgauss procedure (Ref. Chelsea College of Science and Technology (CCST) library procedure).

(iv)
```
real procedure  delta (i,j);  value i,j;  integer i,j;
delta:  =  if i = j then 1 else 0;
```

Using these four real procedures equation (AI.1.6) becomes

```
A[i,j] :  = lambda(h, j+1)*delta(i+1,j+1) +
            nu(h,j+1,ℓ,ki)*delta(i,j+1) +
            mu(h,j+1)*delta(i-1,j+1);
```

```
A[i,j] :  = A[i,j]- hsq * wi[j+1]  *k[i,j+1] ;      (AI.1.8)
```

Note that wi[i] are the Gregory "weights" (Ref. CCST library procedure).

Also from equation (AI.1.7) we have

```
A[i,j] :  = A[i,n] + hsq * wi[1] *k[i,1] ;          (AI.1.9)
```

where

A[i,n] : = -(lambda(h,1)* delta(i+1,1) + nu(h,1,ℓ,ki)*
delta(i,1) + mu(h,1)* delta(i-1,1));

Thus equation (AI.1.5) becomes

$\underline{A}\,\underline{x} = \underline{B}$ (c.f. equation (11.2.10)) (AI.1.11)

As we discussed in § 11.3 all the kernels appearing in our problems of n-He^4 depend on Bessel function of the first kind. Some of the library procedures used are listed below:

(i) Algorithm CACM 221 (Ref: CCST library procedure),

(ii) Algorithm CACM 236 (Ref: CCST library procedure).

(iii) CCST library procedure No. 237. This is the procedure "Gregory Rule" (n,r,t,w).

(iv) CCST library procedure No. 262. This is the "Ilgauss" procedure which solves the matrix elements of the integro-differential equations.

The above procedures were modified by the author to avoid any "exponent overflow" and "division overflow" and when tested were found to be very accurate up to 8D.

Note that the foregoing outlines the programmes for the evaluation of the direct and indirect (kernels) terms. It should be pointed out that it is not always practicable to give every detail of the analysis involved in writing the programmes for solving the integro-differential equations of the scattering of neutron by alpha-particles.

APPENDIX II

COORDINATES AND TRANSFORMATIONS

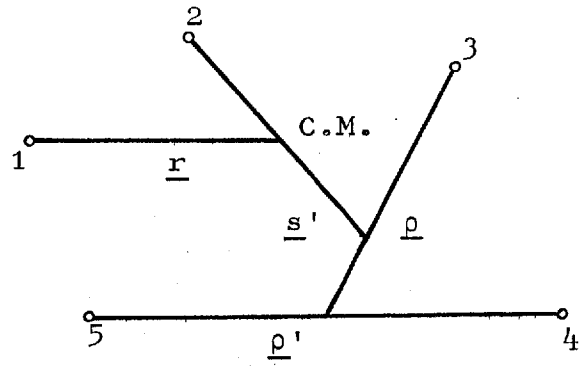


Fig. VII

The incident neutron is labelled as the particle 1 and has the position vector $\underline{r}$. The other neutrons are labelled 2 and 3 and the protons 4 and 5 with respective position vectors $\underline{r}_2$, $\underline{r}_3$, $\underline{r}_4$ and $\underline{r}_5$.

We define $\underline{r}$ as the coordinate of particle 1 relative to the centre of mass (C.M.) of the other four and $\underline{r}'$ as the coordinate of particle 2 relative to the C.M. of the other four.

