THESIS

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by

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N - D SCATTERING WITH CENTRAL, SPIN-ORBIT, TENSOR AND QUADRATIC SPIN-ORBIT FORCES

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ABSTRACT

The following work is discussed.

a). A formulation of the elastic neutron-deuteron scattering using the most general form of the nuclear interaction which includes the central, tensor, linear spin-orbit and quadratic spin-orbit components.

The resonating group method is employed to construct the three-body wave functions and from the Schrödinger's equation a set of simultaneous integro-differential equations is derived. The doublet and the quartet spin states of the system are treated as seperate cases. The radial functions are taken in Gaussian form to permit analytical progress and each of the functions contains two terms so as to maintain accuracy in representing the numerical data. The hard core in the interaction presents a difficulty in the analysis and its effect is taken care of by a modification of the deuteron wave functions.

b). An extension of the n-d scattering formulation to include the D-state of the deuteron wave function.

The S-D interaction due to the quadratic spin-orbit potentials is omitted due to its small contribution and the comparatively complicated algebra involved.

c). The solutions of the resulting integro-differential equations by the method of finite differences.

Programmes for computing the kernels and for the solutions of the equations are prepared for the London Atlas computer. The equations are solved at different incident neutron energies so that the corresponding phase-shifts and cross-sections can be evaluated and compared with previous results.

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INTRODUCTION

In using phenomenological nucleon-nucleon interactions in the calculation of the elastic scattering of neutrons by deuterons we may obtain some information about the nature of nuclear forces. Many detailed studies in this aspect have been carried out and in all, the resonating group technique was employed to derive the integro-differential equations. Among the earlier authors, Buckingham and Massey (1941) calculated phase shifts at energies less than 20 Mev. using ordinary central and exchange potentials. More calculations with the assumption of purely central interactions followed (Buckingham , Hubbard and Massey, 1952; Christian and Gammel, 1953, ~~1955~~; de Borde and Massey, 1955; Burke and Robertson, 1957), but they were more extensive such as to include higher phases or to include a tensor force by representing it with an 'equivalent' central force or to consider both short and long effective ranges of the interaction. The problem with the inclusion of the tensor force in the interaction was considered by Horie, Tamura and Yoshida, 1952, employing the Born Approximation. Bransden, Smith and Tate, 1958, then gave a complete formulation of the neutron-deuteron scattering with both central and tensor forces together with the admixture of the D-state of the deuteron wave functions. The numerical results obtained in these papers were generally in good agreement with experimental data.

Recently a new two-body interaction which satisfies nucleon-nucleon data up to 310 Mev. was derived (Hamada and Johnston, 1962). This interaction includes the linear spin-orbit component and a new type of force namely the quadratic spin-orbit, and this thesis is a study of n-d scattering taking into account all types of forces. It is hoped that this will give a basis for further investigation to determine whether this new interaction can be applied to many-body problems when there is a possibility of other effects such as many-body forces which cannot be revealed in nucleon-nucleon experiments. The phase shifts of the n - d scattering at various incident

neutron energies will be given and the results will be discussed in the Conclusion.

The following formulation of the n - d scattering is prepared as if there was no hard core present and a modification to take care of its effect is given later (in Chapter XIV.)

CHAPTER I

I.1. NUCLEAR INTERACTION

The nucleon-nucleon interaction is considered to include both central and non-central forces. The most general form of this interaction with the invariance and symmetry requirements (Okubo and Marshak, 1958) must be a linear combination of the following terms

a. the Central exchange force,

b. the Tensor force,

$$T(\underline{r}_{ij}) = V(\underline{r}_{ij}) \left[\frac{3(\underline{\sigma}_i \cdot \underline{r}_{ij})(\underline{\sigma}_j \cdot \underline{r}_{ij})}{r_{ij}^2} - \underline{\sigma}_i \cdot \underline{\sigma}_j \right] ,$$

c. the Spin-orbit force

$$A(\underline{r}_{ij}) = V(\underline{r}_{ij}) \, (\underline{s}_i + \underline{s}_j) \cdot (\underline{r}_i - \underline{r}_j) \wedge (\underline{p}_i - \underline{p}_j) ,$$

d. the Quadratic spin-orbit force

$$Q(\underline{r}_{ij}) = V(\underline{r}_{ij}) \left[(\underline{\sigma}_i \cdot \underline{\sigma}_j) \, \underline{L}_{ij}^2 - \tfrac{1}{2} \left\{ (\underline{\sigma}_i \cdot \underline{\sigma}_{ij})(\underline{\sigma}_j \underline{L}_{ij}) + (\underline{\sigma}_j \underline{L}_{ij})(\underline{\sigma}_i \underline{L}_{ij}) \right\} \right] ,$$

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

$V(\underline{r}_{ij})$ is a radial function.

$\underline{s}_i$ is the Pauli spin matrix vector for the ith 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 forms of the tensor and the linear spin-orbit terms has been explained in many papers (Signell & Marshak, 1957, 1958; Gammel and Thaler, 1957). The necessity for the inclusion of the quadratic spin-orbit term is confirmed by Hamada (1960, 1961) in order to produce all the available data of p-p and n-p below 300 Mev. The improved version of the nucleon interaction is given by Hamada and Johnston (1962) whose form of the quadratic spin-orbit term we now use. The choice of parameters is the

set that gave the best fit to the data though this yields a high percentage ($\sim 7\%$) of the admixture of the D-state of the deuteron ground state.

In order to take care of the exchange nature of these forces between nucleons in various states, to each force is attached a combination of projection operators constructed in such a way that each operator will pick out the pair of nucleons ina certain state only.

The projection operators are

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

ν being 1 and 3 to represent the singlet and the triplet states respectively,

$\pm$ representing the even and the odd states.

B_{ij}, M_{ij} and H_{ij} are the usual Bartlett, Majorana and Heisenberg operators for nuclei i and j .

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

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

$$ {}^{3}b_{+} = 1 , \quad {}^{3}b_{-} = 1 , \quad {}^{1}b_{+} = -1 , \quad {}^{1}b_{-} = -1 ,$$

$$ {}^{3}m_{+} = 1 , \quad {}^{3}m_{-} = -1 , \quad {}^{1}m_{+} = 1 , \quad {}^{1}m_{-} = -1 ,$$

$$ {}^{3}h_{+} = 1 , \quad {}^{3}h_{-} = -1 , \quad {}^{1}h_{+} = -1 , \quad {}^{1}h_{-} = 1 .$$

Thus, for example, the operator corresponding to 1 and 2 being in triplet odd state will be

$$\frac{1}{4}\left(1 + B_{ij} - M_{ij} - H_{ij}\right) .$$

The potential wells $V(r_{ij})$ in this work are taken to be of Gaussian form whose parameters were determined by least square fits to the Hamada and Johnston potentials. 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

$$V_{ij} = \sum_{\lambda=0}^{3} \sum_{\nu=1}^{4} \frac{1}{4}(w + b_\nu B_{ij} + m_\nu M_{ij} + h_\nu H_{ij})\ {}^{\nu}V_\lambda(\underline{r}_{ij}, \underline{\sigma}_i, \underline{\sigma}_j)$$

where

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

$$\left[\delta_{\lambda,0} + \delta_{\lambda,1} \left\{ \frac{1}{2}(\underline{\sigma}_i + \underline{\sigma}_j) \cdot \underline{L}_{ij} \right\} + \delta_{\lambda,2} \left\{ \frac{3(\underline{\sigma}_i \cdot \underline{r}_{ij})(\underline{\sigma}_j \cdot \underline{r}_{ij})}{r_{ij}^2} - \underline{\sigma}_i \cdot \underline{\sigma}_j \right\} \right.$$

$$\left. + \delta_{\lambda,3} \left\{ (\underline{\sigma}_i \cdot \underline{\sigma}_j) \underline{L}_{ij}^2 - \frac{1}{2}(\underline{\sigma}_i \cdot \underline{L}_{ij})(\underline{\sigma}_j \cdot \underline{L}_{ij}) - \frac{1}{2}(\underline{\sigma}_j \cdot \underline{L}_{ij})(\underline{\sigma}_i \cdot \underline{L}_{ij}) \right\} \right] .$$

$\delta_{\lambda,\lambda'}$ is the Kronecker delta ,

k represents the kth Gaussian term ,

λ takes the value 0, 1, 2 and 3 for the central forces, the spin-orbit forces, the tensor forces and the quadratic spin-orbit forces respectively. $\nu = 1, 2, 3$ 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

$$\hbar = 1 .$$

I.2 THE DEUTERON WAVE FUNCTIONS

The ground state of the deuteron is in the triplet even state, and it is a mixture of S- and D- states due to the non-central forces. The deuteron wave function can be written

$$\Phi^{m}(\underline{r}_{23}) = \Phi(r_{23}; \underline{\sigma}_2, \underline{\sigma}_3)\, \chi^{1}_{m}(23)$$

where

$$\Phi(r_{23}; \underline{\sigma}_2, \underline{\sigma}_3) = \phi_S(r_{23}) + T(23)\,\phi_D(r_{23}),$$

$T(23)$ being the tensor operator $\dfrac{3(\underline{\sigma}_2 \cdot \underline{r}_{23})(\underline{\sigma}_3 \cdot \underline{r}_{23})}{r_{23}^2} - \underline{\sigma}_2 \cdot \underline{\sigma}_3$.

$\phi_S(23)$ and $\phi_D(23)$ are the S-state and the D-state radial wave functions respectively, and

$\chi^{1}_{m}(23)$ is the spin wave function with total spin 1 and magnetic quantum number m .

The radial wave functions are also taken in Gaussian form, i.e.

$$\phi_S(r_{23}) = \sum_{i=1}^{2} A_i\, e^{-\alpha_i r_{23}^2}$$

and

$$\phi_D(r_{23}) = \sum_{i=1}^{2} A_i'\, r_{23}^2\, e^{-\alpha_i' r_{23}^2} .$$

ϕ_D has a factor r_{23}^2 in order to cancel out the denominator of the tensor operator to simplify the algebra.

The parameters were derived from the same set of results of Hamada and Johnston, and the functions $\phi_S(r_{23})$ and $\phi_D(r_{23})$ are normalised so that

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

I.3. THE THREE-BODY WAVE FUNCTION

In the system which includes non-central forces only the total angular momentum $\underline{J}$ and its z-component J_z with respective eigen values J and M will be constants of the motion, but the orbital angular momentum $\underline{L}$ and the total spin $\underline{S}$ are not conserved.

If we assume particles 1 and 2 to be neutrons.

and particle 3 a proton, then the complete wave function in the resonating group method which describes the system is given by

$$\Psi(\widetilde{12},3) = \Psi(1,\bar{2}\bar{3}) - \Psi(2,\bar{1}\bar{3}) \ .$$

We use the notation of Buckingham & Massey, 1941.

The wave function $\Psi(1,\bar{2}\bar{3})$ can be expanded in eigen functions of J and M thus;

$$\Psi(1,\bar{2}\bar{3}) = \sum_{J,M} \psi_{JM}(1,\bar{2}\bar{3}) \ ,$$

and each of these 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 ($s=\frac{1}{2}$ for doublet states and $s=\frac{3}{2}$ for quartet states). So we can write

$$\psi_{JM}(1,\bar{2}\bar{3}) = \sum_{s} \Phi(23) F^{s}_{JM}(1\text{-}23)$$

and

$$F^{s}_{JM}(1\text{-}23) = \sum_{\ell=|J-s|}^{J+s} \mathcal{Y}^{s}_{JM\ell}(1,\bar{2}\bar{3};\Omega) \frac{1}{r} f^{s}_{JM\ell}(r)$$

where

$$\mathcal{Y}^{s}_{JM\ell}(1,\bar{2}\bar{3};\Omega) = \sum_{m=M-s}^{M+s} C^{s}_{J\ell Mm} Y_{\ell m}(\Omega) \chi^{s}_{M-m}(1,\bar{2}\bar{3}) \ .$$

Using the co-ordinate system as defined in Appendix 1, $\Phi(23)$ is the deuteron wave function,

$f^{S}_{JM\ell}(r)$ is the radial wave function of the incident neutron (particle 1)

$\chi^{S}_{M-m}(1,\bar{23})$ are the spin functions of the three-body system given in Appendix 3.

$Y_{\ell m}(\Omega)$ are the spherical harmonics of the solid angle Ω and

$C^{S}_{JM\ell m}$ are the usual Clebsch-Gordan coefficients.

The classification of the scattering states is given in detail by Bransden, Smith and Tate, 1958, and it shows couplings of states with different ℓ and S. But we shall treat the states with different total spin S, i.e. the doublet and the quartet cases seperately. This is justified because although the contributions of the various values of ℓ to the differential cross-sections are coherent and must be treated together the contributions of the various channel spin S are incoherent, and we can obtain them by attaching appropriate weights to each contribution (Blatt and Weisskopf, 1952, p 424-428). That is to say we regard S as a good quantum number.

The wave function ψ_{JM} given above will satisfy the orthonormality, for each S

$$\iint \left[\Phi(23)\,\mathcal{Y}^{S}_{J\ell Mm}(1,\bar{23};\Omega)\right]^{*}\left[\Phi(23)\,\mathcal{Y}^{S}_{J\ell' M'}(1,\bar{23};\Omega)\right] dr_{23}\,d\Omega = \delta_{JJ'}\,\delta_{MM'}\,\delta_{\ell\ell'}.$$

To abbreviate the algebra the various partial wave-functions are defined in vector and matrix form.

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

$$\chi^{\frac{1}{2}}(1) = \left[\chi^{\frac{1}{2}}_{\frac{1}{2}}(1,\bar{2\bar{3}}),\ \chi^{\frac{1}{2}}_{-\frac{1}{2}}(1,\bar{2\bar{3}})\right],$$

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

$$\mathcal{F}^{\frac{1}{2}}_{JM}(r) = \begin{bmatrix} f^{\frac{1}{2}}_{JM\,J-\frac{1}{2}}(r) \\ f^{\frac{1}{2}}_{JM\,J+\frac{1}{2}}(r) \end{bmatrix}$$

so that

$$F^{S}_{JM}(1\text{-}23) = \frac{1}{r}\chi\mathcal{Y}\mathcal{F} \quad .$$

Here $\mathcal{Y}$ always refers to $\mathcal{Y}^{S}_{JM\ell}(\Omega)$ which involves no spin functions whereas $\mathcal{Y}^{S}_{JM\ell}(1,23;\Omega)$ will be written in full.

I.4 HARD CORES OF THE POTENTIALS

The nuclear potentials of Hamada and Johnston which are used in this work contain hard cores in all states of the interacting nucleons. Though the radii of the cores are assumed to be the same and small ($r_c \sim 0.48\times10^{-13}$ cm.) Their presence constitutes a difficulty in the analysis of the three-body scattering problem. As will be shown in Chapter II the Schrödinger equation involves integrals of the form

$$\int \Phi^{*}(23)\, V(r_{12})\, \Phi(23)\, d\tau_{23} \quad .$$

This integral has to be divided into two regions corresponding to $|\underline{r}_{12}| < r_c$ and $|\underline{r}_{12}| > r_c$ if the hard cores of the potential are considered. The conditions imposed on $|\underline{r}_{12}|$ cause the integration over the spherical harmonics to be restricted to certain solid angles. This results in the dependence of the solutions on the quantum number M which implies the violation of J_z invariance.

Another difficulty arises owing to the integrands over the hard core region not being finite. This may be avoided if either or both of the potentials and the deuteron wave functions are adjusted so as to take care of the hard-core effect.

Brueckner (1958) has shown that, in a two-body problem, the product $V(r)\phi(r)r$ behaves like a Dirac delta function and as $V \to \infty$, $V(r)\, r\phi(r) \to 0$ for $r < r_c$,

where $V(r)$ and $\phi(r)$ are the potential and the radial wave functions respectively.

Since the potential $V(r)$ is infinite inside the hard core, the two body wave function $\phi(r)$ has to vanish there. Thus taking as a hard core effect

$$V(0) = \infty ,$$

we must at the same time put $\phi(0) = 0$.

In this we need not break the integration into two parts and so the difficulty of the M -dependence is avoided.

Thus the hare core effect may be achieved by taking the deuteron

wave function to have the analytical form

$$\Phi_S(r_{23}) = r_{23}^2 \sum_{i=1}^{2} A_i e^{-\alpha_i r_{23}^2} .$$

The D-State function needs no alteration as one additional factor of r_{23}^2 in the wave functions is enough to fulfil the conditions.

Therefore in Appendix 2 the numerical values given by Hamada and Johnston are interpolated into the above Gaussian form for ϕ_S instead of the one previously given in section I.2. But, as mentioned in the Introduction, we leave the analysis of the whole problem as it is and the resulting expressions are differentiated with respect to α_i to obtain the factor r_{23}^2 . These differentiations are discussed in Chapter XIV.

CHAPTER II

II. 1 DERIVATION OF THE INTEGRO-DIFFERENTIAL EQUATIONS.

The Schrödinger's equation for the wave function is

$$(T_{123} + V)\,\Psi(\tilde{12},3) = E\,\Psi(\tilde{12},3) \qquad \ldots\ldots(2.1)$$

where T_{123} is the kinetic energy operator,

V is the potential energy

and E is the total energy of the system.

T_{123} may be written

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

where M is the mass of a neutron or proton,

∇^2_{23} , $\nabla^2_{1\text{-}23}$ are Laplacian operators in the relative co-ordinates of particles 2 and 3 and of particle 1 relative to the centre of mass of the other two respectively.

We have $$V = V_{12} + V_{23} + V_{31} ,$$

V_{ij} being the potential energy of the particles i and j.

$$E = E_n + E_d ,$$

where E_d is the energy of the deuteron ground state (-2.226 Mev)

E_n is the energy of the incident neutron relative to the deuteron (= $\frac{2}{3}$ of the energy in the 'laboratory' system).

Using $\Psi(\tilde{12},3)$ given in Chapter I and dropping the indices J, M, l, s equation (2.1) can be written for both doublet and quartet cases as

$$(T_{1\text{-}23} - E + V_{12} + V_{23} + V_{31})\,\Sigma\,\Phi(23)\,F(1\text{-}23) = (T_{123} - E + V_{12} + V_{23} + V_{31})\,\Sigma\,\Phi(13)\,F(2\text{-}13) .$$

If $\Phi(23)$ used is the exact radial wave function of the deuteron then

$$(T_{23} - E_d + V_{23})\,\Phi(23) = 0 \qquad \ldots\ldots(2.2)$$

and its complex conjugate

$$\Phi^*(23)\,(T_{23} - E_d + V_{23}) = 0 \,. \qquad \ldots\ldots(2.3)$$

Also $$(T_{13} - E_d + V_{13})\,\Phi(13) = 0 \,. \qquad \ldots\ldots(2.4)$$

Conditions (2.2) and (2.4) reduce the Schrödinger's equation to

$$(T_{1-23} - E_n + V_{12} + V_{13})\,\mathcal{A}\,\Phi(23)\,F(1-23) = (T_{2-13} - E_n + V_{12} + V_{23})\,\mathcal{A}\,\Phi(13)\,F(2-13) \,. \qquad \ldots\ldots(2.5)$$

Treating the doublet and the quartet states seperately the only possible coupling in equation (2.5) is that of the states with different l's. To obtain an equation for the radial function $\mathcal{F}^{(r)}_{JMl}$ we multiply (2.5) by $[\Phi(23)\,\mathcal{Y}_{JMl}(\hat{1},\hat{23};\Omega)]^*$, (index s dropped being understood) or $[\Phi(23)\,\chi(1)\,\gamma(1)]^*$ then integrate over all co-ordinates except r and sum over the spins.

Using equation (2.3), we get

$$\int [\Phi(23)\,\chi(1)\,\gamma(\Omega)]^*\,(T_{1-23} - E_n + V_{12} + V_{13})\,\mathcal{A}\,\Phi(23)\,F(1-23)\,d\Omega\,dr_{23}$$

$$= \int [\Phi(23)\,\chi(1)\,\gamma(\Omega)]^*\,(T_{2-13} - T_{23} + E_d - E_n + V_{12})\,\mathcal{A}\,\Phi(13)\,F(2-13)\,d\Omega\,dr_{23} \,.$$

On L.H.S. of the equation, $\int \ldots V_{12} \ldots = \int \ldots V_{13} \ldots$

and on R.H.S., the kernel is symmetrical in 1 and 2 as

$$T_{2-13} - T_{23} \equiv T_{1-23} - T_{13} \,.$$

After working out the operators attached to V_{12} we proceed in the same pattern as previous derivation. Finally the integro-differential equations are found to be

$$\mathcal{D}^2 \mathcal{F}(r)$$

$$= \int d\underline{R}\, d\Omega \left(\frac{4}{3}\frac{M}{\hbar^2}\right) r \left[\Phi(23)\chi(1)\mathcal{Y}(\Omega)\right]^* .$$

$$\cdot \sum_{\lambda,\nu} \Big[\tfrac{1}{4}(2w-h)_\nu \, {}^{\nu}V_{\lambda}(12)\Phi(\underline{\sigma}_2,\underline{\sigma}_3;\underline{r}_{23})\chi(1,\bar{2}\bar{3}) + \tfrac{1}{4}(2b-m)_\nu \, {}^{\nu}V_{\lambda}(12)\Phi(\underline{\sigma}_1,\underline{\sigma}_3;\underline{r}_{23})\chi(2,\bar{1}\bar{3}) \Big] \mathcal{Y}(\Omega)\, \tfrac{1}{r}\mathcal{F}(r)$$

$$- \int d\underline{r}'\, d\Omega \left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r \left[\Phi(23)\chi(1)\mathcal{Y}(\Omega)\right]^* .$$

$$\cdot \sum_{\lambda,\nu} \Big[\tfrac{1}{4}(w-2h)_\nu \, {}^{\nu}V_{\lambda}(12)\Phi(\underline{\sigma}_1,\underline{\sigma}_3;\underline{r}_{13})\chi(2,\bar{1}\bar{3}) + \tfrac{1}{4}(b-2m)_\nu \, {}^{\nu}V_{\lambda}(12)\Phi(\underline{\sigma}_2,\underline{\sigma}_3;\underline{r}_{13})\chi(1,\bar{2}\bar{3}) \Big] \mathcal{Y}(\Omega')\, \tfrac{1}{r'}\mathcal{F}(r')$$

$$+ (E_n - E_d) \int d\underline{r}'\, d\Omega \left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r \left[\Phi(23)\chi(1)\mathcal{Y}(\Omega)\right]^* \Phi(\underline{\sigma}_1,\underline{\sigma}_3;\underline{r}_{13})\chi(2,\bar{1}\bar{3})\mathcal{Y}(\Omega')\, \tfrac{1}{r'}\mathcal{F}(r')$$

$$+ \int d\underline{r}'\, d\Omega \left(\frac{4}{3}\right)^3 r\, \mathcal{Y}^*(\Omega)\chi^*(1)\left[\nabla^2_{r'}\Phi^*(23)\,\Phi(13)\right]\chi(2,\bar{1}\bar{3})\,\mathcal{Y}(\Omega')\,\tfrac{1}{r'}\mathcal{F}(r')$$

$$- \int d\underline{r}'\, d\Omega \left(\frac{4}{3}\right)^4 r \left[\nabla^2_{R}\Phi(23)\,\mathcal{Y}(\Omega)\right]^* \chi^*(1)\,\Phi(13)\chi(2,\bar{1}\bar{3})\,\mathcal{Y}(\Omega')\,\tfrac{1}{r'}\mathcal{F}(r') ,$$

..... (2.6)

where

$$\mathcal{D}^2 = \begin{bmatrix} D^2_{J-S} & & & \\ & D^2_{J-S+1} & & \\ & & \ddots & \\ & & & D^2_{J+S} \end{bmatrix}$$

for all J and S except $J = \frac{1}{2}$, $S = 3/2$ for which

$$\mathcal{D}^2 = \begin{bmatrix} D^2_{J+S-1} & \\ & D^2_{J+S} \end{bmatrix} ,$$

and

$$D^2_\ell = \frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2 ,$$

$$k^2 = \frac{4}{3}\frac{M}{\hbar^2} E_n .$$

II.2 CLASSIFICATION AND PRESENTATION

The equation (2.6) is strictly speaking a 2 x 2 matrix in the doublet case and a 4 x 4 in the quartet. As there is coupling between states with the values of ℓ's differing by 2 only, the doublet case will give two single equations with $\ell = J-1/2$ and $J+1/2$; the quartet case will give two pairs of simultaneous equations when $J > 3/2$ and only two single equations when $J = 1/2$.