CHOICE OF COORDINATES (SEE FIG. VII)

$$\underline{r} = \underline{r}_1 - {}^1/4\ (\underline{r}_2+\underline{r}_3+\underline{r}_4+\underline{r}_5)$$

$$\underline{r}' = \underline{r}_2 - {}^1/4\ (\underline{r}_1+\underline{r}_3+\underline{r}_4+\underline{r}_5)$$

$$\underline{\rho} = \underline{r}_3 - \tfrac{1}{2}(\underline{r}_4+\underline{r}_5)$$

$$\underline{\rho}' = \underline{r}_4 - \underline{r}_5$$

We define

$$\underline{s} = \frac{4}{15}\ (4\underline{r}+\underline{r}')$$

$$\underline{s}' = \frac{4}{15}\ (\underline{r}+4\underline{r}')$$

Thus

$$\underline{s} = \underline{r}_1 - {}^1/3\ (\underline{r}_3+\underline{r}_4+\underline{r}_5)$$

and

$$\underline{s}' = \underline{r}_2 - {}^1/3(\underline{r}_3+\underline{r}_4+\underline{r}_5)$$

We usually write

$$(1\text{-}2345) = (-1) = \underline{s} = (s,\theta,\varphi)$$

$$(2\text{-}1345) = (-2) = \underline{s}' = (s',\theta',\varphi')$$

Other coordinates used in the thesis are defined by:

$$(12) = \underline{r}_{12} = \underline{r}_1-\underline{r}_2 = \underline{r} - {}^3/4\underline{s}' = \tfrac{4}{5}(\underline{r}-\underline{r}') = \underline{s}-\underline{s}'$$

$$(13) = \underline{r}_{13} = \underline{r}_1-\underline{r}_3 = \underline{s} - {}^2/3\underline{\rho}$$

$$(14) = \underline{r}_{14} = \underline{r}_1-\underline{r}_4 = \underline{s} + {}^1/3\underline{\rho} - \tfrac{1}{2}\underline{\rho}'$$

$$(15) = \underline{r}_{15} = \underline{r}_1-\underline{r}_5 = \underline{s} + {}^1/3\underline{\rho} + \tfrac{1}{2}\underline{\rho}'$$

$$(23) = \underline{r}_{23} = \underline{r}_2-\underline{r}_3 = \underline{s}' - {}^2/3\underline{\rho}$$

$$(24) = \underline{r}_{24} = \underline{r}_2-\underline{r}_4 = \underline{s}' + {}^1/3\underline{\rho} - \tfrac{1}{2}\underline{\rho}'$$

$$(25) = \underline{r}_{25} = \underline{r}_2-\underline{r}_5 = \underline{s}' + {}^1/3\underline{\rho} + \tfrac{1}{2}\underline{\rho}'$$

$$(34) = \underline{r}_{34} = \underline{r}_3-\underline{r}_4 = \underline{\rho} - \tfrac{1}{2}\underline{\rho}'$$

$$(35) = \underline{r}_{35} = \underline{r}_3-\underline{r}_5 = \underline{\rho} + \tfrac{1}{2}\underline{\rho}'$$

$$(45) = \underline{r}_{45} = \underline{r}_4-\underline{r}_5 = \underline{\rho}'$$

If $\underline{p}_1$, $\underline{p}_2$, $\underline{p}_3$, $\underline{p}_4$ and $\underline{p}_5$ are the momentum vectors of the particles 1, 2, 3, 4 and 5 respectively referred to a fixed origin, then

$$i\underline{p}_1 = \frac{\partial}{\partial \underline{r}_1} = \frac{\partial}{\partial \underline{r}} - \frac{1}{4}\frac{\partial}{\partial \underline{r}'}$$

$$i\underline{p}_2 = \frac{\partial}{\partial \underline{r}_2} = -\frac{1}{4}\frac{\partial}{\partial \underline{r}} + \frac{\partial}{\partial \underline{r}'}$$

$$i\underline{p}_3 = \frac{\partial}{\partial \underline{r}_3} = -\frac{1}{4}\frac{\partial}{\partial \underline{r}} - \frac{1}{4}\frac{\partial}{\partial \underline{r}'} + \frac{\partial}{\partial \underline{\rho}}$$

$$i\underline{p}_4 = \frac{\partial}{\partial \underline{r}_4} = -\frac{1}{4}\frac{\partial}{\partial \underline{r}} - \frac{1}{4}\frac{\partial}{\partial \underline{r}'} - \frac{1}{2}\frac{\partial}{\partial \underline{\rho}} + \frac{\partial}{\partial \underline{\rho}'}$$

$$i\underline{p}_5 = \frac{\partial}{\partial \underline{r}_5} = -\frac{1}{4}\frac{\partial}{\partial \underline{r}} - \frac{1}{4}\frac{\partial}{\partial \underline{r}'} - \frac{1}{2}\frac{\partial}{\partial \underline{\rho}} - \frac{\partial}{\partial \underline{\rho}'}$$

Hence it follows that

$$i\underline{L}_{12} = (\underline{r}_1-\underline{r}_2)\wedge(\underline{p}_1-\underline{p}_2)$$

$$= (\underline{r}-\underline{r}')\wedge(\frac{\partial}{\partial \underline{r}} - \frac{1}{4}\frac{\partial}{\partial \underline{r}'}), \text{ etc.}$$

The following coordinates systems are also used:

$$\underline{u} = \frac{1}{4}(\underline{r}_2+\underline{r}_3-\underline{r}_4-\underline{r}_5); \quad \underline{v} = \underline{r}_2-\underline{r}_3; \quad \underline{w} = \underline{r}_4-\underline{r}_5.$$

In the calculation for the indirect interaction the transformation used for the volume integration is

$$d\tau_{-1} = d\underline{r}_{2345} = (\frac{16}{15})^3 \, d\underline{r}' \, d\underline{\rho} \, d\underline{\rho}'$$

with

$$d\underline{r}' = r'^2 \, dr' \, d\Omega'$$

Ω' being the solid angle of $\underline{r}'$.

Several transformations have frequent application. These are enumerated below:

(1) $\underline{t} = \underline{\rho} - \eta\underline{r}$, $\underline{t}' = \underline{\rho}' - \delta\underline{s}$ and $\underline{\rho}' = \underline{\rho}'$

where

$$\eta_T(\varkappa) = \frac{3^T\mu_\varkappa^\nu}{12\alpha+12\beta+{}^T\mu_\varkappa^\nu}$$

$$\delta_T(\varkappa) = \frac{3^T\mu_\varkappa^\nu}{2(3\alpha+3\beta+{}^T\mu_\varkappa^\nu)}$$

and $\underline{r} = \frac{1}{2}\underline{\rho}'-\underline{s}$ etc.

Note that the Jacobian is unity. Hence

$$d\underline{\rho}d\underline{\rho}' = d\underline{t}d\underline{t}'$$

(2) $\underline{t} = \underline{s}' - \xi\underline{r}, \quad \underline{t}' = \underline{\rho} - \varepsilon\underline{\rho}'$ and $\underline{\rho}' = \underline{\rho}'$

where

$$\xi = \mu/3\lambda,$$

$$\varepsilon^{c}_{(\nu)} = {}^{c}\mu^{\nu}_{\nu}/2(8\beta+3{}^{c}\mu^{\nu}_{\nu})$$

$$\lambda^{c}_{(\nu)} = 3\beta + {}^{c}\mu^{\nu}_{\nu}$$

and

$$\underline{r} = {}^{3}/_{2}\underline{\rho}' - \underline{\rho}$$

We find that

$$\frac{\partial(\underline{s},\underline{\rho},\underline{\rho}')}{\partial(\underline{t},\underline{t}',\underline{\rho}')} = 1$$

Thus $d\underline{s}d\underline{\rho}d\underline{\rho}' = dtdt'd\underline{\rho}'$ etc.

The following transformation is invariably used in the calculation of the binding energy of alpha-particle (Chapter XI).