The terms on the R.H.S. of equation (2.6) can be classified as 'Direct' and 'Indirect' interactions depending whether they involve the outside neutron (co-ordinates $\underline{r}$). The direct interaction may be evaluated completely, but the indirect interaction terms contain functions of r and r' so the integrals are left as undetermined functions.

Both the direct and indirect interactions terms that contain the same type of force in V_{12} will be treated in the same chapter. The term which is multiplied by $(E_n - E_d)$ will be named the N-kernel, and the two kinetic energy terms with operators $\nabla^2_{r'}$ and ∇^2_R will combine to be called the P-kernel.

The evaluation of these terms will be dealt with in two parts;

a. the S-S terms - the pre and post multiplying deuteron wave functions are both in the S-State.

b. 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 are neglected due to the small percentage of the D-State admixture. Considering the amount of complicated analysis involved and later, the computing time taken in the evaluation of the quadratic spin orbit S-D terms these are also left out. The derivation for the central and tensor forces is repeated here for the sake of completeness.

In the following chapters we shall use the notations for the nuclear potentials and the wave function defined previously. Also we may refer to the co-ordinate system given in Appendix 1 and the spin functions in Appendix 3. The integration formulae quoted in the formulation are in Appendix 4. Owing to the large amount of algebra involved in some parts of the calculation it is not always practicable to give every step explicitly. Also some of the suffice are omitted wherever there is no risk of confusion.

CHAPTER III

THE CENTRAL FORCE TERMS

III. 1 DIRECT INTERACTION

The derivation is straight forward but is given here to illustrate the notation. From equation (2.6) the contribution from the central forces is

$$ {}^{c}D_{s\text{-}s}(r) = \tfrac{4}{3}\frac{M}{\hbar^2}\int d\underline{R}\, d\Omega\, \mathcal{Y}^{*}(\Omega)\chi^{*}(1)\Phi(23)\times $$

$$ \times \sum_{\nu}\left[\tfrac{1}{4}(2w-h)_{\nu}\,{}^{\nu}V_{c}(12)\chi(1)+\tfrac{1}{4}(2b-m)_{\nu}\,{}^{\nu}V_{c}(12)\chi(2)\right]\mathcal{Y}(\Omega)\Phi(23)\mathcal{F}(r)\,. $$

After the spin summation and the spherical harmonic integration, we get

$$ {}^{c}D_{ss}(r) $$

$$ = \tfrac{4}{3}\frac{M}{\hbar^2}\int d\underline{R}\, d\underline{\tau}(23)\sum_{\nu}\tfrac{1}{4}\left[(2w-h)_{\nu}+g(s)(2b-m)_{\nu}\right]{}^{\nu}V_{c}(12)\,\Phi(23)\,\mathcal{F}(r) $$

where

$$ g = -\tfrac{1}{2} \qquad s = \tfrac{1}{2} $$

$$ = 1 \qquad s = \tfrac{3}{2}\,. \qquad \text{.....(3.1)} $$

Hence by the summation over ν the central potential in the direct interaction of the doublet case is

$$ \tfrac{1}{8}\left(V_{c}^{3+}+3V_{c}^{3-}+9V_{c}^{1+}+3V_{c}^{1-}\right). $$

The equivalent Gaussian terms are $\sum_{k=1}^{2} {}^{c}U_{k}^{(1)}\exp.\left[-{}^{c}\mu_{k}^{(1)}r_{12}^{2}\right]$

and the mumerical values are all given in Appendix 2.

Similarly in the quartet case, the potential is

$$\tfrac{1}{2}(V_c^{3+} + 3V_c^{3-}) = \sum_k {}^cU_k^{(3)} \exp.\left[-{}^c\mu_k^{(3)} r_{12}^2\right]$$

The space integration in both cases can nowbe performed viz:

$${}^cD_{s\text{-}s}(r) = \sum_{i,j,k=1}^{2} \tfrac{4}{3}\frac{M}{\hbar^2}\int d\underline{R}\; A_i e^{-\alpha_i r_{23}^2} U_k e^{-\mu_k r_{12}^2} A_j e^{-\alpha_j r_{23}^2} \mathcal{F}(r)$$

$$= \tfrac{4}{3}\frac{M}{\hbar^2}\sum_{i,j,k} A_iA_jU_k\, e^{-(\mu_k-\lambda_{ijk}\gamma_{ijk}^2)r^2}\mathcal{F}(r)\int d\underline{R}\; e^{-\lambda_{ijk}(\underline{R}-\gamma_{ijk}\underline{r})^2}$$

where

$$\lambda_{ijk} = \alpha_i+\alpha_j+\tfrac{1}{4}\mu_k \qquad \gamma_{ijk} = \tfrac{1}{2}\mu_k/\lambda_{ijk}\ .$$

Thus

$${}^cD_{s\text{-}s}(r) = \tfrac{4}{3}\frac{M}{\hbar^2}\sum_{i,j,k}\left(\frac{\pi}{\lambda_{ijk}}\right)^2 A_iA_jU_k\, e^{-(\mu_k-\lambda_{ijk}\gamma_{ijk}^2)r^2}\mathcal{F}(r)$$

after using the relevant integration formula given in App. 4.

In the following sections, only the ijk th term in the summation will be written and the suffices i,j,k may be dropped from the parameters $A, U, \alpha, \mu, \lambda, \gamma$ which still vary according to the interaction (direct or indirect) and the case (doublet or quartet) as well as to the type of forces (Central or Tensor, etc).

Hence the central force direct terms in both cases may be written

$${}^cD_{s\text{-}s} = \tfrac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} AAU\, e^{-(\mu-\lambda\gamma^2)r^2}\mathcal{F}(r)\ .$$

III. 2. THE INDIRECT INTERACTION

The contribution of the indirect terms to equation (2.6) is

$$ {}^{c}I_{S\cdot S}(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r \int dI' d\Omega \, \Phi(23)\, \mathcal{Y}^*(\Omega)\, \mathcal{X}^*(1) \times $$

$$ \times \sum_{\nu} \left[\tfrac{1}{4}(w-2h)_{\nu}\, {}^{\nu}V_c(12)\, \chi(2) + \tfrac{1}{4}(b-2m)_{\nu}\, {}^{\nu}V_c(12)\, \chi(1) \right] \mathcal{Y}(\Omega')\, \Phi(13)\, \frac{1}{r'} \mathcal{F}(r') . $$

The potential in the doublet case is

$$ \sum_{k} {}^{c}U_k^{(2)}\, e^{-{}^{c}\mu_k^{(2)} r_{12}^2} = \sum_{\nu} \tfrac{1}{4}(b-2m-\tfrac{1}{2}w+h)_{\nu}\, {}^{\nu}V_c = \tfrac{1}{8}(-{}^{3+}V_c + 3\,{}^{3-}V_c - 9\,{}^{1+}V_c + 3\,{}^{1-}V_c) $$

and in the quartet case

$$ \sum_{k} {}^{c}U_k^{(4)}\, e^{-{}^{c}\mu_k^{(4)} r_{12}^2} = \sum_{\nu} \tfrac{1}{4}(b-2m+w-2h)_{\nu}\, {}^{\nu}V_c = \tfrac{1}{2}(-{}^{3+}V_c + 3\,{}^{3-}V_c) . $$

Hence in both cases we get ${}^{c}I_{SS}(r)$

$$ = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r \int dI' d\Omega \, \mathcal{Y}^*(\Omega)\, A_i\, e^{-\alpha_i r_{23}^2}\, U_k\, e^{-\mu_k r_{12}^2}\, A_j\, e^{-\alpha_j r_{13}^2}\, \mathcal{Y}(\Omega')\, \frac{1}{r'} \mathcal{F}(r') $$

$$ = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} A_i A_j U_k \int_0^{\infty} dr'\, rr'\, \mathcal{F}(r')\, e^{-a_{ijk} r^2 - b_{ijk} r'^2}\, \delta_{ll'}\, \delta_{mm'} \int Y^*_{lm}(\Omega)\, Y_{l'm'}(\Omega')\, e^{-\delta_{ijk}\, \underline{r}\cdot\underline{r}'}\, d\Omega\, d\Omega' $$

using the fact that $dI' = r'^2 dr' d\Omega'$, where

$$ a_{ijk} = \tfrac{4}{9}(\alpha_i + 4\alpha_j + \mu_k) \quad , \quad b_{ijk} = \tfrac{4}{9}(4\alpha_i + \alpha_j + \mu_k) $$

and

$$ \delta_{ijk} = \tfrac{4}{9}(4\alpha_i + 4\alpha_j - 2\mu_k) , $$

$\delta_{ll'}$ being the Krönecker delta .

l and l' take the values $J-S, J-S+1, \ldots\ldots, J+S$, with the usual exception for $J = \frac{1}{2}$, $S = 3/2$.

m and m' take the values $M-S, M-S+1, \ldots\ldots, M+S$.

We use the formula from Appendix 4

$$\int Y^{*}_{lm}(\theta,\varphi)\, e^{-\partial \underline{r}\cdot\underline{r}'}\, d\Omega = \frac{4\pi}{\partial r r'}\, Y^{*}_{l'm'}(\theta',\varphi')\, \vartheta_{l+\frac{1}{2}}(\partial r r')$$

and define a diagonal matrix

$$\left[\vartheta_{l+\frac{1}{2}}(x)\right] = \begin{pmatrix} \vartheta_{J-S+\frac{1}{2}}(x) & & & \\ & \vartheta_{J-S+3/2}(x) & & \\ & & \ddots & \\ & & & \vartheta_{J+S+\frac{1}{2}}(x) \end{pmatrix}$$

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

and for $J \geq 3/2$ if $S = 3/2$,

and

$$\left[\vartheta_{l+\frac{1}{2}}(x)\right] = \begin{pmatrix} \vartheta_{J+S-\frac{1}{2}}(x) & \\ & \vartheta_{J+S+\frac{1}{2}}(x) \end{pmatrix}$$

for $J = \frac{1}{2}$, $S = 3/2$.

We finally obtain

$${}^{c}_{S\text{-}S}I(r) = -\left(\frac{4}{3}\right)^{4} \frac{M}{\hbar^2} \frac{4\pi}{\partial} A A U \int dr'\, e^{-ar^2-br'^2} \left[\vartheta_{l+\frac{1}{2}}(\partial r r')\right] f^{p}(r') .$$

CHAPTER IV

THE SPIN-ORBIT TERMS

IV.1. THE DIRECT INTERACTION

As we have an account of symmetry

$$\chi^*(1,\bar{2}\bar{3})\,(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\,\chi(2,\bar{1}\bar{3}) \;=\; \chi^*(1,2\bar{3})\,(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\,\chi(1,\bar{2}\bar{3})$$

the spin-orbit terms can be written ${}^{LS}D_{SS}(r)$

$$= \tfrac{4}{3}\tfrac{M}{\hbar^2}\,r\int d\underline{R}\,d\Omega\left[\Phi(23)\chi(1)y(\Omega)\right]^*\sum_\nu \tfrac{1}{4}(2w-h+2b-m)_\nu\,{}^\nu V_{LS}(12)\,\Phi(23)\chi(1)y(\Omega)\,\tfrac{1}{r}\,\mathcal{F}(r)\,.$$

The potential in both cases is

$$\sum_K {}^{LS}U_K^{(1)}\exp.\left[-{}^{LS}\mu_K^{(1)}r_{12}^2\right] \;=\; \sum_\nu \tfrac{1}{4}(2w-h+2b-m)_\nu\,{}^\nu V_{LS}(12)\,.$$

Writing the spin-orbit operator in full

$${}^{LS}D_{SS}(r) \;=\; \tfrac{4}{3}\tfrac{M}{\hbar^2}\,r\int d\underline{R}\,d\Omega\;y^*(\Omega)\chi^*(1)\,A_i\,e^{-\alpha_i R^2}\,U_K\,e^{-\mu_K(\underline{r}-\frac{1}{2}\underline{R})^2}\times$$

$$\times\left[\tfrac{1}{2i}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\left(\tfrac{3}{2}\underline{r}\wedge\tfrac{\partial}{\partial\underline{r}}+\tfrac{1}{2}\underline{R}\wedge\tfrac{\partial}{\partial\underline{R}}-\tfrac{3}{4}\underline{R}\wedge\tfrac{\partial}{\partial\underline{r}}-\underline{r}\wedge\tfrac{\partial}{\partial\underline{R}}\right)\right]A_j\,e^{-\alpha_j R^2}\,\chi(1)y(\Omega)\,\tfrac{1}{r}\,\mathcal{F}(r)\,.$$

Carrying out the $\frac{\partial}{\partial\underline{R}}$ differentiation and then the $d\underline{R}$ integration, we get ${}^{LS}D_{SS}(r)$

$$= \tfrac{4}{3}\tfrac{M}{\hbar^2}\left(\tfrac{\pi}{\lambda}\right)^{3/2}\tfrac{3}{2}\left(1-\tfrac{\gamma}{2}\right)AAU\,e^{-(\mu-\lambda\gamma^2)r^2}\int d\Omega\,y^*(\Omega)\chi^*(1)\,\tfrac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_r\,\chi(1)y(\Omega)\,\mathcal{F}(r)\,.$$

THE EIGEN VALUES OF $(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}$

We represent the values of the operator by

$$\langle(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}\rangle\,.$$

The matrix xy is constructed so that

$$\underline{J}^2 xy = J(J+1)\,xy .$$

Now $$\underline{J} = \underline{L} + \underline{S} ,$$

where $$\underline{S} = \tfrac{1}{2}\underline{\sigma}$$

$$= \tfrac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2+\underline{\sigma}_3) .$$

We have

$$\langle 2\underline{L}\cdot\underline{S}\rangle = \langle \underline{J}^2-\underline{L}^2-\underline{S}^2\rangle$$

i.e. $$\langle \underline{\sigma}\cdot\underline{L}\rangle = \left[J(J+1)-[L(L+1)-S(S+1)]\right][\delta] ,$$

$[\delta]$ being a unit matrix.

For the doublet case we have

$$\langle(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}\rangle = \tfrac{1}{3}\langle\underline{\sigma}\cdot\underline{L}\rangle$$

so that

$$\langle(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}\rangle = \tfrac{1}{3}\left[J(J+1)-[L(L+1)-\tfrac{3}{4}\right][\delta]$$

$$= \left[A^{(\frac{1}{2})}_{JL}\right] \qquad \ldots\ldots \text{(4.1 a)}$$

where

$$\left[A^{(\frac{1}{2})}_{JL}\right] = \begin{bmatrix} \tfrac{1}{3}(J-\tfrac{1}{2}) & \\ & -\tfrac{1}{3}(J+3/2) \end{bmatrix}$$

and for the quartet case

$$\langle(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}\rangle = \tfrac{2}{3}\langle\underline{\sigma}\cdot\underline{L}\rangle$$

$$= \left[A^{(3/2)}_{JL}\right] \qquad \ldots\ldots \text{(4.1 b)}$$

where

$$\left[A^{(3/2)}_{JL}\right] = 2\times\begin{bmatrix} J-3/2 & & & \\ & \tfrac{1}{3}(J-\tfrac{1}{2}) & & \\ & & -\tfrac{1}{3}(J+9/2) & \\ & & & -(J+5/2) \end{bmatrix}$$

for $J \geqslant 3/2$,

and for $J=\frac{1}{2}$, $\quad [A^{3/2}_{J\ell}] = 2\times\begin{bmatrix} \frac{1}{3}(J-\frac{1}{2}) & \\ & -(J+\frac{3}{2}) \end{bmatrix}$.

Hence we obtain finally

$$D^{LS}_{S\text{-}S}(r) = \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2}\frac{3}{2}(1-\tfrac{\gamma}{2})\,AAU\,e^{-(\mu-\lambda\gamma^2)r^2}\,\tfrac{1}{2}[A_{J\ell}]\,\mathcal{F}^0(r).$$

In Appendix 3 an alternative method of derivation is given. In this the spin summation is done before the spherical harmonic integration and it is used in the avaluation of other matrix elements.

IV.2. THE INDIRECT INTERACTION

The potential is

$$\sum_k {}^{LS}U^{(2)}_k\, e^{-{}^{LS}\mu^{(2)}_k r_{12}^2} = \sum_\nu \tfrac{1}{4}(w-2h+b-2m)_\nu\, {}^{\nu}V^{LS}(12).$$

We have to evaluate the integral

$$I^{LS}_{S\text{-}S}(r) = -\left(\tfrac{4}{3}\right)^4\frac{M}{\hbar^2}\,r\int d\underline{r}'d\Omega\, A_i\, e^{-\frac{4}{9}\alpha_i(\underline{r}+2\underline{r}')^2}\, y^*(\Omega)\chi^*(1)\, U_k\, e^{-\frac{4}{9}\mu_k(\underline{r}-\underline{r}')^2}\times$$
$$\times\frac{1}{2i}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\left[(\underline{r}-\underline{r}')_\wedge\frac{\partial}{\partial\underline{r}}-(\underline{r}-\underline{r}')_\wedge\frac{\partial}{\partial\underline{r}'}\right]A_j\, e^{-\frac{4}{9}\alpha_j(2\underline{r}+\underline{r}')^2}\,\chi(2)y(\Omega')\,\frac{1}{r'}\mathcal{F}^0(r').$$

By differentiating w.r.t. $\underline{r}$ and integrating by parts w.r.t. $\underline{r}'$ we get

$$I^{LS}_{S\text{-}S}(r)$$
$$= -\left(\tfrac{4}{3}\right)^4\frac{M}{\hbar^2}\,AAU\,\frac{16}{3}(\alpha_i+\alpha_j)\,r\int d\underline{r}'d\Omega\, e^{-ar^2-br'^2-\partial\underline{r}\cdot\underline{r}'}\, y^*(\Omega)\chi^*(1)\frac{1}{2i}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{r}'_\wedge\underline{r}\,\chi(2)y(\Omega')\,\frac{1}{r'}\mathcal{F}^0(r').$$

By rearranging the factors and using the result

$$\underline{r}' \wedge \underline{r}\; e^{-\partial \underline{r}\cdot\underline{r}'} = -\frac{1}{\partial}\, \underline{r}' \wedge \frac{\partial}{\partial \underline{r}'}\, e^{-\partial \underline{r}\cdot\underline{r}'}$$

and then integrating by parts again we obtain $I^{LS}_{S\cdot S}(r)$

$$= -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\, AAU\, \frac{16}{3}\, \frac{(\alpha_i+\alpha_j)}{\partial} \int dr'\, e^{-ar^2-br'^2}\, rr' \int e^{-\partial \underline{r}\cdot\underline{r}'}\, y^*(\Omega)\chi^*(1)\, \tfrac{1}{2}\, (\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_T\, \chi(2)\, y(\Omega')\, \mathcal{F}(r')\, d\Omega d\Omega'$$

Using equations (4.1a) and (4.1b) we obtain the expression

$$\int d\Omega d\Omega'\, e^{-\partial \underline{r}\cdot\underline{r}'}\, y^*(\Omega)\chi^*(1)\, (\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_T\, \chi(2)\, y(\Omega') = \frac{4\pi}{\partial rr'} \left[\mathcal{I}_{[+\frac{1}{2}}(\partial rr')\right] \left[A_{JI}\right] .$$

So finally we get

$$I^{LS}_{S\cdot S}(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\, AAU\, \frac{4\pi}{\partial}\, \frac{16}{3}\, \frac{(\alpha_i+\alpha_j)}{\partial} \int_0^\infty dr'\, e^{-ar^2-br'^2}\, \tfrac{1}{2} \left[\mathcal{I}_{[+\frac{1}{2}}(\partial rr')\right] \left[A_{JI}\right] \mathcal{F}^*(r') .$$

IV.3 REMARK

The inclusion of the spin-orbit potential introduces no new feature in the integro-differential equations. The matrix $[A_{JI}]$ is diagonal so there is no coupling between the doublet-doublet states, or the quartet-quartet states of the neutron-deuteron system. This may not be the case had we not treated the doublet and the quartet states seperately.

CHAPTER V

THE TENSOR FORCE TERMS

We define the tensor operator which is symmetrical in i,j and $\underline{A},\underline{B}$ as

$$S_{ij}(\underline{A},\underline{B}) = \tfrac{3}{2}(\underline{\sigma}_i\cdot\underline{A})(\underline{\sigma}_j\cdot\underline{B}) + \tfrac{3}{2}(\underline{\sigma}_j\cdot\underline{A})(\underline{\sigma}_i\cdot\underline{B}) - (\underline{\sigma}_i\cdot\underline{\sigma}_j)(\underline{A}\cdot\underline{B}) .$$

This force gives no contribution to the doublet case because of the spins. The formulation given below will be slightly different from the work of Bransden, Smith and Tate (1958) because the operator in the integrats has no denominator, also the calculation is more specific with Gaussian functions.

V.1. DIRECT INTERACTION

The potential is expressed in the form

$$r_{12}^2 \sum_k {}^{T}U_k^{(1)} \exp\left[-{}^{T}\mu_k^{(1)} r_{12}^2\right] = \sum_\nu \tfrac{1}{4}(2w-h+2b-m)_\nu \, {}^{\nu}V_T(12) .$$

The tensor operator in the direct term assumes the form

$$S_{12}(r_{12}^2) = S_{12}(r^2) - S_{12}(\underline{r},\underline{R}) + \tfrac{1}{4}S_{12}(R^2) .$$

We get ${}^{T}_{S\text{-}S}D(r)$

$$= \tfrac{4}{3}\frac{M}{\hbar^2} e^{-(\mu-\lambda\delta^2)r^2} AAU \int d\underline{R}\, d\Omega\, e^{-\lambda(\underline{R}-\delta\underline{r})^2} \times$$

$$\times y^*(\Omega)x^*(1)\left[S_{12}(r^2) - S_{12}(\underline{r},\underline{R}) + \tfrac{1}{4}S_{12}(R^2)\right] x(1)y(\Omega)\mathcal{F}(r)$$

$$= \tfrac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} AAU\left(1-\tfrac{\delta}{2}\right)^2 e^{-(\mu-\lambda\delta^2)r^2} \int d\Omega\, y^*(\Omega)x^*(1)\, S_{12}(r^2)\, x(1)y(\Omega)\mathcal{F}(r) .$$

V.1.1. THE SPIN SUMMATION :

We have to evaluate the matrix: $\langle \chi(1) | S_{12}(\hat{r}) | \chi(1) \rangle$

The elements of this matrix are given in the table below

TABLE I: THE SPIN PRODUCTS OF $S_{12}(\hat{r})$.