(3) $\underline{s} = \underline{u} - \gamma(\underline{w}-\underline{v})$

$$\underline{s}' = \underline{v} - \eta\underline{w}$$

and $\underline{\rho} = \underline{w}$

where

$$\gamma^{Ls}_{(\nu)} = {}^{Ls}\mu^{\nu}_{\nu}/2\xi,$$

$$\xi^{Ls}_{(\nu)} = 4\beta + {}^{Ls}\mu^{\nu}_{\nu},$$

$$\eta^{Ls}_{(\nu)} = {}^{Ls}\mu^{\nu}_{\nu}/(8\beta + 3{}^{Ls}\mu^{\nu}_{\nu}),$$

giving the Jacobian $\dfrac{\partial(\underline{s},\underline{s}',\underline{\rho})}{\partial(\underline{u},\underline{v},\underline{w})} = 1.$

APPENDIX III

INTEGRATION FORMULAE AND SPHERICAL BESSEL FUNCTIONS

§AIII.1 THE DIRECT INTEGRATIONS

In the calculation of the direct integrations, the following formulae are used:

$$K \int \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R} = 1$$

$$K \int \underline{R} \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R} = \gamma\underline{r}$$

$$K \int R^2 \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R} = \frac{3}{2\lambda} + \gamma^2 r^2$$

$$K \int R^3 \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R} = \left(\frac{5}{2\lambda} + \gamma^2 r^2\right) \gamma\underline{r}$$

$$K \int R^4 \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R} = \frac{15}{4\lambda^2} + \frac{5}{\lambda}\gamma^2 r^2 + \gamma^4 r^4$$

$$K \int R^6 \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R} = \frac{105}{8\lambda^3} + \frac{105}{4\lambda^2}\gamma^2 r^2 + \frac{21}{2\lambda}\gamma^4 r^4 + \gamma^6 r^6$$

$$K \int (\underline{R}\wedge\underline{A}).(\underline{R}\wedge\underline{B}) \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R}$$

$$= \gamma^2 (\underline{r}\wedge\underline{A}).(\underline{r}\wedge\underline{B}) + \frac{1}{\lambda}(\underline{A}.\underline{B})$$

$$K \int R^2 (\underline{A}.\underline{R})(\underline{B}.\underline{R}) \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R}$$

$$= \left(\frac{7}{2\lambda} + \gamma^2 r^2\right)\gamma^2 (\underline{A}.\underline{r})(\underline{B}.\underline{r}) + \left(\frac{5}{2\lambda} + \gamma^2 r^2\right)\frac{1}{2\lambda}(\underline{A}.\underline{B})$$

$$K \int (\underline{A}.\underline{R})(\underline{B}.\underline{R})(\underline{C}.\underline{R})(\underline{D}.\underline{R}) \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R}$$

$$= \gamma^4 (\underline{A}.\underline{r})(\underline{B}.\underline{r})(\underline{C}.\underline{r})(\underline{D}.\underline{r}) + \frac{\gamma^2}{2\lambda}\left[(\underline{A}.\underline{B})(\underline{C}.\underline{r})(\underline{D}.\underline{r}) + (\underline{A}.\underline{C})(\underline{B}.\underline{r})(\underline{D}.\underline{r}) + (\underline{A}.\underline{D})(\underline{B}.\underline{r})(\underline{C}.\underline{r}) + (\underline{B}.\underline{C})(\underline{A}.\underline{r})(\underline{D}.\underline{r}) + (\underline{B}.\underline{D})(\underline{A}.\underline{r})(\underline{C}.\underline{r}) + (\underline{C}.\underline{D})(\underline{A}.\underline{r})(\underline{B}.\underline{r})\right] + \frac{1}{4\lambda^2}\left[(\underline{A}.\underline{B})(\underline{C}.\underline{D}) + (\underline{A}.\underline{C})(\underline{B}.\underline{D}) + (\underline{A}.\underline{D})(\underline{B}.\underline{C})\right]$$

$$K \int R^4 \; (\underline{A}.\underline{R})(\underline{B}.\underline{R}) \; \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R}$$

$$= (\gamma^4 r^4 + \frac{9}{\lambda}\gamma^2 r^2 + \frac{63}{4\lambda^2})\gamma^2 (\underline{A}.\underline{r})(\underline{B}.\underline{r})$$

$$+ \frac{1}{2\lambda}(\gamma^4 r^4 + \frac{7}{\lambda}\gamma^2 r^2 + \frac{35}{4\lambda^2})(\underline{A}.\underline{B})$$

$$K \int (\underline{A}.\underline{R})^3 (\underline{B}.\underline{R})^2 \; \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R}$$

$$= \gamma^5 (\underline{A}.\underline{r})^3 (\underline{B}.\underline{r})^2 + \frac{\gamma^3}{2\lambda}\left[3A^2(\underline{B}.\underline{r})^2 + B^2(\underline{A}.\underline{r})^2 + 6(\underline{A}.\underline{B})(\underline{A}.\underline{r})(\underline{B}.\underline{r})\right]$$

$$\times (\underline{A}.\underline{r}) + \frac{3\gamma}{4\lambda^2}\left[A^2 B^2 (\underline{A}.\underline{r}) + 2(\underline{A}.\underline{B})^2 (\underline{A}.\underline{r}) + \right.$$

$$\left. 2A^2 (\underline{A}.\underline{B})(\underline{B}.\underline{r})\right]$$

$$K \int S_{12}(R^2) \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R} = \gamma^2 S_{12}(r^2)$$

$$K \int (\underline{A}.\underline{R}) \; S_{12}(R^2) \; \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R}$$

$$= \gamma^2 (\underline{A}.\underline{r}) \; S_{12}(r^2) + \frac{\gamma}{\lambda} \; S_{12}(\underline{A},\underline{r})$$

$$K \int R^2 \; S_{12}(R^2) \; \exp\left[-\lambda(\underline{R}-\gamma\underline{r})^2\right] d\underline{R}$$

$$= (\frac{7}{2\lambda} + \gamma^2 r^2)\gamma^2 \; S_{12}(r^2) \qquad \text{etc.}$$

where

$$K = (\frac{\lambda}{\pi})^{3/2}$$

and

$$S_{12}(\underline{A},\underline{B}) = S_{12}(\underline{B},\underline{A})$$

$$= 3(\underline{\sigma}_1.\underline{A})(\underline{\sigma}_2.\underline{B}) - (\underline{\sigma}_1.\underline{\sigma}_2)(\underline{A}.\underline{B}).$$

§ AIII.2 THE INDIRECT INTEGRATIONS

The integrations over spherical harmonics in the indirect interaction calculation depend on the use of the following well-known formula:

$$\int Y_{\ell m}(\theta,\varphi)\exp(-\delta \underline{r}.\underline{r}')d\Omega = \frac{4\pi}{\delta rr'} Y_{\ell m}(\theta',\varphi') \, \mathcal{J}_{\ell+\frac{1}{2}}(\delta rr') \qquad \text{(AIII.2.1)}$$

where

$$\left.\begin{aligned} \underline{r} &= (r,\Omega) = (r,\theta,\varphi) \\ \underline{r}' &= (r',\Omega') = (r',\theta',\varphi') \\ d\Omega &= \sin\theta \, d\theta \, d\varphi \\ \text{and} \quad \mathcal{J}_{\ell+\frac{1}{2}}(x) &= i^{\ell-\frac{1}{2}} \left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_{\ell+\frac{1}{2}}(ix) \end{aligned}\right\} \qquad \text{(AIII.2.2)}$$

This formula is well known and has been used by many workers in several related scattering calculations (e.g. Sugie et al., 1957, and Hochberg et al., 1968). The derivation of the above formula (AIII.2.1) can be found in several texts (e.g. Whittaker and Watson, 1952). The first few values of the above Bessel function are given below:

$$\left.\begin{aligned} \mathcal{J}_{\frac{1}{2}}(x) &= \sinh x \\ \mathcal{J}_{3/2}(x) &= \frac{\sinh x}{x} - \cosh x \end{aligned}\right\} \qquad \text{(AIII.2.3)}$$