	$\chi^{3/2}_{3/2}$	$\chi^{3/2}_{1/2}$	$\chi^{3/2}_{-1/2}$	$\chi^{3/2}_{-3/2}$
$\chi^{3/2}_{3/2}$	$3z^2-r^2$	$2\sqrt{3}\, r_- z$	$4\sqrt{3}\, r_-^2$	0
$\chi^{3/2}_{1/2}$	$2\sqrt{3}\, r_+ z$	$-3z^2+r^2$	0	$4\sqrt{3}\, r_-^2$
$\chi^{3/2}_{-1/2}$	$4\sqrt{3}\, r_+^2$	0	$-3z^2+r^2$	$-2\sqrt{3}\, r_- z$
$\chi^{3/2}_{-3/2}$	0	$4\sqrt{3}\, r_+^2$	$-2\sqrt{3}\, r_+ z$	$3z^2-r^2$

We define $r_\pm$ by $r_\pm = \frac{1}{2}(x \pm iy)$.

V. 1.2 THE INTEGRATION OVER SPHERICAL HARMONICS

Each of the matrix elements shown in Table 1 can be represented by a spherical harmonic $Y_{[m}(\theta, \varphi)$ with $[= 2$ and $m = -2, -1, 0, 1$ or 2 . Thus the evaluation of the integral $\int y^* x^* S_{12} \chi y \, d\Omega$ reduces to finding integrals of products of three spherical harmonics.

The formula, given in Edmonds (1957, p,63) is

$$\int\int Y_{l_1 m_1}(\theta,\phi)\, Y_{l_2 m_2}(\theta,\phi)\, Y_{l_3 m_3}(\theta,\phi)\, \sin\theta\, d\theta\, d\phi$$

$$= \left[\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right]^{\frac{1}{2}} \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

where $\begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ is the Wigner 3 - j symbols.

In the actual calculation the Wigner 3 - j symbols simplify but it is still tedious work which involves sums of products of Clebsch-Gordan coefficients.

Write $$\langle S_{12}(r^2)\rangle = \int d\Omega\, y^*(\Omega)\chi^*(1)\, S_{12}(r^2)\chi(1)y(\Omega)$$

The result obtained for $J \geq 3/2$ is

$$\langle S_{12}(r^2)\rangle = r^2 \begin{pmatrix} -\frac{2J-3}{2J} & 0 & \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J} & 0 \\ 0 & \frac{2J+5}{2J+2} & 0 & \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J+2} \\ \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J} & 0 & \frac{2J-3}{2J} & 0 \\ 0 & \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J+2} & 0 & -\frac{2J+5}{2J+2} \end{pmatrix}$$

and for $J = \frac{1}{2}$ only

$$\langle S_{12}(r^2)\rangle = r^2 \begin{pmatrix} \frac{2J-3}{2J} & 0 \\ 0 & -\frac{2J+5}{2J+2} \end{pmatrix} . \qquad \ldots\ldots(5.1)$$

Defining the matrix B_{JI} by $r^2[B_{JI}] = \langle S_{12}(r^2) \rangle$

we finally obtain the tensor force direct interaction ${}^{T}D_{S\text{-}S}(r)$ thus

$$ {}^{T}D_{S\text{-}S}(r) = \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2}\left(1-\frac{\gamma}{2}\right)^2 A_i A_j U_k \, e^{-(\mu-\lambda\gamma^2)r^2} \, r^2[B_{JI}] \, \mathcal{F}^e(r) . $$

V.2. INDIRECT INTERACTION

We write the tensor operator in the form

$$ S_{12}(r_{12}^2) = \frac{4}{9}\left[S_{12}(r^2) + S_{12}(r'^2) - 2S_{12}(\underline{r},\underline{r}') \right] , $$

and the potential radial function as

$$ r_{12}^2 \sum_K {}^{T}U_K^{(2)} \exp\left[-{}^{T}\mu_K^{(2)} r_{12}^2 \right] = \sum_\nu \frac{1}{4}(w-2h+b-2m)_\nu \, {}^{\nu}V_T(12) . $$

The tensor indirect interaction is then given by

$$ {}^{T}I_{S\text{-}S}(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} \, r \, AAU \left(\frac{2}{3}\right)^2 \times $$

$$ \times \int e^{-ar^2-br'^2-d\underline{r}\cdot\underline{r}'} \, y^*(\Omega) x^*(1) \left[S_{12}(r^2) + S_{12}(r'^2) - 2S_{12}(\underline{r},\underline{r}') \right] x(1) y(\Omega') \, r' \mathcal{F}(r') \, d\Omega \, d\Omega' \, dr' $$

The integrals with $S_{12}(r^2)$ and $S_{12}(r'^2)$ are treated by the techniques used previously for tensor operators and indirect terms.

For the term $S_{12}(\underline{r},\underline{r}')$ we have to evaluate the elements of the matrix $\langle \chi^{3/2} | S_{12}(\underline{r},\underline{r}') | \chi^{3/2} \rangle$ given below.

TABLE 2: THE SPIN PRODUCTS OF $S_{12}(\underline{r},\underline{r}')$.

	$\chi^{3/2}_{3/2}$	$\chi^{3/2}_{\frac{1}{2}}$	$\chi^{3/2}_{-\frac{1}{2}}$	$\chi^{3/2}_{-3/2}$
$\chi^{3/2}_{3/2}$	$3zz'-\underline{r}\cdot\underline{r}'$	$2\sqrt{3}(r_-z'+r'_-z)$	$4\sqrt{3}r_-r'_-$	0
$\chi^{3/2}_{\frac{1}{2}}$	$2\sqrt{3}(r_+z'+r'_+z)$	$-3zz'+\underline{r}\cdot\underline{r}'$	0	$4\sqrt{3}r_-r'_-$
$\chi^{3/2}_{-\frac{1}{2}}$	$4\sqrt{3}r_+r'_+$	0	$-3zz'+\underline{r}\cdot\underline{r}'$	$-2\sqrt{3}(r_-z'+r'_-z)$
$\chi^{3/2}_{-3/2}$	0	$4\sqrt{3}r_+r'_+$	$-2\sqrt{3}(r_+z'+r'_+z)$	$3zz'-\underline{r}\cdot\underline{r}'$

Each of the spin elements is equivalent to a product of two spherical harmonics, $Y^*_{1m_s}(\theta,\varphi)\,Y_{1m'_s}(\theta',\varphi')$ where m_s and m'_s take integer values between 1 and -1.

The integration over spherical harmonics takes the form

$$\int e^{-i\underline{r}\cdot\underline{r}'} Y^*_{lm}(\theta,\varphi)\, Y^*_{1m_s}(\theta,\varphi)\, Y_{l'm'}(\theta',\varphi')\, Y_{1m'_s}(\theta',\varphi')\, d\Omega\, d\Omega'$$

This is easily evaluated by expressing the products of two spherical harmonics of the same angle variables as a linear combination of spherical harmonics.

There are also terms of the type

$$\int e^{-\varepsilon \underline{r}\cdot\underline{r}'} Y^{*}_{lm}(\theta,\varphi)\ \underline{r}\cdot\underline{r}'\ Y_{l'm'}(\theta',\varphi')\ d\Omega\, d\Omega'$$

$$= -\frac{\partial}{\partial\varepsilon}\int e^{-\varepsilon \underline{r}\cdot\underline{r}'} Y^{*}_{lm}(\theta,\varphi)\, Y_{l'm'}(\theta',\varphi')\ d\Omega\, d\Omega'$$

$$= \delta_{ll'}\,\delta_{mm'}\,\frac{4\pi}{\varepsilon rr'}\, rr' p_{\varepsilon}\, \mathcal{J}_{l+\frac{1}{2}}(\varepsilon rr')$$

where $\mathcal{J}_{l+\frac{1}{2}}(\varepsilon rr')$ are the Spherical Bessel functions defined in Appendix 4,

and $$rr' p_{\varepsilon}\, \mathcal{J}_{l+\frac{1}{2}}(\varepsilon rr') = -\varepsilon \frac{\partial}{\partial\varepsilon}\left[\frac{1}{\varepsilon}\mathcal{J}_{l+\frac{1}{2}}(\varepsilon rr')\right].$$

By using the recurrence relations between $\mathcal{J}$'s (given in Appendix 4) one may write

$$rr' p_{\varepsilon}\, \mathcal{J}_{l+\frac{1}{2}}(\varepsilon rr') = rr'\, \mathcal{J}_{l+3/2}(\varepsilon rr') - \frac{l}{\varepsilon}\mathcal{J}_{l+\frac{1}{2}}(\varepsilon rr')$$

or $$= \frac{rr'}{2l+1}\left[(l+1)\,\mathcal{J}_{l+3/2}(\varepsilon rr') + l\,\mathcal{J}_{l-\frac{1}{2}}(\varepsilon rr')\right].$$

We define, in the indirect interaction calculation

$$\int d\Omega\, d\Omega'\ e^{-\partial \underline{r}\cdot\underline{r}'}\ y^{*}(\Omega)\, x^{*}(1)\, S_{12}(A^2)\, x(2)\, y(\Omega') = \langle S_{12}(A^2)\rangle$$

Finally the eigen values of the tensor operators in the indirect interaction are found to be

$$\langle S_{12}(\hat{r}^2)\rangle = \frac{4\pi}{\partial r r'} r^2 [B_{Jl}][\vartheta_{l+\frac{1}{2}}(\partial r r')] ,$$

$$\langle S_{12}(\hat{r}'^2)\rangle = \frac{4\pi}{\partial r r'} r'^2 [\vartheta_{l+\frac{1}{2}}(\partial r r')][B_{Jl}] ,$$

and $$\langle S_{12}(\hat{r},\hat{r}')\rangle = \frac{4\pi}{\partial r r'} rr' [P_{Jl}\vartheta_{l+\frac{1}{2}}(\partial r r')] \quad \ldots\ldots (5.2)$$

where $rr'[P_{Jl}\vartheta_{l+\frac{1}{2}}(\partial r r')]$

$$= \begin{pmatrix} -\frac{2J-3}{2J(2J-2)}[(J-2)\vartheta_J + J\vartheta_{J-2}] & 0 & \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J}\vartheta_J & 0 \\ 0 & \frac{2J+5}{2J(2J+2)}[(J-1)\vartheta_{J+1} + (J+1)\vartheta_{J-1}] & 0 & \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J+2}\vartheta_{J+1} \\ \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J}\vartheta_J & 0 & \frac{2J-3}{2J(2J+2}[J\vartheta_{J+2} + (J+2)\vartheta_J] & 0 \\ 0 & \frac{[3(2J-1)(2J+3)]^{\frac{1}{2}}}{2J+2}\vartheta_{J+1} & 0 & -\frac{2J+5}{(2J+2)(2J+4)}[(J+1)\vartheta_{J+3} + (J+3)\vartheta_{J+1}] \end{pmatrix}$$

Hence the tensor indirect interaction is given by

$$T_{S\text{-}S}(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\left(\frac{2}{3}\right)^2 \frac{4\pi}{\partial} AAU \times$$

$$\times \int_0^\infty dr' \, e^{-ar^2-br'^2} \left\{ r^2[B_{Jl}][\vartheta_{l+\frac{1}{2}}(\partial r r')] + r'^2[\vartheta_{l+\frac{1}{2}}(\partial r r')][B_{Jl}] - 2rr'[P_{Jl}\vartheta_{l+\frac{1}{2}}(\partial r r')] \right\} \mathcal{F}^e(r') .$$

CHAPTER VI

THE QUADRATIC SPIN-ORBIT TERMS

The direct ${}^{QS}D_{S\text{-}S}(r)$ and the indirect ${}^{QS}I_{S\text{-}S}(r)$ interactions due to the quadratic spin-orbit forces are as follows

$$ {}^{QS}D_{S\text{-}S}(r) = \frac{4}{3}\frac{M}{\hbar^2} r \int d\underline{R}\, d\Omega \left[\bar{\Phi}(23)\chi(1)y(\Omega)\right]^* \times $$

$$ \times \sum_\nu \left[\frac{1}{4}(2w-h)\,{}^\nu V_{QS}(12) L_{QS}(12)\bar{\Phi}(23)\chi(1) + \frac{1}{4}(2b-m)\,{}^\nu V_{QS}(12) L_{QS}(12)\bar{\Phi}(23)\chi(2)\right] y(\Omega)\frac{1}{r}F(r) $$

and $$ {}^{QS}I_{S\text{-}S}(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r \int d\underline{r}'\, d\Omega \left[\bar{\Phi}(23)\chi(1)y(\Omega)\right]^* \times $$

$$ \times \sum_\nu \left[\frac{1}{4}(w-2h)\,{}^\nu V_{QS}(12) L_{QS}(12)\bar{\Phi}(13)\chi(2) + \frac{1}{4}(b-2m)\,{}^\nu V_{QS}(12) L_{QS}(12)\bar{\Phi}(13)\chi(1)\right] y(\Omega')\frac{1}{r'}F(r'), $$

where $$ L_{QS}(12) = (\underline{\sigma}_1\cdot\underline{\sigma}_2)\underline{L}_{12}^2 - Q_{12} $$

and $$ Q_{12}(r_{12}) = \frac{1}{2}\left[(\underline{\sigma}_1\cdot\underline{L}_{12})(\underline{\sigma}_2\cdot\underline{L}_{12}) + (\underline{\sigma}_2\cdot\underline{L}_{12})(\underline{\sigma}_1\cdot\underline{L}_{12})\right] . $$

Due to the complexity of the operators, we try to simply the integrals by considering the spins first.

VI.1. THE SPIN SIMPLIFICATION

VI.1.1. THE DOUBLET CASE

As $$ \bar{\chi}(2,13) = \frac{1}{2}(1+\underline{\sigma}_1\cdot\underline{\sigma}_2)\,\bar{\chi}(1,23) $$

$$ = \bar{\chi}(1,23) + \frac{1}{2}(\underline{\sigma}_1\cdot\underline{\sigma}_2 - 1)\,\bar{\chi}(1,23) . $$

We can write the spin elements of the integrals for the direct interaction as

$$ \langle\bar{\chi}(1)|\frac{1}{4}(2w-h)\,V_{QS}L_{QS}(12)|\bar{\chi}(1)\rangle + \langle\bar{\chi}(1)|\frac{1}{4}(2b-m)V_{QS}L_{QS}(12)\frac{1}{2}(1+\underline{\sigma}_1\cdot\underline{\sigma}_2)|\bar{\chi}(1)\rangle $$

$$ = \frac{1}{4}(2w-h+2b-m)\,{}^\nu V_{QS}\langle\bar{\chi}(1)|V_{QS}(12)|\bar{\chi}(1)\rangle + \frac{1}{4}(2b-m)\,{}^\nu V_{QS}\langle\bar{\chi}(1)|\frac{1}{2}L_{QS}(12)(\underline{\sigma}_1\cdot\underline{\sigma}_2-1)|\bar{\chi}(1)\rangle . $$

and for the indirect interaction as

$$\tfrac{1}{4}(w-2h+b-2m)\,{}^{\nu}V_{QS}\,\langle\bar{\chi}(1)\,|\,\underline{L}_{QS}(12)\,|\,\bar{\chi}(1)\rangle + \tfrac{1}{4}(b-2m)\,{}^{\nu}V_{QS}\,\langle\bar{\chi}(1)\,|\,\tfrac{1}{2}\underline{L}_{QS}(\underline{\sigma}_1\underline{\sigma}_2-1)\,|\,\bar{\chi}(1)\rangle$$

Applying the relation between the symmetric and the anti-symmetric spin functions (defined in Appendix 4),

$$\chi^{\frac{1}{2}}_{\pm\frac{1}{2}}(1,\bar{23}) = \tfrac{1}{\sqrt{3}}(\underline{\sigma}_1\cdot\underline{\sigma}_2)\,\chi^{\frac{1}{2}}_{\pm\frac{1}{2}}(1,\tilde{23}) \ ,$$

the spin elements can be further reduced.

We work out each component of these elements, using the properties

$$\tilde{\chi}^{*}(1,23)\,\underline{\sigma}_i\,\tilde{\chi}(1,23) = 0 \qquad \text{for} \quad i=2 \text{ and } 3 \ ,$$

$$(\underline{\sigma}_2+\underline{\sigma}_3)\,\tilde{\chi}(1,23) = 0$$

and $$\tilde{\chi}^{*}\,\tilde{\chi} = [\delta] \ .$$

Thus we have $\langle\bar{\chi}(1)|\underline{\sigma}_1\cdot\underline{\sigma}_2\,\underline{L}^2|\bar{\chi}(1)\rangle = \tfrac{1}{3}\langle\tilde{\chi}\,|\,(\underline{\sigma}_1\cdot\underline{\sigma}_2)^3\,|\,\tilde{\chi}(1)\rangle\,\underline{L}^2$

$$= -2\underline{L}^2[\delta]$$

and $\langle\bar{\chi}(1)\,|\,\underline{\sigma}_1\cdot\underline{\sigma}_2(\underline{\sigma}_1\cdot\underline{\sigma}_2-1)\,\underline{L}^2\,|\,\bar{\chi}(1)\rangle = \tfrac{1}{3}\langle\tilde{\chi}\,|\,(\underline{\sigma}_1\cdot\underline{\sigma}_2)^2(\underline{\sigma}_1\cdot\underline{\sigma}_2-1)(\underline{\sigma}_1\cdot\underline{\sigma}_2)\,|\,\tilde{\chi}(1)\rangle\,\underline{L}^2$

$$= 9\,\underline{L}^2[\delta] \ .$$

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

and so $\langle\bar{\chi}(1)\,|\,Q_{12}\,|\,\bar{\chi}(1)\rangle = \langle\bar{\chi}(1)\,|\,\tfrac{1}{3}(\underline{\sigma}_1\cdot\underline{\sigma}_2)\,\underline{L}^2\,|\,\bar{\chi}(1)\rangle$

$$= \tfrac{1}{9}\langle\tilde{\chi}(1)\,|\,(\underline{\sigma}_1\cdot\underline{\sigma}_2)^3\underline{L}^2\,|\,\tilde{\chi}(1)\rangle$$

$$= -\tfrac{2}{3}\underline{L}^2[\delta] \ .$$

We also have

$\langle\bar{\chi}(1)\,|\,Q_{12}\,|\,\bar{\chi}(2)\rangle = \langle\bar{\chi}(1)\,|\,\tfrac{1}{3}(\underline{\sigma}_1\cdot\underline{\sigma}_2)\,\underline{L}^2\,|\,\bar{\chi}(2)\rangle$

$$= \tfrac{1}{18}\langle\tilde{\chi}(1)\,|\,(\underline{\sigma}_1\cdot\underline{\sigma}_2)^2(1+\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{\sigma}_1\cdot\underline{\sigma}_2)\,|\,\tilde{\chi}(1)\rangle\,\underline{L}^2$$

$$= \tfrac{5}{6}\underline{L}^2[\delta]$$

$$= \langle\bar{\chi}(1)\,|\,Q_{12}\,|\,\bar{\chi}(1)\rangle + \tfrac{3}{2}\underline{L}^2[\delta] \ .$$

So the potential and its operator are reduced to the following results.

In the direct interaction, it is given by

$$\frac{1}{4}(2w-h+2b-m)_\nu\, {}^{\nu}V_{QS}^{(12)}\left[-2\underline{L}_{12}^2+\frac{2}{3}\underline{L}_{12}^2\right][\delta]+\frac{1}{4}(2b-m)_\nu\, {}^{\nu}V_{QS}^{(12)}\left[\frac{9}{2}\underline{L}_{12}^2-\frac{3}{2}\underline{L}_{12}^2\right][\delta]$$

$$=\frac{1}{4}(2w-h+2b-m)_\nu\, {}^{\nu}V_{QS}^{(12)}\left[-\frac{4}{3}\underline{L}_{12}^2\right][\delta]+\frac{1}{4}(2b-m)_\nu\, {}^{\nu}V_{QS}^{(12)}\left[3\underline{L}_{12}^2\right][\delta].$$

The potential wells are given by

$$\sum_k {}^{QS}U_k^{(1)}\exp.\left[-{}^{QS}\mu_k^{(1)}r_{12}^2\right]=\sum_\nu \frac{1}{4}(2w-h+2b-m)_\nu\, {}^{\nu}V_{QS}^{(12)}$$

and

$$\sum_k {}^{QS}U_k^{(3)}\exp.\left[-{}^{QS}\mu_k^{(3)}r_{12}^2\right]=\sum_\nu \frac{1}{4}(2b-m)_\nu\, {}^{\nu}V_{QS}^{(12)}.$$

In the indirect interaction it is given by

$$\frac{1}{4}(w-2h+b-2m)_\nu\, {}^{\nu}V_{QS}^{(12)}\left[-\frac{4}{3}\underline{L}_{12}^2\right][\delta]+\frac{1}{4}(b-2m)_\nu\, {}^{\nu}V_{QS}^{(12)}\left[3\underline{L}_{12}^2\right][\delta].$$

The potential wells are $\sum_k {}^{QS}U_k^{(2)}\exp.\left[-{}^{QS}\mu_k^{(2)}r_{12}^2\right]=\sum_\nu \frac{1}{4}(w-2h+b-2m)_\nu\, {}^{\nu}V_{QS}^{(12)}$

and

$$\sum_k {}^{QS}U_k^{(4)}\exp.\left[-{}^{QS}\mu_k^{(4)}r_{12}^2\right]=\sum_\nu \frac{1}{4}(b-2m)_\nu\, {}^{\nu}V_{QS}^{(12)}.$$

VI.1.2. THE QUARTET CASE

As $\mathcal{X}_{m_S}^{3/2}(1,23)$ are symmetrical in 1,2 and 3,

the potential in the direct interaction is

$$\sum_k {}^{QS}U_k^{(1)}\exp.\left[-{}^{QS}\mu_k^{(1)}r_{12}^2\right]=\sum_\nu \frac{1}{4}(2w-h+2b-m)_\nu\, {}^{\nu}V_{QS}^{(12)}.$$

For the indirect interaction, it is

$$\sum_K {}^{QS}U_K^{(2)} \exp.\left[-{}^{QS}\mu_K^{(2)} r_{12}^2\right] = \sum_\nu \frac{1}{A}\left(w\text{-}h + b\text{-}m\right)_\nu {}^{\nu}V_{QS}(12)$$

The spin function in the quartet case offer no simplification of the operator L_{QS}, except that $L_{QS} = \underline{L}_{12}^2 - Q_{12}$.

The evaluation of the direct and the indirect interactions will be done in two section, a. for the operator $\underline{L}_{12}^2$ and b. for Q_{12}.