The recurrance relations between the functions are (from, e.g. Whittaker and Watson, 1952)

$$\frac{2\ell+1}{x} \mathcal{J}_{\ell+\frac{1}{2}}(x) = \mathcal{J}_{\ell+3/2}(x) - \mathcal{J}_{\ell-\frac{1}{2}}(x) \qquad \text{(AIII.2.4)}$$

and

$$\begin{aligned} \mathcal{J}'_{\ell+\frac{1}{2}}(x) &= \frac{d}{dx} \mathcal{J}_{\ell+\frac{1}{2}}(x) \\ &= \frac{\ell+1}{x} \mathcal{J}_{\ell+\frac{1}{2}}(x) - \mathcal{J}_{\ell+3/2}(x) \end{aligned} \qquad \text{(AIII.2.5)}$$

From equations (AIII.2.4) and (AIII.2.5) we deduce the following result:

$$\mathcal{J}''_{\ell+\frac{1}{2}}(x) = \left[\frac{\ell(\ell+1)}{x^2} + 1\right] \mathcal{J}_{\ell+\frac{1}{2}}(x) \quad \text{(see § 6.6)} \quad \text{(AIII.2.6)}$$

Also, from equation (AIII.2.3) we deduce the following relation:

$$\mathcal{J}_{\ell+\frac{1}{2}}(-x) = (-1)^{\ell+1} \mathcal{J}_{\ell+\frac{1}{2}}(x) \quad \text{(AIII.2.7)}$$

APPENDIX IV

NUMERICAL CONSTANTS

(A) THE ALPHA RADIAL WAVE FUNCTIONS

The S- and D-state alpha radial wave function parameters α, β and c are determined from the variational calculation of the binding energy of He^4 by the direct search method.

The value of α obtained from the variational calculation of the binding energy of He^4 is not used in our calculations in this thesis, instead α is taken to be $0.140\ fm^{-2}$. This value assigned to α is established from high energy e-He^4 scattering. The numerical values of these parameters are listed below:

$$\alpha = 0.140$$

$$\beta = 0.262$$

and $$c = -0.145$$

Both α and β have the same unit of fm^{-2} (i.e. 10^{26} cm^{-2}). Other constants used are given below:

$$\frac{M}{\hbar^2} = 0.024148 \times 10^{26}\ cm^{-2}\ (MeV)^{-1}$$

$$E_\alpha(\text{experimental}) = -28.2\ MeV$$

$$E_\alpha(\text{variational}) = -26.038\ MeV$$

and $$e^2 = 1.445 \times 10^{-13}\ cm\ MeV.$$

(B) THE NUCLEAR INTERACTION

The interactions defined in various chapters are defined in general by:

$$V(r) \sim \sum_{\kappa=1}^{2} \lambda_{U_\kappa}(\nu)\ \exp\left[-\ \lambda_{\mu_\kappa}(\nu)\ r^2\right]$$

and in the case of the tensor force only by:

$$V(r) \sim r^2 \sum_{\nu=1}^{2} \lambda_{U_\nu}(\nu) \exp[-\lambda_{\mu_\nu}(\nu) r^2]$$

The numerical values of U_ν and μ_ν are given in Table V.

TABLE V

λ	ν	U_1	μ_1	U_2	μ_2
Central	1	-57.30048745	0.7813030618	-227.7522931	3.090637232
	2	-19.51929806	1.047131587	- 45.08092453	2.859980282
	3	-150.4331204	0.961409294	-1331.300511	3.569316324
	4	-9.768369285	0.3780574533	2171.754221	4.094385782
Spin-Orbit	1	8.720315489	0.9561013786	38.27868688	3.351005841
	2	-220.6591852	1.825849870	-1926.807671	4.711770074
Tensor	1	-72.68042879	0.8477295439	-2230.867772	3.149339284
	2	14.01647580	0.7368709121	231.4471582	2.755371243
Quadratic Spin-Orbit	1	36.93418652	1.619715442	673.3739529	4.909374710
	2	11.66989625	1.963875693	-2332.307031	9.035133669
	3	5.049903637	1.387305140	-61.79157312	4.379654329
	4	-129.2988328	2.031807456	-4459.021051	5.750887105

U_ν are given in MeV and μ_ν in fm^{-2}.

APPENDIX V

COLLECTION OF PARAMETERS

The parameters defined in the direct interation calculation are as follows:

S-S

$$P_{c(\kappa)} \equiv \frac{16\alpha}{16\alpha + {}^{3c}\mu_{\kappa}(\nu)}$$

$$P_{Ls(\kappa)} \equiv \frac{16\alpha}{16\alpha + {}^{3Ls}\mu_{\kappa}(\nu)}$$

$$\gamma_{LL(\kappa)} \equiv \frac{{}^{4LL}\mu_{\kappa}(\nu)}{16\alpha + {}^{3LL}\mu_{\kappa}(\nu)}$$

$$\sigma \equiv 3\alpha \left[\frac{3\alpha}{\lambda'_{LL(\kappa)}} - (1 + \frac{5}{4}\gamma_{LL(\kappa)})(1 - \frac{3}{4}\gamma_{LL(\kappa)})\right]$$

$$\eta \equiv \frac{15}{16}\left[(1 + \frac{5}{4}\gamma_{LL(\kappa)})(1 - \frac{3}{4}\gamma_{LL(\kappa)}) - \frac{3\alpha}{\lambda'_{LL(\kappa)}}\right]$$

$$\lambda'_{LL(\kappa)} \equiv \frac{3}{16}(16\alpha + {}^{3LL}\mu_{\kappa}(\nu))$$

In the indirect calculation the following parameters are defined.

S-S

$$\lambda_{c(\kappa)} = \frac{32}{75}(4\alpha - {}^{3c}\mu_{\kappa}(\nu))$$

$$\lambda_{Ls(\kappa)} = \frac{32}{75}(4\alpha - {}^{3Ls}\mu_{\kappa}(\nu))$$

$$\lambda_{LL(\kappa)} \equiv \frac{32}{75}(4\alpha - {}^{3LL}\mu_{\kappa}(\nu))$$

$$\eta_c \equiv \frac{6\alpha}{6\alpha + {}^{c}\mu_{\kappa}(\nu)}$$

$$\varepsilon \equiv \frac{128\alpha}{75}$$

$$\zeta_{c(\varkappa)} \equiv \frac{128\alpha}{25}\left(\frac{2\alpha + {}^{c}\mu_{\varkappa}(\nu)}{6\alpha + {}^{c}\mu_{\varkappa}(\nu)}\right)$$

$$\omega \equiv \frac{128\alpha}{15}$$

$$\zeta_{LL(\varkappa)} \equiv \frac{32}{75}\left(16\alpha + 3\,{}^{LL}\mu_{\varkappa}(\nu)\right)$$

S-D

$$a \equiv \frac{{}^{T}\mu_{\varkappa}(\nu)}{3(\alpha+\beta)+{}^{T}\mu_{\varkappa}(\nu)}$$

$$b \equiv 3(\alpha+\beta)/\left[3(\alpha+\beta)+{}^{T}\mu_{\varkappa}(\nu)\right]$$

$$d \equiv (\alpha+\beta)/(\alpha+\beta+{}^{T}\mu_{\varkappa}(\nu))$$

$$\lambda_{T} \equiv 3\left(\frac{8}{15}\right)^{2}(1+2a)(\alpha+\beta)$$

$$\gamma^{(1)} \equiv \frac{24}{225}(\alpha+16\beta) + 3\left(\frac{16}{15}\right)^{2}(\alpha+\beta)a$$