VI.2. THE DIRECT INTERACTION

We have for the doublet case of the spin-orbit direct interaction

$$\begin{aligned}
&{}^{QS}D_{S\text{-}S}(r) \\
&= \frac{4}{3}\frac{M}{\hbar^2} r\, AAU^{(1)} \int d\underline{R}\, d\Omega\; e^{-\alpha R^2 - \mu^{(1)}(\underline{r}-\frac{1}{2}\underline{R})^2} y^*(\Omega)\left[-\frac{4}{3}\underline{L}_{12}^2\right][\delta]\, y(\Omega)\, e^{-\alpha R^2} \frac{1}{r} F(r) \\
&+ \frac{4}{3}\frac{M}{\hbar^2} r\, AAU^{(3)} \int d\underline{R}\, d\Omega\; e^{-\alpha R^2 - \mu^{(3)}(\underline{r}-\frac{1}{2}\underline{R})^2} y^*(\Omega)\left[3\underline{L}_{12}^2\right][\delta]\, y(\Omega)\, e^{-\alpha R^2} \frac{1}{r} F(r).
\end{aligned} \qquad \ldots\ldots (6.1)$$

Similarly for the quartet case we obtain

$$\begin{aligned}
&{}^{QS}D_{S\text{-}S}(r) \\
&= \frac{4}{3}\frac{M}{\hbar^2} r\, AAU^{(1)} \int d\underline{R}\, d\Omega\; \exp.\left[-\alpha R^2 - \mu^{(1)}(\underline{r}-\tfrac{1}{2}\underline{R})^2\right] y^*(\Omega) x^*(1)\, \underline{L}_{12}^2\, x(1) y(\Omega)\, e^{-\alpha_j R^2} \frac{1}{r} F(r) \\
&- \frac{4}{3}\frac{M}{\hbar^2} r\, AAU^{(1)} \int d\underline{R}\, d\Omega\; \exp.\left[-\alpha R^2 - \mu^{(1)}(\underline{r}-\tfrac{1}{2}\underline{R})^2\right] y^*(\Omega) x^*(1)\, Q_{12}(r_{12})\, x(1) y(\Omega)\, e^{-\alpha_j R^2} \frac{1}{r} F(r).
\end{aligned} \qquad \ldots\ldots (6.2)$$

VI.2.1. THE MATRIX ELEMENTS OF $\underline{L}_{12}^2$

The operator $\underline{L}_{12}$ is given by

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

$\underline{L}_{12}^2$ has on its right the functions $Y_{lm}(\Omega)\, e^{-\alpha R^2}\, \frac{1}{r} f_l(r)$ and we aim to eliminate $e^{-\alpha R^2}$ first. To be brief the terms $Y_{lm}(\Omega)\, \frac{1}{r} f_l(r)$ are left out in what follows. We shall be integrating first and various formulae in Appendix 3 will be used.

The Space Integration

We have

$$i\,\underline{L}_{12}\, e^{-\alpha R^2} = \left[\tfrac{3}{2} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} + 2\alpha\, \underline{r} \wedge \underline{R} \right] e^{-\alpha R^2} .$$

Thus

$$(i)^2 \underline{L}_{12}^2\, e^{-\alpha R^2} = \left[\tfrac{3}{2} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} - (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{R}} \right] \cdot \left[\tfrac{3}{2} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} + 2\alpha\, \underline{r} \wedge \underline{R} \right] e^{-\alpha R^2}$$

$$= e^{-\alpha R^2} \left[\tfrac{3}{2} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} - (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{R}} \right] \cdot \left[\tfrac{3}{2} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} + 2\alpha\, \underline{r} \wedge \underline{R} \right]$$

$$+ 2\alpha\, (\underline{r} \wedge \underline{R}) \cdot \left[\tfrac{3}{2} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} + 2\alpha\, \underline{r} \wedge \underline{R} \right] e^{-\alpha R^2} .$$

We also write $(i)^2\, \underline{L}_{12}^2\, e^{-\alpha R^2}$

$$= \tfrac{9}{4} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} \cdot (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} \qquad \ldots\ldots A$$

$$+ 3\alpha (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} \cdot \underline{r} \wedge \underline{R} \qquad \ldots\ldots B$$

$$- \tfrac{3}{2} (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{R}} \cdot (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} \qquad \ldots\ldots C$$

$$- 2\alpha (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{R}} \cdot \underline{r} \wedge \underline{R} \qquad \ldots\ldots D$$

$$+ 3\alpha\, \underline{r} \wedge \underline{R} \cdot (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} \qquad \ldots\ldots E$$

$$+ 4\alpha^2 (\underline{r} \wedge \underline{R})^2 \qquad \ldots\ldots F$$

The term A gives

$$\tfrac{9}{4} \left[\left(\underline{r} \wedge \frac{\partial}{\partial \underline{r}} \right)^2 - \tfrac{1}{2} \left(\underline{r} \wedge \frac{\partial}{\partial \underline{r}} \right) \cdot \left(\underline{R} \wedge \frac{\partial}{\partial \underline{r}} \right) - \tfrac{1}{2} \left(\underline{R} \wedge \frac{\partial}{\partial \underline{r}} \right) \cdot \left(\underline{r} \wedge \frac{\partial}{\partial \underline{r}} \right) + \tfrac{1}{4} \left(\underline{R} \wedge \frac{\partial}{\partial \underline{r}} \right)^2 \right]$$

and after the $d\underline{R}$ integration we obtain A

$$= \left(\frac{\pi}{\lambda}\right)^{3/2} \frac{9}{4}\left[\left(\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right)^2 - \frac{\gamma}{2}\left(\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right)\cdot\left(\underline{r}_c\wedge\frac{\partial}{\partial \underline{r}}\right) - \frac{\gamma}{2}\left(\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right)^2 + \frac{\gamma^2}{4}\left(\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right)\cdot\left(\underline{r}_c\wedge\frac{\partial}{\partial \underline{r}}\right) + \frac{1}{4\lambda^2}\left(\frac{\partial}{\partial \underline{r}}\right)^2 \right]$$

where $\underline{r}_c$ is the vector $\underline{r}$ to be kept constant under the differentiation $\frac{\partial}{\partial \underline{r}}$, i.e. $\frac{\partial}{\partial \underline{r}}\,\underline{r}_c = \underline{r}\,\frac{\partial}{\partial \underline{r}}$.

Now $$\left(\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right)^2 = \left(\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right)\cdot\left(\underline{r}_c\wedge\frac{\partial}{\partial \underline{r}}\right) - 2\,\underline{r}\cdot\frac{\partial}{\partial \underline{r}} ,$$

and hence $$A = \left(\frac{\pi}{\lambda}\right)^{3/2} \frac{9}{4}\left[\left(1-\gamma+\frac{\gamma^2}{4}\right)\left(\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right)^2 - \gamma\,\underline{r}\cdot\frac{\partial}{\partial \underline{r}} + \frac{\gamma^2}{2}\,\underline{r}\cdot\frac{\partial}{\partial \underline{r}} + \frac{1}{4\lambda}\left(\frac{\partial}{\partial \underline{r}}\right)^2 \right]$$

$$= \left(\frac{\pi}{\lambda}\right)^{3/2} \left[-\frac{9}{4}\left(1-\frac{\gamma}{2}\right)^2 \underline{L}_r^2 - \frac{9}{4}\gamma\left(1-\frac{\gamma}{2}\right)\,\underline{r}\cdot\frac{\partial}{\partial \underline{r}} + \frac{9}{16\lambda}\left(\frac{\partial}{\partial \underline{r}}\right)^2 \right] .$$

Similarly we obtain for the term B

$$3\alpha\left[\left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\wedge\frac{\partial}{\partial \underline{r}}\cdot\underline{r}\wedge\underline{R} \right]$$

$$= 3\alpha\left[\left(r^2\underline{R}\cdot\frac{\partial}{\partial \underline{r}} - 2\underline{r}\cdot\underline{R} - \underline{r}\cdot\underline{R}\;\underline{r}\cdot\frac{\partial}{\partial \underline{r}} - \frac{1}{2}(\underline{r}\cdot\underline{R})(\underline{R}\cdot\frac{\partial}{\partial \underline{r}}) + R^2 + \frac{1}{2}R^2\left(\underline{r}\cdot\frac{\partial}{\partial \underline{r}}\right)\right)\right]$$

which after $d\underline{R}$ integration reduces to

$$B = \left(\frac{\pi}{\lambda}\right)^{3/2} \left[-6\alpha\gamma\left(1-\frac{\gamma}{2}\right)r^2 + \frac{9\alpha}{2\lambda} + \frac{3\alpha}{2\lambda}\left(\underline{r}\cdot\frac{\partial}{\partial \underline{r}}\right) \right]$$

We further get for term C

$$-\frac{3}{2}\left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\wedge\frac{\partial}{\partial \underline{R}}\cdot\left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\wedge\frac{\partial}{\partial \underline{r}} = -\frac{3}{2}\left[-\frac{1}{2}\left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\cdot\frac{\partial}{\partial \underline{r}} + \frac{3}{2}\left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\cdot\frac{\partial}{\partial \underline{r}} \right]$$

which after $d\underline{R}$ integration, reduces to

$$C = \left(\frac{\pi}{\lambda}\right)^{3/2} \left(-\frac{3}{2}\right)\left(1-\frac{\gamma}{2}\right)\,\underline{r}\cdot\frac{\partial}{\partial \underline{r}} .$$

Also term D gives

$$-2\alpha\left[\left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\wedge\frac{\partial}{\partial \underline{R}}\cdot\underline{r}\wedge\underline{R} \right] = -2\alpha\left[3\left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\cdot\underline{r} - \left(\underline{r}-\tfrac{1}{2}\underline{R}\right)\cdot\underline{r} \right] ,$$

and after $d\underline{R}$ integration,

$$D = \left(\frac{\pi}{\lambda}\right)^{3/2} (-4\alpha)(1-\tfrac{\gamma}{2})r^2 .$$

Then <u>term E</u> gives

$$3\alpha\ \underline{r}\wedge\underline{R}\cdot(\underline{r}-\tfrac{1}{2}\underline{R})\wedge\frac{\partial}{\partial\underline{r}} = 3\alpha\left[r^2(\underline{R}\cdot\frac{\partial}{\partial\underline{r}}) - \underline{r}\cdot\underline{R}\,(\underline{r}\cdot\frac{\partial}{\partial\underline{R}}) - \tfrac{1}{2}\,\underline{r}\cdot\underline{R}\,(\underline{R}\cdot\frac{\partial}{\partial\underline{r}}) + \tfrac{1}{2}R^2(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right]$$

and after $d\underline{R}$ integration ,

$$E = \left(\frac{\pi}{\lambda}\right)^{3/2} 3\alpha\left[-\frac{1}{4\lambda}\,\underline{r}\cdot\frac{\partial}{\partial\underline{r}} + \frac{3}{4\lambda}\,\underline{r}\cdot\frac{\partial}{\partial\underline{r}}\right]$$

$$= \left(\frac{\pi}{\lambda}\right)^{3/2} \frac{3\alpha}{2\lambda}\,\underline{r}\cdot\frac{\partial}{\partial\underline{r}} .$$

Finally <u>term F</u> gives $4\alpha^2(\underline{r}\wedge\underline{R})\cdot(\underline{r}\wedge\underline{R})$

which, after $d\underline{R}$ integration, reduces to

$$F = \left(\frac{\pi}{\lambda}\right)^{3/2} \frac{4\alpha^2}{\lambda}r^2 .$$

Hence collecting all terms, we obtain finally

$$\left(\frac{\pi}{\lambda}\right)^{3/2}\left[-\frac{9}{4}(1-\tfrac{\gamma}{2})^2\underline{L}_r^2 + \frac{9\alpha}{2\lambda} + 4\alpha\left\{\frac{\alpha}{\lambda} - (1-\tfrac{\gamma}{2})(1+3\tfrac{\gamma}{2})\right\}r^2 + \frac{3}{2}\left\{\frac{2\alpha}{\lambda} - (1-\tfrac{\gamma}{2})(1+3\tfrac{\gamma}{2})\right\}\underline{r}\cdot\frac{\partial}{\partial\underline{r}} + \frac{9}{16\lambda}\left(\frac{\partial}{\partial\underline{r}}\right)^2\right]$$

$$= \left(\frac{\pi}{\lambda}\right)^{3/2}\left[-\frac{9}{4}(1-\tfrac{\gamma}{2})^2\underline{L}_r^2 + \frac{9\alpha}{2\lambda} + 2\sigma r^2 - 2\nu(\underline{r}\cdot\frac{\partial}{\partial\underline{r}}) + \frac{9}{16\lambda}\left(\frac{\partial}{\partial\underline{r}}\right)^2\right] ,$$

where $\sigma = 2\alpha\left\{\frac{\alpha}{\lambda} - (1-\frac{\gamma}{2})(1+3\frac{\gamma}{2})\right\}$

and $\nu = -\frac{3}{4}\left\{\frac{2\alpha}{\lambda} - (1-\frac{\gamma}{2})(1+3\frac{\gamma}{2})\right\}$.

<u>The Spherical harmonic integrations</u>

The following results are standard :

$$\underline{L}_r^2\, Y_{lm}(\theta,\varphi)\,\frac{1}{r}f_l(r) = l(l+1)\,Y_{lm}(\theta,\varphi)\,\frac{1}{r}f_l(r) ,$$

$$(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\,Y_{lm}(\theta,\varphi)\,\frac{1}{r}f_l(r) = \left[f_l'(r) - \frac{1}{r}f_l(r)\right]Y_{lm}(\theta,\varphi) ,$$

and $$\left(\frac{\partial}{\partial r}\right)^2 Y_{lm}(\theta,\phi)\,\frac{1}{r}\,f_l(r) = \left[\frac{1}{r}f_l''(r) - \frac{l(l+1)}{r^3}f_l(r)\right] Y_{lm}(\theta,\phi)\ .$$

We are using the notation

$$\mathcal{F}'(r) = \frac{d}{dr}\mathcal{F}(r)$$

and

$$\mathcal{F}''(r) = \frac{d^2}{dr^2}\mathcal{F}(r)\ .$$

With the above results we get , for $\nu = 1, 3$,

$$D^{(\nu)}_{l_{12}}(r) = AAU^{(\nu)}\, r\int d\underline{R}\, d\Omega\; e^{-\alpha R^2-\mu^{(\nu)}(\underline{r}-\frac{1}{2}\underline{R})^2}\, Y^*(\Omega)\left[\underline{L}^2_{12}\right][\delta]\, Y(\Omega)\, e^{-\alpha R^2}\,\frac{1}{r}\mathcal{F}(r)$$

$$= \left(\frac{\pi}{\lambda}\right)^{3/2} AAU^{(\nu)}\, exp.\left[-(\mu-\lambda\delta^2)r^2\right]\ \times$$

$$\times\left[\left\{\frac{9}{4}\left(1-\frac{\delta}{2}\right)^2+\frac{9}{16\lambda r^2}\right\}\left[\Omega_{jl}\right]\mathcal{F}(r) - \left(\frac{9}{2}\frac{\alpha}{\lambda}+2\nu+2\delta r^2\right)\mathcal{F}(r) + 2\nu r\,\mathcal{F}'(r) - \frac{9}{16\lambda}\mathcal{F}''(r)\right]$$

..... (6.3)

where $\left[\Omega_{jl}\right]$ is a diagonal matrix with elements $l(l+1)$.

VI.2.2. THE MATRIX ELEMENTS OF $Q_{12}(r_{12})$.

We write $$Q_{12}(r_{12}) = \frac{1}{2}\left(q_{12}+q_{21}\right)$$

where $$q_{12}(r_{12}) = (\underline{\sigma}_1\cdot\underline{L}_{12})(\underline{\sigma}_2\cdot\underline{L}_{12})$$

and $$q_{21}(r_{12}) = (\underline{\sigma}_2\cdot\underline{L}_{12})(\underline{\sigma}_1\cdot\underline{L}_{12})\ .$$

The evaluation follows in exactly the same steps as used for $\underline{L}^2_{12}$ except that the terms are more complicated.

The space integration

We have $$(i)^2 q_{12}(r_{12})\, e^{-\alpha R^2}$$

$$= \left[\frac{\partial}{2}\underline{\sigma}_1\cdot(\underline{r}-\tfrac{1}{2}\underline{R})\wedge\frac{\partial}{\partial\underline{r}} - \underline{\sigma}_1\cdot(\underline{r}-\tfrac{1}{2}\underline{R})\wedge\frac{\partial}{\partial\underline{R}}\right]\left[\frac{\partial}{2}\underline{\sigma}_2\cdot(\underline{r}-\tfrac{1}{2}\underline{R})\wedge\frac{\partial}{\partial\underline{r}} - \underline{\sigma}_2\cdot(\underline{r}-\tfrac{1}{2}\underline{R})\wedge\frac{\partial}{\partial\underline{R}}\right] e^{-\alpha R^2}$$

The terms involving $\underline{\sigma}_2 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{R}}$ will be zero after the $\underline{R}$ differentiation and so will the term $(\underline{\sigma}_1 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{R}}) \cdot (\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}})$, being proportional to $\underline{R} \wedge \underline{R}$.

The term $(\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{R}})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}})$ which is proportional to $(\underline{\sigma}_1 \cdot \underline{r} \wedge \underline{R})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}})$ after differentiation, is zero on integration over $\underline{R}$ since it contains a factor $\underline{r} \wedge \underline{r}$.

We write

$$
\begin{aligned}
(i)^2 q_{12}(r_{12}) &= \frac{9}{4}(\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}}) && \ldots\ldots A \\
&- \frac{9}{8}(\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}})(\underline{\sigma}_2 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{r}}) && \ldots\ldots B \\
&- \frac{3}{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}}) && \ldots\ldots C \\
&- \frac{9}{8}(\underline{\sigma}_1 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{r}})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}}) && \ldots\ldots D \\
&+ \frac{9}{16}(\underline{\sigma}_1 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{r}})(\underline{\sigma}_2 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{r}}) && \ldots\ldots E \\
&+ \frac{3}{4}(\underline{\sigma}_1 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{r}})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{R}}) && \ldots\ldots F \\
&+ \frac{3}{4}(\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{R}})(\underline{\sigma}_2 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{r}}) && \ldots\ldots G \\
&+ (\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{R}})(\underline{\sigma}_2 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{R}}) && \ldots\ldots H \\
&- \frac{3}{8}(\underline{\sigma}_1 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{R}})(\underline{\sigma}_2 \cdot \underline{R} \wedge \frac{\partial}{\partial \underline{r}}) && \ldots\ldots I \\
&- \frac{1}{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}}) && \ldots\ldots J
\end{aligned}
$$

The <u>term A</u>, after $d\underline{R}$ integration, results in

$$A = \left(\frac{\pi}{\lambda}\right)^{3/2} (i)^2 (\underline{\sigma}_1 \cdot \underline{L}_1)(\underline{\sigma}_2 \cdot \underline{L}_1) .$$

Similarly the <u>term B</u>, after $d\underline{R}$ integration, reads

$$B = \left(\frac{\pi}{\lambda}\right)^{3/2} \left(-\frac{9}{8}\gamma\right)\left(\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}}\right)\left(\underline{\sigma}_2 \cdot \underline{r}_C \wedge \frac{\partial}{\partial \underline{r}}\right) .$$

The operator

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

and hence we get

$$B = \left(\frac{\pi}{\lambda}\right)^{3/2}\left(-\frac{9}{8}\gamma\right)\left[(i)^2(\underline{\sigma}_1\cdot\underline{L}_1)(\underline{\sigma}_2\cdot\underline{L}_1) - \left\{(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right\}\right] .$$

The <u>term C</u> leads to

$$3\alpha\,(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_2\cdot\underline{r}\wedge\underline{R})$$

which, after $d\underline{R}$ integration, gives

$$C = \left(\frac{\pi}{\lambda}\right)^{3/2} 3\alpha\gamma\left[(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)r^2\right] .$$

The <u>term D</u> gives after integration, $\left(\frac{\pi}{\lambda}\right)^{3/2}\left(-\frac{9}{8}\gamma\right)(i)^2(\underline{\sigma}_1\cdot\underline{L}_1)(\underline{\sigma}_2\cdot\underline{L}_1)$.

Similarly the <u>term E</u>, after integration, results in

$$E = \left(\frac{\pi}{\lambda}\right)^{3/2}\frac{9}{16}\left[\gamma^2(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_2\cdot\underline{r}_c\wedge\frac{\partial}{\partial\underline{r}}) + \frac{1}{2\lambda}\left\{(\underline{\sigma}_1\cdot\underline{\sigma}_2)\left(\frac{\partial}{\partial\underline{r}}\right)^2 - (\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}})\right\}\right]$$

$$= \left(\frac{\pi}{\lambda}\right)^{3/2}\frac{9}{16}\left[\gamma^2 i^2(\underline{\sigma}_1\cdot\underline{L}_1)(\underline{\sigma}_2\cdot\underline{L}_1) - \gamma^2\left\{(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right\} + \frac{1}{2\lambda}\left\{(\underline{\sigma}_1\cdot\underline{\sigma}_2)\left(\frac{\partial}{\partial\underline{r}}\right)^2 - (\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}})\right\}\right] .$$

Also the <u>term F</u> leads to $-\frac{3}{2}\alpha\left[(\underline{\sigma}_1\cdot\underline{R}\wedge\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_2\cdot\underline{r}\wedge\underline{R})\right]$

$$= -\frac{3}{2}\alpha\left[(\underline{\sigma}_1\cdot\underline{R}\wedge\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_2\cdot\underline{r}_c\wedge\underline{R}) + \left\{(\underline{\sigma}_1\cdot\underline{R})(\underline{\sigma}_2\cdot\underline{R}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)R^2\right\}\right] ,$$

which, after $d\underline{R}$ integration, produces

$$F = \left(\frac{\pi}{\lambda}\right)^{3/2}\left(-\frac{3}{2}\alpha\right)\left[\frac{1}{2\lambda}\left\{(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right\} + \gamma^2\left\{(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)r^2\right\} - \frac{1}{\lambda}\underline{\sigma}_1\cdot\underline{\sigma}_2\right] .$$

Further the <u>term G</u> gives $\frac{3}{4}\left[-2\alpha(\underline{\sigma}_1\cdot\underline{r}\wedge\underline{R})(\underline{\sigma}_2\cdot\underline{R}\wedge\frac{\partial}{\partial\underline{r}}) + \left\{(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right\}\right]$

and after $d\underline{R}$ integration we obtain

$$G = \left(\frac{\pi}{\lambda}\right)^{3/2}\frac{3}{4}\left(1-\frac{\alpha}{\lambda}\right)\left[(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right] .$$

Term H on differentiation reads

$$4\alpha^2(\underline{\sigma}_1\cdot\underline{r}\wedge\underline{R})(\underline{\sigma}_2\cdot\underline{r}\wedge\underline{R}) - 2\alpha\left\{(\underline{\sigma}_1\cdot\underline{\sigma}_2)r^2 - (\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r})\right\}$$

and after $d\underline{R}$ integration we get

$$H = \left(\frac{\pi}{\lambda}\right)^{3/2}\left(\frac{4\alpha^2}{2\lambda} - 2\alpha\right)\left\{(\underline{\sigma}_1\cdot\underline{\sigma}_2)r^2 - (\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r})\right\} .$$

Term I after differentiation reads

$$-\frac{3}{8}\left[(\underline{\sigma}_2\cdot\underline{R})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{R}\cdot\frac{\partial}{\partial\underline{r}})\right]$$

which after integration, results in

$$I = \left(\frac{\pi}{\lambda}\right)^{3/2}\left(-\frac{3}{8}\gamma\right)\left[(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right] .$$

Finally term J , by differentiations, is

$$\alpha\left[(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\underline{R}) - (\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{R})\right]$$

leading to

$$J = \left(\frac{\pi}{\lambda}\right)^{3/2}\alpha\gamma\left[(\underline{\sigma}_1\cdot\underline{\sigma}_2)r^2 - (\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r})\right] .$$

Hence the full operator $(i)^2 Q_{12}(\underline{r}_{12})$ after integration w.r.t. $\underline{R}$, gives

$$\left(\frac{\pi}{\lambda}\right)^{3/2}\left[-\frac{9}{4}\left(1-\frac{\gamma}{2}\right)^2 Q_{12}(r^2) - \frac{9}{32\lambda}\left\{\frac{1}{2}(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}}) + \frac{1}{2}(\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)\left(\frac{\partial}{\partial\underline{r}}\right)^2\right\}\right.$$

$$+\nu\left\{\frac{1}{2}(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}}) + \frac{1}{2}(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial\underline{r}}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right\}$$

$$\left.-\sigma\left\{(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)r^2\right\} + \frac{3\alpha}{2\lambda}\underline{\sigma}_1\cdot\underline{\sigma}_2\right] .$$