$$\delta^{(1)} \equiv \frac{24}{225}(16\alpha+\beta) + \frac{3}{16}\left(\frac{16}{15}\right)^{2}(\alpha+\beta)a$$

$$S_{\ell}^{(1)} \equiv \frac{5}{2}b^{2} + \frac{20}{3}\ell bd(2a+b) + 8\ell(\ell-1)ad^{2}\left(a+\frac{2}{3}b\right)$$

$$T_{\ell}^{(1)} \equiv \frac{10}{3}b^{2}(2a+b) + 8\ell abd(a+{}^{2}/3b)$$

$$T'^{(1)}_{\ell} \equiv \frac{5}{24}b^{2}(2a+b) + \tfrac{1}{2}\ell abd(a+{}^{2}/3b)$$

$$U^{(1)} \equiv 2ab^{2}(a+{}^{2}/3b)$$

$$U'^{(1)} = {}^{3}/16\ U^{(1)}$$

$$U''^{(1)} = \frac{1}{256}U^{(1)}$$

$$V^{(1)} \equiv \frac{5}{3}b^{2}(2a+b) - 4abd(a+{}^{2}/3b)$$

$$W^{(1)} = U^{(1)}$$

$$W'^{(1)} = {}^{1}/_{16}\, U^{(1)}$$

$$\rho^{(1)} \equiv \frac{24}{225}(\alpha+16\beta)$$

$$\xi^{(1)} \equiv \frac{24}{225}(16\alpha+\beta)$$

$$\tau \equiv {}^{3}/_{4}\,(\frac{16}{15})^2(\alpha+\beta)$$

$$Y'^{(1)} \equiv \frac{16}{15}\,ab$$

$$Y^{(1)} = \frac{1}{16}\,Y'^{(1)}$$

D-S

$$\gamma^{(2)} \equiv \frac{24}{225}(16\alpha+\beta)+3(\frac{16}{15})^2(\alpha+\beta)a$$

$$\delta^{(2)} \equiv \frac{24}{225}(\alpha+16\beta) + \frac{3}{16}(\frac{16}{15})^2(\alpha+\beta)a$$

$$S_{\ell}^{(2)} \equiv \frac{5}{2}\,b^2 + \frac{5}{6}\,\ell bd(25a+17b)+2\ell(\ell-1)ad^2(7a+\frac{17}{3}b)$$

$$T_{\ell}^{(2)} \equiv \frac{5}{6}\,b^2(5a+b)+\ell abd(9a+\frac{19}{3}\,b)$$

$$T'^{(2)}_{\ell} \equiv \frac{5}{24}\,b^2(5a+4b)+\frac{1}{16}\ell abd(19a+\frac{49}{3}\,b)$$

$$U^{(2)} \equiv ab^2(a+{}^{1}/3b)$$

$$U'^{(2)} \equiv \frac{1}{32}\,ab^2(21a+17b)$$

$$U''^{(2)} \equiv \frac{1}{128}\,ab^2(3a+\frac{8b}{3})$$

$$V^{(2)} \equiv \frac{5}{24}\,b^2(25a+17b)-abd(7a+\frac{17}{3}\,b)$$

$$W^{(2)} \equiv \frac{1}{4}\,ab^2(9a+\frac{19}{3}b)$$

$$W'^{(2)} \equiv \frac{1}{64}\,ab^2(19a+\frac{49}{3}\,b)$$

$$X_{\ell} \equiv \frac{8}{3}\,b + \frac{32}{15}\,\ell ad$$

$$Y^{(2)} \equiv \frac{16}{15}\, ab$$

$$Y'^{(2)} = \frac{1}{16}\, Y^{(2)}$$

$$Z = \tfrac{1}{2} Y^{(2)}$$

$$\rho^{(2)} \equiv \frac{24}{225}\, (16\alpha+\beta)$$

$$\xi^{(2)} \equiv \frac{24}{225}\, (\alpha+16\beta)$$

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