With the notation

$$T_{12}(\underline{A},\underline{B}) = \frac{1}{2}(\underline{\sigma}_1\cdot\underline{A})(\underline{\sigma}_2\cdot\underline{B}) + \frac{1}{2}(\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_1\cdot\underline{B}) - (\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{A}\cdot\underline{B}) ,$$

this becomes finally

$$\left(\frac{\pi}{\lambda}\right)^{3/2}\left[-\frac{9}{4}\left(1-\frac{\gamma}{2}\right)^2 Q_{12}(r^2) - \frac{9}{32\lambda}T_{12}\left(\frac{\partial}{\partial\underline{r}},\frac{\partial}{\partial\underline{r}}\right) + \nu T_{12}\left(\underline{r},\frac{\partial}{\partial\underline{r}}\right) - \sigma T_{12}(\underline{r}^2) + \frac{3\alpha}{2\lambda}\underline{\sigma}_1\cdot\underline{\sigma}_2\right] .$$

The spherical harmonic integration

It can easily be verified that

$$T_{12}(I,\frac{\partial}{\partial I})\,Y_{lm}(\theta,\varphi)\,\frac{1}{r}f(r) = \frac{1}{r}f\,T_{12}(I,\frac{\partial}{\partial I})\,Y + \left[\frac{1}{r^2}f'(r)-\frac{1}{r^3}f\right]T_{12}(r^2)\,Y$$

and

$$T_{12}(\frac{\partial}{\partial I},\frac{\partial}{\partial I})\,Y_{lm}(\theta,\varphi)\,\frac{1}{r}f(r) = \frac{1}{r}f\,T_{12}(\frac{\partial}{\partial I},\frac{\partial}{\partial I})\,Y + \left[\frac{2}{r^2}f'-\frac{2}{r^3}f\right]T_{12}(I,\frac{\partial}{\partial I})\,Y$$
$$+\left[\frac{1}{r^3}f''(r)-\frac{3}{r^4}f'+\frac{3}{r^5}f\right]T_{12}(r^2)\,Y\,.$$

Using the results we get

$$\gamma\int d\underline{R}\,d\Omega\; e^{-\alpha R^2-\mu(r-\frac{1}{2}R)^2}\,y^*(\Omega)x^*(1)\,Q_{12}(r_{12}^2)\,x(1)y(\Omega)\,e^{-\alpha_j R^2}\,\frac{1}{\gamma}\mathcal{F}(r)$$
$$=\left(\frac{\pi}{\lambda}\right)^{3/2} e^{-(\mu-\lambda\delta^2)r^2}\int d\underline{R}\; y^*(\Omega)x^*(1)[\quad]x(1)y(\Omega)[\quad]$$

where the terms in the brackets are

$$\left[\frac{9}{4}(1-\frac{\delta}{2})^2 Q_{12}(r^2)\right]\ldots\left[\mathcal{F}(r)\right] + \frac{9}{32\lambda}\left[T_{12}(\frac{\partial}{\partial I},\frac{\partial}{\partial I})\right]\ldots\left[\mathcal{F}(r)\right]$$
$$+\left[T_{12}(I,\frac{\partial}{\partial I})\right]\ldots\left[\frac{9}{16\lambda}\frac{1}{r}\mathcal{F}'(r)-\left(\nu+\frac{9}{16\lambda r^2}\right)\mathcal{F}(r)\right]-\left[\frac{3}{2}\frac{\alpha}{\lambda}\right]\ldots\left[\mathcal{F}(r)\right]$$
$$+\left[T_{12}(r^2)\right]\ldots\left[\frac{9}{32\lambda r^2}\mathcal{F}''(r)-\left(\nu+\frac{27}{32\lambda r^2}\right)\frac{1}{r}\mathcal{F}'(r)+\left(\sigma+\frac{\nu}{r^2}+\frac{27}{32\lambda r^4}\right)\mathcal{F}(r)\right].$$

The $\frac{\partial}{\partial I}$ operates here on the spherical harmonics only. The symmetric property of the spin functions is used so that $(\underline{\sigma}_1\cdot\underline{\sigma}_2)=1$.

We now define the following matrix elements w.r.t. the eigen functions xy:

$$\left\langle \tfrac{1}{2}(\underline{\sigma}_1\cdot I)(\underline{\sigma}_2\cdot\frac{\partial}{\partial I}) + \tfrac{1}{2}(\underline{\sigma}_2\cdot I)(\underline{\sigma}_1\cdot\frac{\partial}{\partial I})\right\rangle = [D_{jl}]\,,$$

$$\left\langle \tfrac{1}{2}(\underline{\sigma}_1\cdot\frac{\partial}{\partial I})(\underline{\sigma}_2\cdot\frac{\partial}{\partial I}) + \tfrac{1}{2}(\underline{\sigma}_2\cdot\frac{\partial}{\partial I})(\underline{\sigma}_1\cdot\frac{\partial}{\partial I})\right\rangle = \frac{1}{r^2}[E_{jl}]\,,$$

$$\left\langle \tfrac{1}{2}(\underline{\sigma}_1\cdot L)(\underline{\sigma}_2\cdot L) + \tfrac{1}{2}(\underline{\sigma}_2\cdot L)(\underline{\sigma}_1\cdot L)\right\rangle = [F_{jl}]\,.$$

These elements are evaluated in the usual way. We obtain the spin products of the operators in the form given in Table 3. Then after the components of $\underline{r}$, $\frac{\partial}{\partial \underline{r}}$ and $\underline{L}_r$ have been transformed into equivalent spherical harmonics, the integrations are performed.

Table 3: THE SPIN PRODUCTS OF $\frac{1}{2}(\underline{\sigma}_1\cdot\underline{A})(\underline{\sigma}_2\cdot\underline{B})+\frac{1}{2}(\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_1\cdot\underline{B})$.

	$\chi^{3/2}_{3/2}$	$\chi^{3/2}_{1/2}$	$\chi^{3/2}_{-1/2}$	$\chi^{3/2}_{-3/2}$
$\chi^{3/2}_{3/2}$	$A^z B^z$	$\frac{2}{\sqrt{3}}(A^z B^- + A^- B^z)$	$\frac{4}{\sqrt{3}} A^- B^-$	0
$\chi^{3/2}_{1/2}$	$\frac{2}{\sqrt{3}}(A^z B^+ + A^+ B^z)$	$\frac{2}{3}\underline{A}\cdot\underline{B} - A^z B^z$	0	$\frac{4}{\sqrt{3}} A^- B^-$
$\chi^{3/2}_{-1/2}$	$\frac{4}{\sqrt{3}} A^+ B^+$	0	$\frac{2}{3}\underline{A}\cdot\underline{B} - A^z B^z$	$-\frac{2}{\sqrt{3}}(A^z B^- + A^- B^z)$
$\chi^{3/2}_{-3/2}$	0	$\frac{4}{\sqrt{3}} A^+ B^+$	$-\frac{2}{\sqrt{3}}(A^z B^+ + A^+ B^z)$	$A^z B^z$

where

$$A^{\pm} = \tfrac{1}{2}(A^x \pm iA^y)$$

and

$$B^{\pm} = \tfrac{1}{2}(B^x \pm iB^y) .$$

The full arrays of these elements are found to be

$$[P_{Jl}] = \begin{pmatrix} -\frac{2J-3}{4J} & & & \\ & \frac{2J+5}{4(J+1)} & & \\ & & \frac{2J-3}{4J} & \\ & & & -\frac{2J+5}{4(J+1)} \end{pmatrix} ,$$

$$[E_{JI}] = \begin{pmatrix} -\frac{(2J+1)(2J-3)}{8J} & 0 & \frac{(2J+1)(2J+3)}{8J}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} & 0 \\ 0 & \frac{-16J^3-28J^2+16J+37}{24(J+1)} & 0 & \frac{(2J+3)(2J+5)}{8(J+1)}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} \\ \frac{(2J-1)(2J-3)}{8J}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} & 0 & \frac{-16J^3-20J^2+24J-9}{24J} & 0 \\ 0 & \frac{(2J-1)(2J+1)}{8(J+1)}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} & 0 & \frac{(2J+1)(2J+5)}{8(J+1)} \end{pmatrix}$$

$$[F_{JI}] = \begin{pmatrix} (J-\frac{3}{2})^2 & & & \\ & \frac{-4J^2-12J+19}{12} & & \\ & & \frac{-4J^2+4J+27}{12} & \\ & & & (J+\frac{5}{2})^2 \end{pmatrix} \quad \ldots\ldots (6.3.a)$$

with the usual exception for $S = 3/2$, $J = \frac{1}{2}$.

With these we are able to write down concisely the direct term namely

$$D^{(\nu)}_{Q_{12}}(\tau) = AAU^{(\nu)}\, \tau \int d\underline{R}\, d\Omega\; e^{-\alpha R^2 - \mu^{(\nu)}(\underline{r}-\frac{1}{2}\underline{R})^2} y^*(\Omega)\chi^*(1)\, Q_{12}(\tau_{12}^2)\, \chi(1) y(\Omega)\, \frac{1}{\tau} F(\tau)$$

$$= \left(\frac{\pi}{\lambda}\right)^{3/2} AAU\; e^{-(\mu-\lambda\delta^2)\tau^2} \times$$

$$\times \Big[\Big\{ \frac{9}{4}(1-\tfrac{\delta}{2})^2 [F_{JI}] + \frac{9}{32\lambda\tau^2}[E_{JI}] - (\nu + \frac{9}{16\lambda\tau^2})[D_{JI}] + \frac{9}{32\lambda\tau^2}[\Omega_{JI}]$$

$$+ (\tfrac{8}{3}\sigma\tau^2 + \tfrac{1}{5}\nu + \frac{9}{32\lambda\tau^2})[B_{JI}] - (\tfrac{2}{3}\sigma\tau^2 + \tfrac{2}{5}\nu + \tfrac{3}{2}\tfrac{\alpha}{\lambda} + \frac{9}{16\lambda\tau^2})[\delta] \Big\} F(\tau)$$

$$+ \Big\{ \frac{9}{16\lambda}[D_{JI}] - (\tfrac{1}{3}\nu\tau^2 + \frac{9}{32\lambda})[B_{JI}] + (\tfrac{2}{3}\nu\tau^2 + \frac{9}{16\lambda})[\delta] \Big\} \frac{1}{\tau} F'(\tau)$$

$$+ \Big\{ \frac{3}{32\lambda}[B_{JI}] - \frac{3}{16\lambda}[\delta] \Big\} F''(\tau) \Big] . \qquad \ldots\ldots (6.4)$$

VI.2.3 RESULTS AND REMARK

From equation (6.1) the direct interaction due to the quadratic spin-orbit force for the doublet case is given by

$$ {}^{Q}D_{S\cdot S}(r) = \frac{4}{3}\frac{M}{\hbar^2}\left[-\frac{4}{3}D^{(1)}_{L_{12}}(r) + 3D^{(3)}_{L_{12}}(r)\right] . $$

where $D^{(\nu)}_{L_{12}}(r)$ are given by (6.3) .

From equation (6.2) the quartet term has the form

$$ {}^{Q}D_{S\cdot S}(r) = \frac{4}{3}\frac{M}{\hbar^2}\left[D^{(1)}_{L_{12}}(r) - D^{(1)}_{Q_{12}}(r)\right] $$

where $D^{(1)}_{Q_{12}}(r)$ is given by (6.4).

We note that the quadratic spin-orbit interaction introduces three new terms, namely those containing $1/r^2$, and first and second derivatives of the unknown radial function $f(r)$. These integro-differential equations therefore differ from those of previous calculations which did not include this interaction. Because of the presence of $f'(r)$ a modified numerical procedure is needed to solve the equations which will be discussed in Chapter XV.

Although the operators $\frac{1}{2}\left[(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\frac{\partial}{\partial r}) + (\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial r})\right]$ and $\frac{1}{2}\left[(\underline{\sigma}_1\cdot\frac{\partial}{\partial r})(\underline{\sigma}_2\cdot\frac{\partial}{\partial r}) + (\underline{\sigma}_2\cdot\frac{\partial}{\partial r})(\underline{\sigma}_1\cdot\frac{\partial}{\partial r})\right]$ are symmetrical with regards to the spins, their matrix elements $[D_{Jl}]$ and $\frac{1}{r^2}[E_{Jl}]$ are not symmetrical with regards to the angular momentum l . The symmetrisation of the operators is given in Chapter XII.

VI.3 THE INDIRECT INTERACTION

The doublet indirect term $^{QS}I_{SS}(r)$ is given by

$$\underset{SS}{^{QS}I}(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r AAU^{(2)} \int d\underline{r}' d\Omega \, e^{-\alpha_i r_{23}^2 - \mu^{(2)} r_{12}^2} y^*(\Omega) \left[-\frac{4}{3} \underline{L}_{12}^2\right] y(\Omega') \, e^{-\alpha_j r_{13}^2} \underset{r'}{\perp} F^e(r')$$

$$-\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r AAU^{(4)} \int d\underline{r}' d\Omega \, e^{-\alpha_i r_{23}^2 - \mu^{(4)} r_{12}^2} y^*(\Omega) \left[3 \underline{L}_{12}^2\right] y(\Omega') \, e^{-\alpha_j r_{13}^2} \underset{r'}{\perp} F^e(r') \quad \ldots\ldots (6.5)$$

and the quartet term by $^{QS}\underset{SS}{I}(r)$

$$= -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r AAU^{(2)} \int d\underline{r}' d\Omega \, e^{-\alpha_i r_{23}^2 - \mu^{(2)} r_{12}^2} y^*(\Omega) x^*(1) \underline{L}_{12}^2 x(2) y(\Omega') \, e^{-\alpha_j r_{13}^2} \underset{r'}{\perp} F^e(r')$$

$$+\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r AAU^{(2)} \int d\underline{r}' d\Omega \, e^{-\alpha_i r_{23}^2 - \mu^{(2)} r_{12}^2} y^*(\Omega) x^*(1) \left[Q_{12}(r_{12}^2)\right] x(2) y(\Omega') \, e^{-\alpha_j r_{13}^2} \underset{r'}{\perp} F^e(r') \quad \ldots\ldots (6.6)$$

VI.3.1 THE MATRIX ELEMENTS OF $\underline{L}_{12}^2$

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

Considering space co-ordinates only, we have on the right of the operator $\underline{L}_{12}$ the function $e^{-\alpha_j r_{13}^2} y(\Omega') \underset{r'}{\perp} F^e(r')$ and on its left $e^{-\alpha_i r_{23}^2 - \mu_k r_{12}^2} y^*(\Omega)$.

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

1. Differentiation w.r.t. $\underline{r}$ on $e^{-\alpha_j r_{13}^2}$.

We have $$\underline{r}_{13} = \frac{2}{3}(2\underline{r} + \underline{r}'),$$

so it follows that

$$\frac{\partial}{\partial \underline{r}} e^{-\alpha_j r_{13}^2} = -\frac{16}{9}\alpha_j(2\underline{r}+\underline{r}')\, e^{-\alpha_j r_{13}^2}$$

and

$$(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial \underline{r}} e^{-\alpha_j r_{13}^2} = \frac{16}{3}\alpha_j(\underline{r}'\wedge\underline{r})\, e^{-\alpha_j r_{13}^2}.$$

2. Integration by parts wrt. $\underline{r}'$ (in order to transfer the unknown $f(r')$ to the left of the operator) followed by differentiation w.r.t. $\underline{r}'$.

Since $$\underline{r}_{23} = \frac{2}{3}(\underline{r}+2\underline{r}')$$

and $$\underline{r}_{12} = \frac{2}{3}(\underline{r}-\underline{r}')$$

we have the result

$$\frac{\partial}{\partial \underline{r}'} e^{-\alpha_i r_{23}^2-\mu r_{12}^2} = \left[-\frac{16}{9}\alpha_i(\underline{r}+2\underline{r}')+\frac{8}{9}\mu(\underline{r}-\underline{r}')\right] e^{-\alpha r_{23}^2-\mu r_{12}^2}$$

$$= (\eta\underline{r}+\xi\underline{r}')\, e^{-\alpha r_{23}^2-\mu r_{12}^2}$$

where

$$\xi = -\frac{8}{9}(4\alpha_i+\mu_k)$$

and

$$\eta = -\frac{8}{9}(2\alpha_i-\mu_k).$$

We thus obtain two operator identities

$$\underline{r}\wedge\frac{\partial}{\partial \underline{r}'} e^{-\alpha r_{23}^2-\mu r_{12}^2} = \xi\,\underline{r}\wedge\underline{r}'\, e^{-\alpha r_{23}^2-\mu r_{12}^2}$$

and

$$\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'} e^{-\alpha r_{23}^2-\mu r_{12}^2} = \eta\,\underline{r}'\wedge\underline{r}\, e^{-\alpha r_{23}^2-\mu r_{12}^2}.$$

The forgoing results for step 1 and 2 will now be used (often implicitely) in evaluating the matrix elements of operators $\underline{L}_{12}^2$ and Q_{12}.

Only relevant functions involved in the calculation will be written down.

We have the identity

$$(i)^2 \, \underline{L}_{12}^2 \, e^{-\alpha_j I_{13}^2} = \left[(\underline{I}-\underline{I}') \wedge \frac{\partial}{\partial \underline{I}} - (\underline{I}-\underline{I}') \wedge \frac{\partial}{\partial \underline{I}'} \right] \cdot \left[(\underline{I}-\underline{I}') \wedge \frac{\partial}{\partial \underline{I}} - (\underline{I}-\underline{I}') \wedge \frac{\partial}{\partial \underline{I}'} \right] e^{-\alpha_j r_{23}^2}.$$

Consider the expressions on the right hand side.

The term $\left[(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{I}} \right] \cdot \left[(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{I}} \right] \exp.\left[-\alpha_j r_{13}^2\right]$ becomes

$$\frac{16}{3}\alpha \left[\frac{16}{3}\alpha \left\{ r^2 r'^2 - (\underline{r}\cdot\underline{r}')^2 \right\} + 2\,(\underline{r}\cdot\underline{r}' - r'^2) \right] \exp.\left[-\alpha_j r_{13}^2\right].$$

The term $\left[(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{I}} \right] \cdot \left[-(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{I}'} \right] \exp.\left[-\alpha_j r_{13}^2\right]$ becomes

$$\left[\frac{16}{9}\alpha\,(\underline{r}-\underline{r}')^2 \frac{\partial}{\partial \underline{r}'} \cdot (2\underline{I}+\underline{r}') - \frac{16}{9}\alpha \left\{ (\underline{r}-\underline{r}') \cdot \frac{\partial}{\partial \underline{r}'} \right\} (\underline{r}-\underline{r}_c') \cdot (2\underline{I}+\underline{r}') + 2\,(\underline{r}-\underline{r}') \cdot \frac{\partial}{\partial \underline{I}'} \right] \exp.\left[-\alpha_j r_{13}^2\right].$$

On using step 2 we get the result for this term

$$\left[-\frac{16}{9}\alpha_j \left\{ (2\underline{I}+\underline{r}') \cdot \frac{\partial}{\partial \underline{I}'} \right\} (\underline{I}-\underline{I}')^2 + \frac{16}{9}\alpha_j \left\{ \frac{\partial}{\partial \underline{I}'} \cdot (\underline{I}-\underline{I}') \right\} (\underline{I}-\underline{I}') \cdot (2\underline{I}+\underline{r}_c') - 2\frac{\partial}{\partial \underline{I}'} \cdot (\underline{I}-\underline{I}') \right] \exp.\left[-\alpha_i r_{23}^2 - \mu r_{12}^2\right]$$

$$= \left[-\frac{32}{9}\alpha_j (2r^2 - \underline{I}\cdot\underline{r}' - r'^2) - 2\left\{ \eta r^2 + (\xi-\eta)\,\underline{I}\cdot\underline{r}' - \xi r'^2 \right\} + 6 + \frac{16}{3}\alpha_j (\xi+\eta) \left\{ (\underline{I}\cdot\underline{r}')^2 - r^2 r'^2 \right\} \right] \exp.\left[-\alpha_i r_{23}^2 - \mu r_{12}^2\right].$$

The term $\left[-(\underline{I}-\underline{I}') \wedge \frac{\partial}{\partial \underline{I}'} \right] \cdot \left[(\underline{I}-\underline{I}') \wedge \frac{\partial}{\partial \underline{I}} \right] \exp.\left[-\alpha_j r_{13}^2\right]$ gives

$$\frac{16}{3}\alpha_j (\xi+\eta) \left\{ (\underline{I}\cdot\underline{r}')^2 - r^2 r'^2 \right\} \exp.\left[-\alpha_i r_{23}^2 - \mu r_{12}^2\right].$$

Finally the term $\left[-(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}'} \right] \cdot \left[-(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}'} \right] \exp.\left[-\alpha_j r_{13}^2\right]$ becomes

$$\left[(\underline{r}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}'} \right] \cdot \left[(\underline{I}-\underline{r}') \wedge \frac{\partial}{\partial \underline{r}'} \right] \exp.\left[-\alpha_i r_{23}^2 - \mu r_{12}^2\right]$$

$$= \left[(\xi+\eta)^2 \left\{ r^2 r'^2 - (\underline{r}\cdot\underline{r}')^2 \right\} + 2(\xi+\eta)(r^2 - \underline{I}\cdot\underline{r}') \right] \exp.\left[-\alpha_i r_{23}^2 - \mu r_{12}^2\right].$$

Combining these four terms we get

$$9w^2\left\{r^2r'^2-(\underline{r}\cdot\underline{r}')^2\right\}-2\zeta(r^2-2\underline{r}\cdot\underline{r}'+r'^2)+6$$

where $$w_{ij} = \frac{16}{9}(\alpha_i+\alpha_j)$$

and $$\zeta_{ijk} = \frac{8}{9}(4\alpha_i+4\alpha_j+\mu_k)\ .$$

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

We find in general

$$\int d\Omega\, d\Omega'\ Y^*_{lm}(\theta,\varphi)\ (\underline{r}\cdot\underline{r}')^n\ Y_{l'm'}(\theta',\varphi')\ e^{-\varepsilon\underline{r}\cdot\underline{r}'} = \frac{4\pi}{\varepsilon rr'}\, r^n r'^n\, \mathfrak{p}^{(n)}_{\varepsilon}\, \mathfrak{I}_{l+\frac{1}{2}}(\varepsilon rr')\ \delta_{ll'}\,\delta_{mm'}$$

where $$r^n r'^n\, \mathfrak{p}^{(n)}_{\varepsilon}\, \mathfrak{I}_{l+\frac{1}{2}}(\varepsilon rr') \equiv (-1)^n \varepsilon\, \frac{d^n}{d\varepsilon^n}\left[\frac{1}{\varepsilon}\, \mathfrak{I}_{l+\frac{1}{2}}(\varepsilon rr')\right] .$$

Hence the indirect integral of the operator $\underline{L}^2_{12}$ becomes finally

$$I^{(\nu)}_{L_{12}}(r) = r\int d\underline{r}'\, d\Omega\ e^{-\alpha r_{23}^2-\mu^{(\nu)}r_{12}^2}\, AAU^{(\nu)}\, y^*(\Omega)\chi(1)\ \underline{L}^2_{12}\,\chi(2)y(\Omega')\, e^{-\alpha r_{13}^2}\, \frac{1}{r'}\, \mathfrak{F}(r')$$

$$= \frac{4\pi}{\delta} AAU^{(\nu)}\int dr'\, e^{-ar^2-br'^2}\left[9w^2r^2r'^2-2\zeta(r^2+r'^2)+6+4\zeta rr'\,\mathfrak{p}^{(1)}_{\delta}-9w^2r^2r'^2\,\mathfrak{p}^{(2)}_{\delta}\right]\left[\mathfrak{I}_{l+\frac{1}{2}}(\delta rr')\right]\mathfrak{F}(r')$$

where $\chi^*(1)\chi(2) = [\delta]$ . ..... (6.7)

VI.3.2. THE MATRIX ELEMENTS OF $Q_{12}(r_{12}^2)$

Again we put

$$Q_{12}(r_{12}^2) = \tfrac{1}{2}(q_{12}+q_{21})\ ,$$

and follow the steps of section VI.3. thus:

$$(i)^2 q_{12} = \left[\underline{\sigma}_1\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}} \right]\left[\underline{\sigma}_2\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}} \right] \quad \ldots\ldots A_{12}$$

$$+\left[\underline{\sigma}_1\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}} \right]\left[-\underline{\sigma}_2\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}'} \right] \quad \ldots\ldots B_{12}$$

$$+\left[-\underline{\sigma}_1\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}'} \right]\left[\underline{\sigma}_2\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}} \right] \quad \ldots\ldots C_{12}$$

$$+\left[-\underline{\sigma}_1\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}'} \right]\left[-\underline{\sigma}_2\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}'} \right] \quad \ldots\ldots D_{12}$$

The term A_{12} gives

$$\left(\frac{16}{3}\alpha\right)^2(\underline{\sigma}_1\cdot\underline{I}'\wedge\underline{I})(\underline{\sigma}_2\cdot\underline{I}'\wedge\underline{I}) + \frac{16}{3}\alpha\left[(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{I}\cdot\underline{I}') - (\underline{\sigma}_1\cdot\underline{I}')(\underline{\sigma}_2\cdot\underline{I}') - (\underline{\sigma}_1\cdot\underline{\sigma}_2)r'^2 + (\underline{\sigma}_1\cdot\underline{I}')(\underline{\sigma}_2\cdot\underline{I}')\right].$$

We put $U_{12} = (\underline{\sigma}_1\cdot\underline{I}'\wedge\underline{I})(\underline{\sigma}_2\cdot\underline{I}'\wedge\underline{I})$, and use $T_{12}(\underline{A},\underline{B})$ as defined previously. Also $U_{12} = U_{21}$ in our case.

We have $T_{12}(\underline{A},\underline{B}) = T_{12}(\underline{B},\underline{A})$ if $\underline{A}$ and $\underline{B}$ commute.

Hence $\frac{1}{2}(A_{12}+A_{21}) = \left(\frac{16}{3}\alpha\right)^2 U_{12} + \frac{16}{3}\alpha\left[T_{12}(r'^2) - T_{12}(\underline{I},\underline{I}')\right]$.

The term B_{12}, after applying step 1, gives

$$\left[(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{I}-\underline{I}')\cdot\frac{\partial}{\partial \underline{I}'} - \underline{\sigma}_2\cdot(\underline{I}-\underline{I}')\ \underline{\sigma}_1\cdot\frac{\partial}{\partial \underline{I}'}\right] - \frac{16}{3}\alpha\left[(\underline{\sigma}_1\cdot\underline{I}'\wedge\underline{I})\ \underline{\sigma}_2\cdot(\underline{I}-\underline{I}')\wedge\frac{\partial}{\partial \underline{I}'}\right]$$

$$+\frac{16}{9}\alpha\left[(\underline{\sigma}_1\cdot\underline{\sigma}_2)(\underline{I}-\underline{I}')^2 - \underline{\sigma}_1\cdot(\underline{I}-\underline{I}')\ \underline{\sigma}_2\cdot(\underline{I}-\underline{I}')\right].$$

Hence we obtain the result

$$\frac{1}{2}(B_{12}+B_{21})$$

$$= \left[T_{12}(\underline{I}',\frac{\partial}{\partial \underline{I}'}) - T_{12}(\underline{I},\frac{\partial}{\partial \underline{I}'})\right] + \frac{16}{3}\alpha\left[\frac{1}{2}(\underline{\sigma}_1\cdot\underline{I}'\wedge\underline{I})\ \underline{\sigma}_2\cdot(\underline{I}'-\underline{I})\wedge\frac{\partial}{\partial \underline{I}'} + \frac{1}{2}(\underline{\sigma}_2\cdot\underline{I}'\wedge\underline{I})\ \underline{\sigma}_1\cdot(\underline{I}'-\underline{I})\wedge\frac{\partial}{\partial \underline{I}'}\right]$$

$$+\frac{16}{9}\alpha\left[2T_{12}(\underline{I},\underline{I}') - T_{12}(r^2) - T_{12}(r'^2)\right].$$

On using step 2, $\frac{1}{2}(B_{12}+B_{21})$ becomes

$$-\left[T_{12}\left(\frac{\partial}{\partial \underline{r}'},\underline{r}'\right)-T_{12}\left(\frac{\partial}{\partial \underline{r}'},\underline{r}\right)\right]-\frac{16}{3}\alpha_j\left[\frac{1}{2}\underline{\sigma}_2\cdot(\underline{r}'-\underline{r})\wedge\frac{\partial}{\partial \underline{r}'}(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})+\frac{1}{2}\underline{\sigma}_1\cdot(\underline{r}'-\underline{r})\wedge\frac{\partial}{\partial \underline{r}'}(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})\right]$$

$$+\frac{16}{9}\alpha_j\left[2T_{12}(\underline{r},\underline{r}')-T_{12}(r^2)-T_{12}(r'^2)\right]$$

operating on $\exp.\left[-\alpha_i r_{23}^2-\mu r_{12}^2\right]$

which reduces to

$$-\frac{16}{3}\alpha_j(\xi+\eta)U_{12}+(\eta+\tfrac{32}{9}\alpha_j)T_{12}(r^2)+(\xi-\eta-\tfrac{16}{9}\alpha_j)T_{12}(\underline{r},\underline{r}')-(\xi+\tfrac{16}{9}\alpha_j)T_{12}(r'^2)+2.$$

Now consider the term C_{12}. By step 1, $\frac{1}{2}(C_{12}+C_{21})$ becomes

$$\frac{16}{3}\alpha_j\left[\frac{1}{2}\underline{\sigma}_1\cdot(\underline{r}'-\underline{r})\wedge\frac{\partial}{\partial \underline{r}'}(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})+\frac{1}{2}\underline{\sigma}_2\cdot(\underline{r}'-\underline{r})\wedge\frac{\partial}{\partial \underline{r}'}(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})\right].$$

Then using step 2 we have further

$$-\frac{16}{3}\alpha_j\left[\frac{1}{2}(\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})\,\underline{\sigma}_2\cdot(\underline{r}'-\underline{r})\wedge\frac{\partial}{\partial \underline{r}'}+\frac{1}{2}(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r})\,\underline{\sigma}_1\cdot(\underline{r}'-\underline{r})\wedge\frac{\partial}{\partial \underline{r}'}\right]\exp.\left[-\alpha r_{23}^2-\mu r_{12}^2\right]$$

$$=-\frac{16}{3}\alpha_j(\xi+\eta)U_{12}\exp.\left[-\alpha r_{23}^2-\mu r_{12}^2\right].$$

In evaluating the term D_{12} we apply Green's Theorem and obtain the resulting expression in the form

$$(\underline{\sigma}_1\cdot\underline{A}\wedge\frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_2\cdot\underline{B}\wedge\frac{\partial}{\partial \underline{r}'})\;e^{-\alpha r_{23}^2-\mu r_{12}^2}$$

where $\underline{A}$ and $\underline{B}$ are either $\underline{r}$ or $\underline{r}'$.

The differentiations w.r.t. $\underline{r}'$ can then be carried out, for example,

$$(\underline{\sigma}_1\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}'})(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'})\,e^{-\alpha r_{23}^2-\mu r_{12}^2}=\left[-\xi\eta U_{12}+\eta T_{12}(r^2)\right]e^{-\alpha r_{23}^2-\mu r_{12}^2}.$$

Finally the contribution from $\frac{1}{2}(D_{12}+D_{21})$ is found to be

$$(\xi+\eta)^2U_{12}+(\xi+\eta)\left[T_{12}(\underline{r},\underline{r}')-T_{12}(r^2)\right].$$

Collecting the terms we obtain the integral $I^{(\nu)}_{Q_{12}}$

$$= AAU^{(\nu)}\, r \int d\underline{r}'\, d\Omega\; e^{-\alpha_i r_{23}^2 - \mu^{(\nu)} r_{12}^2}\, \mathcal{Y}^*(\Omega)\chi(1)\, Q_{12}(r_{12}^2)\, \chi(2)\mathcal{Y}(\Omega')\, e^{-\alpha_j r_{13}^2}\, \frac{1}{r'}\, \mathcal{F}(r')$$

$$= AAU^{(\nu)}\, r \int d\underline{r}'\, d\Omega\; e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'}\, \mathcal{Y}^*(\Omega)\chi(1)\left[-9w^2 U_{12} - \zeta T_{12}(r^2) + 2\zeta T_{12}(\underline{r},\underline{r}') - \zeta T_{12}(r'^2) - 2\right] \times$$

$$\times\, \chi(2)\mathcal{Y}(\Omega')\, \frac{1}{r'}\, \mathcal{F}(r') .$$

A third step is needed to evaluate the integral

$$I_{U_{12}} = \int r\, d\underline{r}'\, d\Omega\; e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'}\, \mathcal{Y}^*(\Omega)\chi(1)\, U_{12}(\underline{r},\underline{r}')\, \chi(2)\mathcal{Y}(\Omega')\, \frac{1}{r'}\, \mathcal{F}(r') .$$

By simple differentiation we obtain the identities

$$\left(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}\right)\left(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}\right) e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'} = \left[\partial^2 (\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r})(\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r}) + \partial\left\{(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_2\cdot\underline{r}') - (\underline{\sigma}_1\cdot\underline{\sigma}_2)\, r\cdot r'\right\}\right] e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'}$$

Thus $U_{12}(\underline{r},\underline{r}')\, e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'}$

$$= \frac{1}{\partial^2}\left[\frac{1}{2}\left(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}\right)\left(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}\right) + \frac{1}{2}\left(\underline{\sigma}_2\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}\right)\left(\underline{\sigma}_1\cdot\underline{r}'\wedge\frac{\partial}{\partial \underline{r}'}\right)\right] e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'} + \frac{1}{\partial} T_{12}(\underline{r},\underline{r}')\, e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'} .$$

The integrand of $I_{U_{12}}(r)$ is then rearranged so that Green's theorem may be applied, and we get

$$I_{U_{12}} = r \int d\underline{r}'\, d\Omega\; e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'}\, \mathcal{Y}^*(\Omega)\chi(1)\left[-\frac{1}{\partial^2} Q_{12}(r'^2) + \frac{1}{\partial} T_{12}(\underline{r},\underline{r}')\right]\chi(2)\mathcal{Y}(\Omega')\, \frac{1}{r'}\, \mathcal{F}(r') .$$

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

$I^{(r)}_{Q_{12}}$ reduces to

$$I^{(r)}_{Q_{12}} = AAU\, r \int d\underline{r}'\, d\Omega\; e^{-ar^2 - br'^2 - \partial \underline{r}\cdot\underline{r}'}\, \mathcal{Y}^*(\Omega)\chi(1)\left[\quad\right]_Q \chi(2)\mathcal{Y}(\Omega')\, \frac{1}{r'}\, \mathcal{F}(r')$$

where

$$\left[\quad\right]_Q = \frac{9w^2}{\partial^2} Q_{12}(r'^2) - \frac{1}{3}\zeta\left[S_{12}(r^2) + S_{12}(r'^2)\right] - \frac{1}{3}\left(\frac{9w^2}{\partial} - 2\zeta\right) S_{12}(\underline{r},\underline{r}')$$

$$+ \frac{2}{3}\zeta(r^2 + r'^2)(\underline{\sigma}_1\cdot\underline{\sigma}_2) + \frac{2}{3}\left(\frac{9w^2}{\partial} - 2\zeta\right)(\underline{r}\cdot\underline{r}')(\underline{\sigma}_1\cdot\underline{\sigma}_2) - 2\,\underline{\sigma}_1\cdot\underline{\sigma}_2 .$$

The matrix elements of the operators in $[\ ]_Q$ have already been evaluated for the direct interaction (Chapters V - VI, pages 33,49)

Hence we finally obtain $I^{(2)}_{Q_{12}}(r)$ given by

$$I^{(2)}_{Q_{12}}(r) = \frac{4\pi}{\delta} AAU^{(2)} \int dr' e^{-ar^2-br'^2} \times \qquad \ldots\ldots (6.8)$$

$$\times \Big[\Big\{ \frac{9w^2}{\delta^2} [F_{JL}] + \frac{2}{3}\zeta(r^2+r'^2) - 2 + \frac{2}{3}\Big(\frac{9w^2}{\delta} - 2\zeta\Big) rr' P^{(1)}_{\delta} \Big\} [\mathcal{I}_{L+\frac{1}{2}}(\delta rr')]$$

$$- \frac{1}{3}\zeta \Big\{ r^2 [B_{JL}] [\mathcal{I}_{L+\frac{1}{2}}(\delta rr')] + r'^2 [\mathcal{I}_{L+\frac{1}{2}}(\delta rr')] [B_{JL}] \Big\} - \frac{1}{3}\Big(\frac{9w^2}{\delta} - 2\zeta\Big) [P_{JL} \mathcal{I}_{L+\frac{1}{2}}(\delta rr')] \Big] F^2(r')$$

VI.3.3 SUMMARY OF RESULTS

From equation (6.5) the indirect interaction of the doublet case is given by

$$^{QS}I_{S\text{-}S}(r) = -\Big(\frac{4}{3}\Big)^4 \frac{M}{\hbar^2} \Big[-\frac{4}{3} I^{(2)}_{L_{12}}(r) + 3 I^{(4)}_{L_{12}}(r) \Big]$$

where the $I^{(\nu)}_{L_{12}}(r)$ are given by equation (6.7)

For the quartet case (using equation (6.6)) we obtain finally

$$^{QS}I_{S\text{-}S}(r) = -\Big(\frac{4}{3}\Big)^4 \frac{M}{\hbar^2} \Big[I^{(2)}_{L_{12}}(r) - I^{(2)}_{Q_{12}}(r) \Big]$$

where $I^{(2)}_{Q_{12}}(r)$ is given by equation (6.8).

CHAPTER VII

THE ENERGY TERMS

VII.1 THE N. KERNEL

This kernel is given by the expression

$$N_{S\text{-}S}(r) = (E_n - E_d)\left(\tfrac{4}{3}\right)^4 \frac{M}{\hbar^2} r \int d\underline{r}' d\Omega\, \psi^*(\Omega)\chi^*(1)\Phi(23)\Phi(13)\chi(2)\psi(\Omega')\frac{1}{r'}\mathcal{F}(r').$$

Again we take $\chi^*(1)\chi(2) = g(s)$ where $g(s)$ is given by equation (3.1).

The kernel is easily evaluated and we find

$$N_{S\text{-}S}(r) = (E_n - E_d)\left(\tfrac{4}{3}\right)^4 \frac{M}{\hbar^2} g(s) \frac{4\pi}{w_{ij}} A_i A_j \int e^{-er^2 - fr'^2} \left[\mathcal{J}_{l+\frac{1}{2}}(wrr')\right] \mathcal{F}(r')\, dr'$$

where $$e_{ij} = \tfrac{4}{9}(\alpha_i + 4\alpha_j) = f_{ji},$$

$$f_{ij} = \tfrac{4}{9}(4\alpha_i + \alpha_j) = e_{ji},$$

and $$w_{ij} = \tfrac{4}{9}(4\alpha_i + 4\alpha_j) = w_{ji}.$$

VII.2 THE KINETIC ENERGY KERNELS

These Kernels are given by the expressions

$$P^{(1)}_{S\text{-}S}(r) = \left(\tfrac{4}{3}\right)^3 r \int d\underline{r}' d\Omega\, \psi^*(\Omega)\chi^*(1)\left[\nabla^2_{r'}\Phi^*(23)\Phi(13)\right]\chi(2)\psi(\Omega')\frac{1}{r'}\mathcal{F}(r')$$

and

$$P^{(2)}_{S\text{-}S}(r) = -\left(\tfrac{4}{3}\right)^4 r \int d\underline{r}' d\Omega \left[\nabla^2_R \Phi(23)\psi(\Omega)\right]^* \chi^*(1)\Phi(13)\chi(2)\psi(\Omega')\frac{1}{r'}\mathcal{F}(r').$$

Let us put $P_{S\text{-}S}(r) = P^{(1)}_{S\text{-}S}(r) + P^{(2)}_{S\text{-}S}(r)$.

The kernel of $P_{S\text{-}S}(r)$ is symmetrical in the spatial co-ordinates of particles 1 and 2. This can be seen from the T operator identities:

$$T_{2\text{-}13} - T_{23} \equiv T_{1\text{-}23} - T_{13} \equiv \tfrac{1}{2}(T_{2\text{-}13} + T_{1\text{-}23}) - \tfrac{1}{2}(T_{23} + T_{13}).$$

Hence it follows that

$$P_{S\text{-}S}(r) = P^{(1)}_{S\text{-}S}(r) + P^{(2)}_{S\text{-}S}(r)$$
$$= \tfrac{1}{2}\left[P^{'(1)}_{S\text{-}S}(r) + P^{''(1)}_{S\text{-}S}(r)\right] + \tfrac{1}{2}\left[P^{'(2)}_{S\text{-}S}(r) + P^{''(2)}_{S\text{-}S}(r)\right],$$

where

$$P^{'(1)}_{S\text{-}S}(r) = \left(\tfrac{4}{3}\right)^3 r \int d\underline{r}' d\Omega\, \psi^*(\Omega)\chi^*(1)\left[\nabla^2_{r'}\Phi(23)\Phi(13)\right]\chi(2)\psi(\Omega')\,\frac{1}{r'}\,f(r'),$$

$$P^{''(1)}_{S\text{-}S}(r) = \left(\tfrac{4}{3}\right)^3 r \int d\underline{r}' d\Omega\, \psi^*(\Omega)\chi^*(1)\left[\nabla^2_{r}\Phi(23)\Phi(13)\right]\chi(2)\psi(\Omega')\,\frac{1}{r'}\,f(r')$$

and

$$P^{'(2)}_{S\text{-}S}(r) = -\left(\tfrac{4}{3}\right)^4 r \int d\underline{r}' d\Omega\left[\nabla^2_{23}\Phi(23)\psi(\Omega)\right]^*\chi^*(1)\Phi(13)\chi(2)\psi(\Omega')\,\frac{1}{r'}\,f(r'),$$

$$P^{''(2)}_{S\text{-}S}(r) = -\left(\tfrac{4}{3}\right)^4 r \int d\underline{r}' d\Omega\left[\nabla^2_{13}\Phi(23)\psi(\Omega)\right]^*\chi^*(1)\Phi(13)\chi(2)\psi(\Omega')\,\frac{1}{r'}\,f(r')$$

which is further equal to

$$-\left(\tfrac{4}{3}\right)^4 r \int d\underline{r}' d\Omega\left[\Phi(23)\psi(\Omega)\right]^*\chi^*(1)\left[\nabla^2_{13}\Phi(13)\right]\chi(2)\psi(\Omega')\,\frac{1}{r'}\,f(r')$$

by Green's Theorem (as ∇^2_{13} does not operate on $r' \equiv (2\text{-}13)$).

VII.2.1. THE KERNELS $P^{(1)}_{S\text{-}S}(r)$.

Replacing $\underline{r}_{23}$ by $\frac{2}{3}(2\underline{r}' + \underline{r})$

and $\underline{r}_{13}$ by $\frac{2}{3}(2\underline{r} + \underline{r}')$,

We find that

$$\nabla_r^2 \Phi(23)\Phi(13) = A_i A_j \left[-6f_{ij} + w_{ij}^2 r^2 + 4f_{ij}^2 r'^2 + 4f_{ij} w_{ij}\, r\cdot r'\right] e^{-e_{ij}r^2 - f_{ij}r'^2 - w_{ij} r\cdot r'}$$

and $$\nabla_r^2 \Phi(23)\Phi(13) = A_i A_j \left[-6e_{ij} + 4e_{ij}^2 r^2 + w_{ij}^2 r'^2 + 4e_{ij} w_{ij}\, r\cdot r'\right] e^{-e_{ij}r^2 - f_{ij}r'^2 - w_{ij} r\cdot r'}$$

Hence it follows that $P^{(1)}_{S\cdot S}(r)$

$$= \left(\tfrac{4}{3}\right)^3 A_i A_j\, r \int d\underline{r}' d\Omega\, e^{-er^2 - fr'^2 - w\, r\cdot r'} Y^*(\Omega) X(1) \left[-\tfrac{15}{4}w + \tfrac{1}{2}\{(4e^2+w^2)r^2 + (4f^2+w^2)r'^2 + 5w^2 r\cdot r'\}\right] X(2) Y(\Omega') \tfrac{1}{r'} \mathcal{F}(r')$$

$$= \left(\tfrac{4}{3}\right)^3 \tfrac{4\pi}{w}\, g(s) A_i A_j \int dr'\, e^{-er^2 - fr'^2} \left[-\tfrac{15}{4}w + \tfrac{1}{2}(4e^2+w^2)r^2 + \tfrac{1}{2}(4f^2+w^2)r'^2 + \tfrac{5}{2}w^2 rr' p_w\right] \left[\mathcal{I}_{l+\frac{1}{2}}(wrr')\right] \mathcal{F}(r')$$

where $g(s)$ and $rr'p_w$ are as defined previously.

VII.2.2 <u>THE KERNELS</u> $P^{(2)}_{S\cdot S}(r)$.

We find that

$$\nabla_{23}^2 \Phi(23) = A_i (4\alpha_i^2 r_{23}^2 - 6\alpha_i)\, e^{-\alpha_i r_{23}^2}$$

and $$\nabla_{13}^2 \Phi(13) = A_j (4\alpha_j^2 r_{13}^2 - 6\alpha_j)\, e^{-\alpha_j r_{13}^2}.$$

Hence we get $P^{(2)}_{S\cdot S}(r)$

$$= -\left(\tfrac{4}{3}\right)^4 A_i A_j\, r \int d\underline{r}' d\Omega\, e^{-er^2 - fr'^2 - w\, r\cdot r'} Y^*(\Omega) X(1) \left[-\tfrac{27}{16}w + \tfrac{8}{9}(\alpha_i^2 + 4\alpha_j^2)r^2 + \tfrac{8}{9}(4\alpha_i^2 + \alpha_j^2)r'^2 + \tfrac{32}{9}(\alpha_i^2 + \alpha_j^2) r\cdot r'\right] X(2) Y(\Omega') \tfrac{1}{r'} \mathcal{F}(r')$$

$$= -\left(\tfrac{4}{3}\right)^4 \tfrac{4\pi}{w}\, g(s) A_i A_j \int dr'\, e^{-er^2 - fr'^2} \left[-\tfrac{27}{16}w + \tfrac{8}{9}(\alpha_i^2 + 4\alpha_j^2)r^2 + \tfrac{8}{9}(4\alpha_i^2 + \alpha_j^2)r'^2 + \tfrac{32}{9}(\alpha_i^2 + \alpha_j^2) rr' p_w\right] \left[\mathcal{I}_{l+\frac{1}{2}}(wrr')\right] \mathcal{F}(r').$$

VII. 2.3 THE TOTAL KERNEL

Combining the expressions in VII.2.2 and VII.2.3, the total kinetic energy term is given by $P_{s.s}(r)$

$$= \left(\frac{4}{3}\right)^3 \frac{4\pi}{w}\, q(s)\, A_i A_j \int dr'\, e^{-er^2-fr'^2} \left[-\frac{3}{2}w + \frac{64}{81}\left(\phi_{ij} r^2 + \psi_{ij} r'^2 + 4\chi_{ij} rr' p_w\right)\right] \left[J_{l+\frac{1}{2}}(wrr')\right] F^e(r')$$

where

$$\phi_{ij} = \alpha_i^2 + 8\alpha_i\alpha_j + 4\alpha_j^2 = \psi_{ji} ,$$

$$\psi_{ij} = 4\alpha_i^2 + 8\alpha_i\alpha_j + \alpha_j^2 = \phi_{ij} ,$$

$$\chi_{ij} = \alpha_i^2 + 5\alpha_i\alpha_j + \alpha_j^2 = \chi_{ji} .$$

CHAPTER VIII

THE CENTRAL FORCE S-D TERMS

The evaluation of the S-D terms is done in the same way as that of the S-S terms. There is an additional operator namely the tensor operator of the deuteron D-state wave function. Because of this operator, the central force gives no contribution to the doublet case.

VIII.1 THE DIRECT INTERACTION

The central force S-D term is $\underset{S\text{-}D}{{}^{c}D}(r)$

$$= \frac{4}{3}\frac{M}{\hbar^2}\int d\underline{R}\, d\Omega\, \mathcal{Y}^{*}(\Omega)\chi^{*}(1)\,\phi_S(23)\sum_{\nu}\tfrac{1}{4}(2w-h+2b-m)_{\nu}\,{}^{\nu}V_c(12)\,T(23)\,\phi_D(23)\,\chi(1)\,\mathcal{Y}(\Omega)\,\mathcal{F}(r)$$

where $T(23)$ is defined in section I.2.

The potential is the same as in the S-S term.

With $\phi_D(23)$ given in section I.2 we have

$$\underset{S\text{-}D}{{}^{c}D}(r) = \frac{4}{3}\frac{M}{\hbar^2}A_i A'_j\,{}^{c}U^{(3)}_{k}\, e^{-(\mu-\lambda'\gamma'^2)r^2}\int d\underline{R}\, d\Omega\, \mathcal{Y}^{*}(\Omega)\chi(1)\,S_{23}(r_{23}^2)\,\chi(1)\,\mathcal{Y}(\Omega)\,\mathcal{F}(r)\, e^{-\lambda'(\underline{R}-\gamma'\underline{r})^2}$$

where $$\lambda'_{ijk} = \alpha_i + \alpha'_j + \tfrac{1}{4}\mu_k$$

and $$\gamma'_{ijk} = \tfrac{1}{2}\mu_k / \lambda'_{ijk}\ .$$

We leave out all primes whenever there is a no loss in clarity.

For the space integration, $d\underline{R}$, we need the formula

$$\int d\underline{R}\; S_{23}(R^2)\, e^{-\lambda(\underline{R}-\gamma\underline{r})^2} = \left(\frac{\pi}{\lambda}\right)^{3/2}\gamma^2 S_{23}(r^2)\ .$$

The factor for the spin summation and the spherical harmonic integration is of the form

$$\int Y^{*}(\Omega) X^{*}(1)\, S_{23}(r^2)\, X(1)\, Y(\Omega)\, d\Omega \;=\; r^2 [B_{Jl}] \,.$$

Hence it follows that

$$D^{C}_{S\text{-}D}(r) \;=\; \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda'}\right)^{3/2} \gamma'^{2} A_i A'_j U^{(3)}_{K} \; e^{-(\mu-\lambda'\gamma'^2)r^2}\; r^2 [B_{Jl}]\, F^{e}(r) \,.$$

VIII.2 THE INDIRECT INTERACTION

This is given by the expression $I^{C}_{S\text{-}D}(r)$

$$= -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\, r \int dr'\, d\Omega\, Y^{*}(\Omega) X^{*}(1)\, \phi_{S}(23) \sum_{\nu} \frac{1}{4}(w-2h+b-2m)^{\nu} V_{C}(12)\, T(13)\, \phi_{D}(13)\, X(2)\, Y(\Omega') \frac{1}{r'} F^{e}(r') \,.$$

The potential is the same as in the S-S indirect interaction term.

Similar to the case of the direct interaction we get $I^{C}_{S\text{-}D}(r)$

$$= -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\, r\, A_i A'_j\, U^{C(4)}_{K} \int dr'\, d\Omega\; Y^{*}(\Omega) X^{*}(1)\, S_{13}(r_{13}^2)\, X(2)\, Y(\Omega') \frac{1}{r'} F^{e}(r')\; e^{-a'r^2 - b'r'^2 - \delta' r\cdot r'}$$

where
$$a'_{ijk} \;=\; \frac{4}{9}(\alpha_i + 4\alpha'_j + \mu_K) \,,$$
$$b'_{ijk} \;=\; \frac{4}{9}(4\alpha_i + \alpha'_j + \mu_K) \,,$$
and
$$\delta'_{ijk} \;=\; \frac{4}{9}(4\alpha_i + 4\alpha'_j - 2\mu_K) \,.$$

We use the results from section V.2 for the integral and finally get the result:

$$I^{C}_{S\text{-}D}(r) \;=\; -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\left(\frac{2}{3}\right)^2 \frac{4\pi}{\delta'}\, A_i A'_j\, U^{C(4)}_{K} \int dr'\; e^{-a'r^2 - b'r'^2} \times$$

$$\times \left\{ 4r^2 [B_{Jl}] [J_{l+\frac{1}{2}}(\delta' r r')] + r'^2 [J_{l+\frac{1}{2}}(\delta' r r')] [B_{Jl}] + 4rr' [P_{Jl} J_{l+\frac{1}{2}}(\delta' r r')] \right\} F^{e}(r') \,.$$

CHAPTER IX

THE SPIN-ORBIT FORCE S-D TERMS

IX.1. THE DIRECT INTERACTION

This is given by the terms $\overset{LS}{D}_{S.D}(r)$

$$= \frac{4}{3}\frac{M}{\hbar^2} r \int d\underline{R}\, d\Omega\, y^*(\Omega)\chi^*(1)\,\phi_S(23)\sum_\nu \frac{1}{4}(2w-h+2b-m)_\nu\, {}^{\nu}V_{LS}(12)\,T(23)\,\phi_D(23)\,\chi(1)\,y(\Omega)\,\frac{1}{r}\,\overline{F}(r).$$

The operator $V_{LS}(12)\,T(23)$ in this integral is

$$\tfrac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\;\; S_{23}(r_{23}^2)$$

with

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

IX.11. THE SPACE INTEGRATION

We follow closely the steps and the explanation given for the case of the quadratic spin-orbit operator (see section VI.2)

Consider the above operator namely

$$i(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\; S_{23}(r_{23}^2) = i(\underline{\sigma}_1\cdot\underline{L}_{12})\,S_{23}(r_{23}^2) + i(\underline{\sigma}_2\cdot\underline{L}_{12})\left[3(\underline{\sigma}_3\underline{R})(\underline{\sigma}_3\underline{R}) - \underline{\sigma}_3\underline{\sigma}_3 R^2\right].$$

This may be seperated into four terms,

A. $i(\underline{\sigma}_1\cdot\underline{L}_{12})\,S_{23}(r_{23}^2)$

B. $3i(\underline{L}_{12}\underline{R})(\underline{\sigma}_3\underline{R})$

C. $-3(\underline{\sigma}_2\underline{L}_{12\wedge}\underline{R})(\underline{\sigma}_3\underline{R})$

and D. $-i(\underline{\sigma}_3\cdot\underline{L}_{12})R^2$.

The term containing $(\underline{\sigma}_2 \underline{L}_{12} \wedge \underline{\sigma}_3)\ \mathcal{R}^2$ vanishes on account of the symmetry of the spin functions.

TERM A After differentiation term A reads

$$A = \frac{3}{2} S_{23}(\mathcal{R}^2)\ \underline{\sigma}_1 \cdot (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \frac{\partial}{\partial \underline{r}} + 2\alpha_j' S_{23}(\mathcal{R}^2)\ \underline{\sigma}_1 \cdot \underline{r} \wedge \underline{R} + 3(\underline{\sigma}_1 \wedge \underline{\sigma}_2 \cdot \underline{r})(\underline{\sigma}_3 \cdot \underline{R})$$

$$+ 3(\underline{\sigma}_1 \wedge \underline{\sigma}_3 \cdot \underline{r})(\underline{\sigma}_2 \cdot \underline{R}) - \frac{3}{2}(\underline{\sigma}_1 \wedge \underline{\sigma}_2 \cdot \underline{R})(\underline{\sigma}_3 \cdot \underline{R}) - \frac{3}{2}(\underline{\sigma}_1 \wedge \underline{\sigma}_3 \cdot \underline{R})(\underline{\sigma}_2 \cdot \underline{R}) + 2\,\underline{\sigma}_1 \cdot \underline{r} \wedge \underline{R}\ .$$

After $d\underline{R}$ integration this term contributes a factor

$$\left(\frac{\pi}{\lambda}\right)^{3/2} \Big[\frac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 S_{23}(r^2)\ \underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}} + 3\gamma(1-\tfrac{\gamma}{2}) \left\{ (\underline{\sigma}_1 \wedge \underline{\sigma}_2 \cdot \underline{r})(\underline{\sigma}_3 \cdot \underline{r}) + (\underline{\sigma}_1 \wedge \underline{\sigma}_3 \cdot \underline{r})(\underline{\sigma}_2 \cdot \underline{r}) \right\}$$

$$+ 2\alpha_j' \frac{\gamma}{2\lambda} \left\{ (\underline{\sigma}_2 \cdot \underline{\sigma}_1 \wedge \underline{r})(\underline{\sigma}_3 \cdot \underline{r}) + 3(\underline{\sigma}_3 \cdot \underline{\sigma}_1 \wedge \underline{r})(\underline{\sigma}_2 \cdot \underline{r}) \right\}$$

$$- \frac{3}{4} \cdot \frac{\gamma}{2\lambda} \left\{ 3(\underline{\sigma}_2 \cdot \underline{r})(\underline{\sigma}_1 \wedge \underline{\sigma}_3 \cdot \frac{\partial}{\partial \underline{r}}) + 3(\underline{\sigma}_3 \cdot \underline{r})(\underline{\sigma}_1 \wedge \underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{r}}) - 2(\underline{\sigma}_2 \cdot \underline{\sigma}_3)(\underline{\sigma}_1 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}}) \right\} \Big]\ .$$

TERM B On differentiation in term B we obtain

$$B = \frac{9}{2}(\underline{\sigma}_3 \cdot \underline{R})(\underline{R} \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}}) - 3\,\underline{\sigma}_3 \cdot \underline{R} \wedge \underline{r}$$

and after $d\underline{R}$ integration we get the result

$$B \rightarrow \left(\frac{\pi}{\lambda}\right)^{3/2} \frac{9}{4\lambda}\ \underline{\sigma}_3 \cdot \underline{r} \wedge \frac{\partial}{\partial \underline{r}}\ .$$

TERM C After the differentiation term C becomes

$$C = 3i \Big[\frac{3}{2}(\underline{\sigma}_3 \cdot \underline{R})\ \underline{\sigma}_2 \cdot (\underline{r} \wedge \frac{\partial}{\partial \underline{r}}) \wedge \underline{R} - \frac{3}{4}(\underline{\sigma}_3 \cdot \underline{R}) \left\{ \mathcal{R}^2\, \underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{r}} - (\underline{\sigma}_2 \cdot \underline{R})(\underline{R} \cdot \frac{\partial}{\partial \underline{r}}) \right\}$$

$$+ S_{23}(\underline{r}, \underline{R}) - \frac{1}{2} S_{23}(\mathcal{R}^2) + 2\alpha_j' (\underline{\sigma}_2 \cdot \underline{R})(\underline{\sigma}_3 \cdot \underline{R})(\underline{r} \cdot \underline{R}) - 2\alpha_j' (\underline{\sigma}_2 \cdot \underline{r})(\underline{\sigma}_3 \cdot \underline{R})\, \mathcal{R}^2 \Big]\ .$$

This is followed by $d\underline{R}$ integration to give a factor

$$\left(\frac{\pi}{\lambda}\right)^{3/2} 3i \Big[\frac{3}{2}\gamma^2(1-\tfrac{\gamma}{2}) \left\{ r^2 (\underline{\sigma}_3 \cdot \underline{r})(\underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{r}}) - (\underline{\sigma}_2 \cdot \underline{r})(\underline{\sigma}_3 \cdot \underline{r})(\underline{r} \cdot \frac{\partial}{\partial \underline{r}}) \right\} + \frac{\gamma \alpha_i}{\lambda} S_{23}(r^2) - \frac{3}{4} \cdot \frac{\gamma}{2\lambda} S_{23}(\underline{r}, \frac{\partial}{\partial \underline{r}}) \Big]\ .$$

TERM D After the differentiation, term D reads

$$D = -\frac{3}{2}R^2\,\underline{\sigma_3}\cdot(\underline{r}-\tfrac{1}{2}\underline{R})\wedge\frac{\partial}{\partial \underline{r}} + 2\,\underline{\sigma_3}\cdot\underline{r}\wedge\underline{R} - 2\alpha_j' R^2\,\underline{\sigma_3}\cdot\underline{r}\wedge\underline{R}$$

and so after $d\underline{R}$ integration we finally obtain

$$D \to \left(\frac{\pi}{\lambda}\right)^{3/2}\left[-\frac{3}{2}\left(1-\frac{\gamma}{2}\right)\gamma^2 r^2\,\underline{\sigma_3}\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}} - \frac{3}{2}\cdot\frac{1}{2\lambda}\left(3-\frac{5}{2}\gamma\right)\underline{\sigma_3}\cdot\underline{r}\wedge\frac{\partial}{\partial \underline{r}}\right].$$

Collecting all the terms we finally have the resulting expression for the operators $\frac{1}{2}(\underline{\sigma_1}+\underline{\sigma_2})\cdot\underline{L}_{12}\,S_{23}(r_{23}^2)$ given by

$$\begin{aligned}\underline{LS} = \left(\frac{\pi}{\lambda}\right)^{3/2}\frac{1}{2}\Bigg[&\frac{3}{2}\left(1-\frac{\gamma}{2}\right)\gamma^2 S_{23}(r^2)\,\underline{\sigma_1}\cdot\underline{L}_\gamma + \frac{3\gamma}{4\lambda}\,\underline{\sigma_1}\cdot\underline{L}_\gamma + \left\{\frac{15\gamma}{8\lambda} - \frac{3}{2}\left(1-\frac{\gamma}{2}\right)\gamma^2 r^2\right\}\underline{\sigma_3}\cdot\underline{L}_\gamma \\ &+ 3\frac{\gamma}{\lambda}\alpha_i\,S_{23}(r^2) - \frac{9\gamma}{8\lambda}\,S_{23}\left(r,\frac{\partial}{\partial r}\right) \\ &+ \frac{9}{2}\gamma^2\left(1-\frac{\gamma}{2}\right)\left\{r^2(\underline{\sigma_3}\cdot\underline{r})\left(\underline{\sigma_2}\cdot\frac{\partial}{\partial \underline{r}}\right) - (\underline{\sigma_2}\cdot\underline{r})(\underline{\sigma_3}\cdot\underline{r})\left(\underline{r}\cdot\frac{\partial}{\partial \underline{r}}\right)\right\} \\ &+ \left\{3\gamma\left(1-\frac{\gamma}{2}\right) + \frac{\gamma}{\lambda}\alpha_j'\right\}\frac{1}{i}\left\{(\underline{\sigma_1}\wedge\underline{\sigma_2}\cdot\underline{r})(\underline{\sigma_3}\cdot\underline{r}) + (\underline{\sigma_1}\wedge\underline{\sigma_3}\cdot\underline{r})(\underline{\sigma_2}\cdot\underline{r})\right\} \\ &- \frac{9\gamma}{8\lambda}\cdot\frac{1}{i}\left\{(\underline{\sigma_2}\cdot\underline{r})(\underline{\sigma_1}\wedge\underline{\sigma_3}\cdot\frac{\partial}{\partial \underline{r}}) + (\underline{\sigma_3}\cdot\underline{r})(\underline{\sigma_1}\wedge\underline{\sigma_2}\cdot\frac{\partial}{\partial \underline{r}})\right\}\Bigg].\end{aligned}$$

Further reductions due to spin summation will be obtained in each case seperately.

IX.1.2. THE DOUBLET CASE

The spin functions in the doublet case help to eliminate some of the terms which have the form of atensor operator.

Thus the expression $$3r^2(\sigma_3\cdot r)\left(\sigma_2\cdot\frac{\partial}{\partial r}\right) - 3(\sigma_2 r)(\sigma_3 r)\left(r\cdot\frac{\partial}{\partial r}\right)$$

which is really $$r^2 S_{23}\left(r,\frac{\partial}{\partial r}\right) - S_{23}(r^2)\left(r\cdot\frac{\partial}{\partial r}\right)$$

vanishes on the spin summation.

We make use of the following results for further reduction of the spins:

$$\langle\bar{\chi}^{\frac{1}{2}}|\underset{23}{S}(r^2)\,\sigma_1\cdot L_r|\bar{\chi}^{\frac{1}{2}}\rangle = \tfrac{4}{3}r^2\langle\tilde{\chi}^{\frac{1}{2}}|\sigma_1\cdot L_r|\tilde{\chi}^{\frac{1}{2}}\rangle ,$$

$$\langle\bar{\chi}^{\frac{1}{2}}|(\sigma_1\wedge\sigma_2\cdot A)(\sigma_3\cdot B)|\bar{\chi}^{\frac{1}{2}}\rangle = -\langle\tilde{\chi}^{\frac{1}{2}}|\sigma_1\cdot A\wedge B|\tilde{\chi}^{\frac{1}{2}}\rangle$$

$$= 0 \quad \text{if} \quad A\equiv B ,$$

$$\langle\bar{\chi}^{\frac{1}{2}}|\sigma_1\cdot L_r|\bar{\chi}^{\frac{1}{2}}\rangle = -\tfrac{1}{3}\langle\tilde{\chi}^{\frac{1}{2}}|\sigma_1\cdot L_r|\tilde{\chi}^{\frac{1}{2}}\rangle$$

and $$\langle\bar{\chi}^{\frac{1}{2}}|\sigma_3\cdot L_r|\bar{\chi}^{\frac{1}{2}}\rangle = \tfrac{2}{3}\langle\tilde{\chi}^{\frac{1}{2}}|\sigma_1\cdot L_r|\tilde{\chi}^{\frac{1}{2}}\rangle .$$

With these results the operator in the integral of the spin-orbit S-D term reduces to

$$LS = \left(\frac{\pi}{\lambda}\right)^{3/2}\frac{1}{2}\left\{(1-\tfrac{\gamma}{2})\gamma^2r^2-\frac{5\gamma}{4\lambda}\right\}\langle\tilde{\chi}^{\frac{1}{2}}|\sigma_1\cdot L_r|\tilde{\chi}^{\frac{1}{2}}\rangle .$$

It can be easily verified that

$$\langle\tilde{\chi}^{\frac{1}{2}}y\,|\,\sigma_i\cdot L\,|\,\tilde{\chi}^{\frac{1}{2}}y\rangle = 3[A_{jl}]$$

where $[A_{jl}]$ is defined in section IV.1.

Therefore the direct interaction is given by

$$\underset{S\text{-}D}{{}^{LS}D(r)} = \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} A_i A_j' \, {}^{LS}U_k^{(1)} \, e^{-(\mu+\lambda\gamma^2)r^2} \, \frac{3}{2}\left[(1-\tfrac{\gamma}{2})\gamma^2 r^2 - \frac{5\gamma}{4\lambda}\right][A_{jl}]\, \mathcal{F}(r) \, .$$

IX.1.3. THE QUARTET CASE

Employing the full symmetry of the spin functions, the expression $\underline{LS}$ in IX.1.1 becomes

$$\begin{aligned}\underline{LS} = \left(\frac{\pi}{\lambda}\right)^{3/2}\frac{1}{2}\Big[& \tfrac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 S_{23}(r^2)\,\underline{\sigma}_1\cdot\underline{L}_r + \left\{\frac{21\gamma}{8\lambda} - \tfrac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 r^2\right\}\underline{\sigma}_1\cdot\underline{L}_r \\ & + \frac{3\gamma}{\lambda}\sigma_i S_{23}(r^2) + \left\{-\frac{9\gamma}{8\lambda} + \tfrac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 r^2\right\} S_{23}(\underline{r},\tfrac{\partial}{\partial\underline{r}}) \\ & - \tfrac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 S_{23}(r^2)\;\underline{r}\cdot\frac{\partial}{\partial\underline{r}}\Big] \, .\end{aligned}$$

We now eliminate terms involving $\frac{\partial}{\partial\underline{r}}$ in this expression which has on its right the expression $\mathcal{Y}(\Omega)\frac{1}{r}\mathcal{F}(r)$.

Again we have

$$(\underline{r}\cdot\tfrac{\partial}{\partial\underline{r}})\, Y_{lm}(\theta,\varphi)\,\tfrac{1}{r}f(r) = Y_{lm}(\theta,\varphi)\left[f'(r) - \tfrac{1}{r}f(r)\right]$$

and $S_{23}(\underline{r},\tfrac{\partial}{\partial\underline{r}})\, Y_{lm}(\theta,\varphi)\,\tfrac{1}{r}f(r) = \tfrac{1}{r}f\, S_{23}(\underline{r},\tfrac{\partial}{\partial\underline{r}})\, Y_{lm} + \tfrac{1}{r^2}S_{23}(r^2)\, Y_{lm}\left[f'(r) - \tfrac{1}{r}f\right]$.

Hence the operator in the integral of the quartet case is now

$$\begin{aligned}\left(\frac{\pi}{\lambda}\right)^{3/2}\frac{1}{2}\Big[& \tfrac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 S_{23}(r^2)\,\underline{\sigma}_1\cdot\underline{L}_r + \left\{\frac{21\gamma}{8\lambda} - \tfrac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 r^2\right\}\underline{\sigma}_1\cdot\underline{L}_r \\ & + \left\{3(1-\tfrac{\gamma}{2})\gamma - 3\alpha\frac{\gamma}{\lambda} + \frac{9\gamma}{8\lambda r^2}\right\} S_{23}(r^2) + \left\{-\frac{9\gamma}{8\lambda} + \tfrac{3}{2}(1-\tfrac{\gamma}{2})\gamma^2 r^2\right\} S_{23}(\underline{r},\tfrac{\partial}{\partial\underline{r}})\Big]\,\mathcal{Y}(\Omega)\,\mathcal{F}(r) \\ & + \left(\frac{\pi}{\lambda}\right)^{3/2}\frac{1}{2}\left[-\frac{9\gamma}{8\lambda}S_{23}(r^2)\right]\mathcal{Y}(\Omega)\,\mathcal{F}'(r) \, ,\end{aligned}$$

where $\frac{\partial}{\partial \underline{r}}$ only operates on the solid angles of $\underline{r}$.

The matrix elements of these operators, except the term $S_{23}(r^2)\,\underline{\sigma}_1\cdot\underline{L}_r$ have already been found, and they are given by

$$\langle \underline{\sigma}_1\cdot\underline{L}_r \rangle = \tfrac{1}{2}[A_{JL}] \quad ,$$

$$\langle S_{23}(r^2) \rangle = r^2[B_{JL}] \quad ,$$

and

$$\langle S_{23}(r,\frac{\partial}{\partial \underline{r}}) \rangle = 3\langle T_{23}(\underline{r},\frac{\partial}{\partial \underline{r}} \rangle = 3[D_{JL}] \quad .$$

The matrix elements of $S_{23}(r^2)\,\underline{\sigma}_1\cdot\underline{L}_r$

With usual procedure we obtain the spin array of the operator as given in Table 4 below

TABLE 4: THE SPIN PRODUCTS OF $S_{23}(r^2)\,\underline{L}_r\cdot\underline{\sigma}_1$

	$\chi^{3/2}_{3/2}$	$\chi^{3/2}_{1/2}$	$\chi^{3/2}_{-1/2}$	$\chi^{3/2}_{-3/2}$
$\chi^{3/2}_{3/2}$	$(3z^2-r^2)\,L_z$	$2/\sqrt{3}$ $(3z^2-r^2)L_- + 6zr_-L_z$	$4/\sqrt{3}$ $2zr_-L_- + r_-^2L_z$	$2\sqrt{4}\,r_-^2L_-$
$\chi^{3/2}_{1/2}$	$2/\sqrt{3}$ $(3z^2-r^2)L_+ + 6zr_+L_z$	$(2r^2-5z^2)L_z$ $+8z(r_+L_- + r_-L_+)$	$\frac{2}{3}(5r^2-12z^2)L_-$ $+8r_-(r_+L_+ - zL_z)$	$-4/\sqrt{3}$ $2zr_-L_- + r_-^2L_z$
$\chi^{3/2}_{-1/2}$	$4/\sqrt{3}$ $2zr_+L_+ + r_+^2L_z$	$\frac{2}{3}(5r^2-12z^2)L_+$ $+12r_+(r_+L_- - zL_z)$	$(5z^2-2r^2)L_z$ $-8z(r_+L_+ + r_-L_+)$	$2/\sqrt{3}$ $(3z^2-r^2)L_- + 6zr_-L_z$
$\chi^{3/2}_{-3/2}$	$2\sqrt{4}\,r_+^2L_+$	$-4/\sqrt{3}$ $2zr_+L_+ + r_+^2L_z$	$2\sqrt{/3}$ $(3z^2-r^2)L_+ + 6zr_+L_z$	$-(3z^2-r^2)\,L_z$

where $L^{\pm} = \frac{1}{2}(L^x \pm iL^y)$.

As $$L^2 Y_{[m}(\theta,\varphi) = m Y_{[m}(\theta,\varphi) \quad ,$$

and $$L^{\pm} Y_{[m}(\theta,\varphi) = \tfrac{1}{2}\left[([\mp m)([\pm m+1)\right]^{\frac{1}{2}} Y_{[m\pm1}(\theta,\varphi) \quad ,$$

the integration again involves products of three spherical harmonics. The result of this integration is

$$\int d\Omega\, \mathcal{Y}^*(\Omega)\, \chi^*(1)\, S_{23}(\tau^2)\, \underline{\sigma}_1 \cdot \underline{L}_\tau\, \chi(1)\, \mathcal{Y}(\Omega) = \tau^2 [C_{J[}] \qquad \ldots\ldots \quad (9.1)$$

where

$$[C_{J[}] = \begin{pmatrix} -\frac{(2J-3)^2}{4J} & 0 & \frac{2J-3}{4J}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} & 0 \\ 0 & \frac{20J^2+4J-43}{12(J+1)} & 0 & -\frac{2J+5}{4(J+1)}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} \\ \frac{2J-3}{4J}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} & 0 & \frac{-20J^2-36J+27}{12J} & 0 \\ 0 & -\frac{2J+5}{4(J+1)}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} & 0 & \frac{(2J+5)^2}{4(J+1)} \end{pmatrix}$$

for $J \geqslant 3/2$,

and $$[C_{J[}] = \begin{pmatrix} \frac{-20J^2-36J+27}{12J} & \\ & \frac{(2J+5)^2}{4(J+1)} \end{pmatrix}$$

for $J = \frac{1}{2}$.

Now we are able to write down the direct interaction of the spin-orbit S-D term namely:

$$D^{LS}_{S\text{-}D}(r) = \tfrac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} A_i A_j' \, {}^{LS}U^{(1)}_k \, e^{-(\mu-\lambda\gamma^2)r^2} \times$$

$$\times \left\{ \left[\frac{21\gamma}{32\lambda} - \frac{3}{8}\left(1-\frac{\gamma}{2}\right)\gamma^2 r^2\right][A_{J[}]\, \mathcal{F}(r) + \left[\frac{9\gamma}{16\lambda} + \frac{3}{2}\left(1-\frac{\gamma}{2}\right)\gamma r^2 - \frac{3}{2\lambda}\gamma\alpha_j' r^2\right][B_{J[}]\, \mathcal{F}(r) \right.$$

$$\left. + \frac{3}{4}\left(1-\frac{\gamma}{2}\right)\gamma^2 r^2 [C_{J[}]\, \mathcal{F}(r) + \left\{-\frac{27\gamma}{16\lambda} + \frac{9}{4}\left(1-\frac{\gamma}{2}\right)\gamma^2 r^2\right][D_{J[}]\, \mathcal{F}(r) - \frac{9\gamma}{16\lambda} r^2 [B_{J[}]\, \mathcal{F}'(r) \right\} .$$

IX.2. THE INDIRECT INTERACTION

The integral for the spin-orbit S-D terms is given by $^{LS}I_{S\text{-}D}(r)$

$$= -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r \int d\underline{r}' d\Omega\, \mathcal{Y}^*(\Omega)\chi^*(1)\phi_S(23) \sum_\nu \tfrac{1}{4}(w-2h+b-2m)_\nu V_{LS}(12)T(13)\phi_D(13)\chi(2)\mathcal{Y}(\Omega)\frac{1}{r'}F^\nu(r').$$

The operator $V_{LS}(12)T(13)$ in the integral is

$$\tfrac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\; S_{13}(r_{13}^2)$$

with $$\underline{L}_{12} = \frac{1}{i}(\underline{r}-\underline{r}')\wedge\left(\frac{\partial}{\partial\underline{r}}-\frac{\partial}{\partial\underline{r}'}\right).$$

IX.2.1. THE SPACE INTEGRATION

For the space integration, the integrals are conveniently considered in two parts.

a. The part which involves $\frac{\partial}{\partial\underline{r}}$ of $\underline{L}_{12}$.

The relevant function on the right of the operator is $e^{-\alpha_j' r_{13}^2}$

We perform the differentiation and combine the spin products to obtain the following result:

$$\left(\frac{3}{2}\right)^2 e^{+\alpha_j' r_{13}^2}\; \tfrac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}}\; S_{13}(r_{13}^2)\; e^{-\alpha_j' r_{13}^2}$$

$$= \frac{16}{3}\alpha'\Big[\left\{4S_{13}(r^2)+4S_{13}(\underline{r},\underline{r}')+4S_{13}(r'^2)\right\}\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r} - (4r^2+4\underline{r}\cdot\underline{r}'+r'^2)\underline{\sigma}_3\cdot\underline{r}'\wedge\underline{r}$$
$$+ i(4\underline{r}\cdot\underline{r}'+2r'^2)S_{13}(r^2) - i(2r^2+\underline{r}\cdot\underline{r}')S_{13}(r'^2)$$
$$- \tfrac{i}{3}(4r^2-2\underline{r}\cdot\underline{r}'-2r'^2)R_{13}(\underline{r},\underline{r}') - \tfrac{i}{3}(8r^2+2\underline{r}\cdot\underline{r}'-r'^2)R_{13}(\underline{r}',\underline{r})\Big]$$

$$+ 12\,\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r} + 12\left[W(r^2)-W(\underline{r},\underline{r}')\right] + 6\left[W(\underline{r}',\underline{r})-W(r'^2)\right]$$

$$+ 30\,\underline{\sigma}_3\cdot\underline{r}'\wedge\underline{r} - 12iS_{13}(r^2) - 2iR_{13}(\underline{r},\underline{r}') + 8iR_{13}(\underline{r}',\underline{r}) + 6iS_{13}(r'^2),$$

where

$$\mathcal{R}_{13}(\underline{r},\underline{r}') = 3(\underline{\sigma}_1\cdot\underline{r})(\underline{\sigma}_3\cdot\underline{r}') - \underline{\sigma}_1\cdot\underline{\sigma}_3\,(\underline{r}\cdot\underline{r}')$$

and $$W(\underline{A},\underline{B}) = (\underline{\sigma}_1\cdot\underline{A})(\underline{\sigma}_3\wedge\underline{\sigma}_2\cdot\underline{B}) + (\underline{\sigma}_3\cdot\underline{A})(\underline{\sigma}_1\wedge\underline{\sigma}_2\cdot\underline{B})\ .$$

b. The part which involves $\frac{\partial}{\partial \underline{r}'}$.

This is $$-\frac{1}{2i}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot(\underline{r}-\underline{r}')\wedge\frac{\partial}{\partial\underline{r}'}\,S_{13}(r_{13}^2)\ .$$

After integration by parts, the relevant function which has to be differentiated w.r.t $\underline{r}'$ is now $\exp.\left[-\alpha_i r_{23}^2-\mu r_{12}^2\right]$ and we get

$$\frac{1}{2i}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot(\underline{r}-\underline{r}')\,S_{13}(r_{13}^2)\wedge\frac{\partial}{\partial\underline{r}'}\,e^{-\alpha_i r_{23}^2-\mu r_{12}^2} = \frac{1}{2i}\cdot\frac{16}{3}\alpha_i(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{r}'\wedge\underline{r}\;S_{13}(r_{13}^2)\,e^{-\alpha_i r_{23}^2-\mu r_{12}^2}\ .$$

Carrying out the spin product, we have the result:

$$\left(\frac{3}{2}\right)^2(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{r}'\wedge\underline{r}\;S_{13}(r_{13}^2)$$

$$= \left\{4S_{13}(r^2)+4S_{13}(\underline{r},\underline{r}')+S_{13}(r'^2)\right\}\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r} - (4r^2+4\underline{r}\cdot\underline{r}'+r'^2)\,\underline{\sigma}_3\cdot\underline{r}'\wedge\underline{r} + i(4\underline{r}\cdot\underline{r}'+2r'^2)S_{13}(r^2)$$

$$-i(2r^2+\underline{r}\cdot\underline{r}')S_{13}(r'^2) - \frac{i}{3}(4r^2-2\underline{r}\cdot\underline{r}'-2r'^2)\mathcal{R}_{13}(\underline{r},\underline{r}') - \frac{i}{3}(8r^2+2\underline{r}\cdot\underline{r}'-2r'^2)\mathcal{R}_{13}(\underline{r}',\underline{r})\ .$$

The above two parts of the integral are now combined.

We thus obtain

$$I^{LS}_{S\cdot D}(r)$$

$$= -\left(\frac{4}{3}\right)^4\frac{M}{\hbar^2}\,\frac{1}{2}\left(\frac{2}{3}\right)^2 A_i A_j' {}^{LS}U_K^{(2)}\,r\int d\underline{r}'d\Omega\;e^{-ar^2-br'^2-d\underline{r}\cdot\underline{r}'}\,y^*(\Omega)\chi^*(1)\Big[\ \Big]^{LS}_{LS}\chi(2)y(\Omega')\frac{1}{r'}\mathcal{F}(r')\ ,$$

where the square bracket denotes the factor

$$\frac{16}{3}(\alpha_i+\alpha_j')\Big[\Big\{4S_{13}(r^2)+4S_{13}(\underline{r},\underline{r}')+S_{13}(r'^2)\Big\}\frac{1}{i}\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r}-(4r^2+4\underline{r}\cdot\underline{r}'+r'^2)\frac{1}{i}\underline{\sigma}_3\cdot\underline{r}'\wedge\underline{r}$$

$$+(4\underline{r}\cdot\underline{r}'+2r'^2)S_{13}(r^2)-(2r^2+\underline{r}\cdot\underline{r}')S_{13}(r'^2)$$

$$-\tfrac{1}{3}(4r^2-2\underline{r}\cdot\underline{r}'-2r'^2)R_{13}(\underline{r},\underline{r}')-\tfrac{1}{3}(8r^2+2\underline{r}\cdot\underline{r}'-\underline{r}'^2)R_{13}(\underline{r}',\underline{r})\Big]$$

$$+\frac{12}{i}\underline{\sigma}_3\cdot\underline{r}'\wedge\underline{r}+\frac{12}{i}\left[W(r^2)-W(\underline{r},\underline{r}')\right]+\frac{6}{i}\left[W(\underline{r}',\underline{r})-W(r^2)\right]$$

$$+\frac{30}{i}\underline{\sigma}_3\cdot\underline{r}'\wedge\underline{r}-12S_{13}(r^2)-2R_{13}(\underline{r},\underline{r}')+8R_{13}(\underline{r}',\underline{r})+6S_{13}(r'^2)\ .$$

Here again the spin simplification will be done in each case seperately.

IX.2.2. THE DOUBLET CASE

The following results are quoted for further use

$$\langle\bar{\chi}^{\frac{1}{2}}(1)\,|\,S_{13}(\underline{A},\underline{B})\,\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r}\,|\,\bar{\chi}^{\frac{1}{2}}(2,13)\rangle=-\frac{2}{3}\underline{A}\cdot\underline{B}\,\langle\tilde{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r}\,|\,\tilde{\chi}^{\frac{1}{2}}(1)\rangle$$

if vectors $\underline{A}$ and $\underline{B}$ are either $\underline{r}$ or $\underline{r}'$.

Further identitites are

$$\langle\bar{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_1\cdot\underline{A}\,(\underline{\sigma}_3\wedge\underline{\sigma}_2\cdot\underline{B})\,|\,\bar{\chi}^{\frac{1}{2}}(2,13)\rangle=\langle\tilde{\chi}^{\frac{1}{2}}(1)\,|\,i\,\underline{A}\cdot\underline{B}+\underline{\sigma}_1\cdot\underline{A}\wedge\underline{B}\,|\,\tilde{\chi}^{\frac{1}{2}}(1)\rangle\ ,$$

$$\langle\bar{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_3\cdot\underline{A}\,(\underline{\sigma}_1\wedge\underline{\sigma}_2\cdot\underline{B})\,|\,\bar{\chi}^{\frac{1}{2}}(2,13)\rangle=\langle\tilde{\chi}^{\frac{1}{2}}(1)\,|\,-i\,\underline{A}\cdot\underline{B}\,|\,\tilde{\chi}^{\frac{1}{2}}(1)\rangle\ .$$

Thus by the definition given in IX.2.1 (a) we have

$$\langle\bar{\chi}^{\frac{1}{2}}(1)\,|\,W(\underline{A},\underline{B})\,|\,\bar{\chi}^{\frac{1}{2}}(2,13)\rangle=\langle\tilde{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_1\cdot\underline{A}\wedge\underline{B}\,|\,\tilde{\chi}^{\frac{1}{2}}(1)\rangle\ .$$

It follows also that

$$\langle\bar{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_2\cdot\underline{r}'\wedge\underline{r}\,|\,\bar{\chi}^{\frac{1}{2}}(2,13)\rangle=\frac{1}{6}\langle\tilde{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r}\,|\,\tilde{\chi}^{\frac{1}{2}}(1)\rangle\ ,$$

$$\langle\bar{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_3\cdot\underline{r}'\wedge\underline{r}\,|\,\bar{\chi}^{\frac{1}{2}}(2,13)\rangle=-\frac{5}{6}\langle\tilde{\chi}^{\frac{1}{2}}(1)\,|\,\underline{\sigma}_1\cdot\underline{r}'\wedge\underline{r}\,|\,\tilde{\chi}^{\frac{1}{2}}(1)\rangle\ .$$

The term R_{13} gives no contribution in the doublet case.

We make use of the above results and simplify the spin products of $[\ ]_{LS}$ to give

$$\langle \chi^{-\frac{1}{2}}(1) | [\ ]_{LS} | \chi^{-\frac{1}{2}}(2) \rangle = \left[\tfrac{1}{2} w'_{ij}(4r^2+4\underline{r}\cdot\underline{r}'+r'^2)-5\right]\langle \tilde{\chi}^{\frac{1}{2}} | \tfrac{1}{i}\underline{\sigma}_i \underline{r}'_\wedge \underline{r} | \tilde{\chi}^{\frac{1}{2}}\rangle ,$$

where $$w'_{ij} = \frac{16}{9}(\alpha_i+\alpha'_j) .$$

Before the spherical harmonic integration may be performed it is convenient to transform the terms involving $\underline{\sigma}\cdot\underline{r}'_\wedge\underline{r}$ into the angular momentum operator $\underline{\sigma}\cdot\underline{L}_{r'}$ thus:

Consider the integral $$\int d\Omega\, d\Omega'\, e^{-\partial \underline{r}\cdot\underline{r}'} \langle (Ar^2+B\underline{r}\cdot\underline{r}'+Cr'^2)\tfrac{1}{i}\underline{\sigma}\cdot\underline{r}'_\wedge\underline{r}\rangle f(r') .$$

We have $\underline{r}'_\wedge\underline{r}\, e^{-\partial \underline{r}\cdot\underline{r}'} = -\frac{1}{\delta}\,\underline{r}'_\wedge\frac{\partial}{\partial \underline{r}'}\, e^{-\delta \underline{r}\cdot\underline{r}'}$ and on integration by parts we find that the integral is

$$\frac{1}{\delta}\int d\Omega\, d\Omega'\, e^{-\partial \underline{r}\cdot\underline{r}'} \langle (Ar^2+B\underline{r}\cdot\underline{r}'+Cr'^2)\,\underline{\sigma}\cdot\underline{L}_{r'} + \frac{B}{\delta}\,\underline{\sigma}\cdot\underline{L}_{r'}\rangle f(r')$$

which can be easily evaluated using the fact that

$$\int d\Omega\, d\Omega'\, e^{-\partial \underline{r}\cdot\underline{r}'}(\underline{r}\cdot\underline{r}')\langle \underline{\sigma}\cdot\underline{L}_{r'}\rangle f(r') = rr' p_\delta \int d\Omega\, d\Omega'\, e^{-\partial \underline{r}\cdot\underline{r}'}\langle \underline{\sigma}\cdot\underline{L}_{r'}\rangle f(r') .$$

Finally the indirect interaction of the spin-orbit force S-D terms is found to be

$$I^{LS}_{S\text{-}D}(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\left(\frac{2}{3}\right)^2 \frac{4\pi}{\delta^2} A_i A'_j\, {}^{LS}U^{(2)}_k \int dr'\, e^{-ar^2-br'^2} \times$$

$$\times \left[\frac{w'}{4}(4r^2+4rr'p_\delta+r'^2) + \frac{w'}{4\delta} - \frac{5}{2}\right]\left[3A_{J\ell}\right]\left[\mathcal{J}_{\ell+\frac{1}{2}}(\delta rr')\right] f(r') .$$

IX.2.3. THE QUARTET CASE

The spin products of the terms in the bracket $[\quad]_{LS}$ in IX.2.1 can be reduced to

$$\chi^{*3/2}\,[\quad]_{LS}\,\chi^{3/2}$$

$$= 3W'\Big[\Big\{4S_{13}(r'^2)+4S_{13}(\underline{r}.\underline{r}')+S_{13}(r^2)\Big\}\tfrac{1}{i}\underline{\sigma}_2.\underline{r}'\wedge\underline{r}-(4r^2+4\underline{r}.\underline{r}'+r'^2)\tfrac{1}{i}\underline{\sigma}_2.\underline{r}'\wedge\underline{r}$$

$$+(4\underline{r}.\underline{r}'+2r'^2)S_{13}(r'^2)-(4r^2-r'^2)S_{13}(\underline{r}.\underline{r}')-(2r^2+\underline{r}.\underline{r}')S_{13}(r^2)\Big]$$

$$+42\tfrac{1}{i}\underline{\sigma}_2.\underline{r}'\wedge\underline{r}\;-12S_{13}(r^2)+6S_{13}(\underline{r}.\underline{r}')+6S_{13}(r'^2)\,.$$

The terms $W(\underline{A},\underline{B})$ vanish due to spin symmetry.

Similar to the transformation of $\underline{\sigma}.\underline{r}'\wedge\underline{r}$ to $\underline{\sigma}.\underline{L}_{r'}$ given in IX.2.2 the following additional results are obtained.

$$\int d\Omega\,d\Omega'\,e^{-\partial\underline{r}.\underline{r}'}\langle S_{13}(A^2)\tfrac{1}{i}\underline{\sigma}_2.\underline{r}'\wedge\underline{r}\rangle f(r') \;=\; \frac{1}{\delta}\int d\Omega\,d\Omega'\,e^{-\partial\underline{r}.\underline{r}'}\langle S_{13}(A^2)\,\underline{\sigma}_2.\underline{L}_{r'}\rangle f(r')$$

and

$$\int d\Omega\,d\Omega'\,e^{-\partial\underline{r}.\underline{r}'}\langle S_{13}(\underline{r}.\underline{r}')\tfrac{1}{i}\underline{\sigma}_2.\underline{r}'\wedge\underline{r}\rangle f(r') \;=\; \frac{1}{\delta}\int d\Omega\,d\Omega'\,e^{-\partial\underline{r}.\underline{r}'}\langle S_{13}(\underline{r}.\underline{r}')\,\underline{\sigma}_2.\underline{L}_{r'}-\tfrac{1}{\delta}\underline{\sigma}_2.\underline{L}_{r'}\rangle f(r')\,.$$

The matrix elements of $S_{13}(\underline{A}^2)\,\underline{\sigma}_2.\underline{L}_{r'}$ for $\underline{A}=\underline{r}$ or $\underline{r}'$ can easily be dervied using Table 4 in IX.1.3 and the usual technique. They are given by

$$\int d\Omega\,d\Omega'\,e^{-\partial\underline{r}.\underline{r}'}\langle S_{13}(r^2)\,\underline{\sigma}_2.\underline{L}_{r'}\rangle \;=\; \frac{4\pi}{\partial r r'}\,r'^2\big[C_{Jl}\big]\big[\vartheta_{l+\frac{1}{2}}(\partial r r')\big] \qquad \ldots\ldots (9.2\text{ a})$$

and

$$\int d\Omega\,d\Omega'\,e^{-\partial\underline{r}.\underline{r}'}\langle S_{13}(r'^2)\,\underline{\sigma}_2.\underline{L}_{r'}\rangle \;=\; \frac{4\pi}{\partial r r'}\,r'^2\big[\vartheta_{l+\frac{1}{2}}(\partial r r')\big]\big[C_{Jl}\big] \qquad \ldots\ldots (9.2\text{ b})$$

where $[C_{Jl}]$ is defined in IX.1.3.

To evaluate the matrix elements of $S_{13}(\underline{r},\underline{r}')\,\underline{\sigma}_2\cdot\underline{L}_{r'}$, the spin products of the operator are needed and they are given in Table No. 5 below.

TABLE 5: THE SPIN PRODUCTS OF $S_{13}(\underline{r},\underline{r}')\,\underline{\sigma}_2\cdot\underline{L}_{r'}$.

	$\chi^{3/2}_{3/2}$	$\chi^{3/2}_{\frac{1}{2}}$	$\chi^{3/2}_{-\frac{1}{2}}$	$\chi^{3/2}_{-3/2}$
$\chi^{3/2}_{3/2}$	$(3zz'-\underline{r}\cdot\underline{r}')L_{z'}$	$2/\sqrt{3}$ $(3zz'-\underline{r}\cdot\underline{r}')L_{-}+3(zr_{-}'+r_{-}z')L_{z'}$	$4/\sqrt{3}$ $(zr_{-}'+r_{-}z')L_{-}+r_{-}r_{-}'L_{z}$	$24\,r_{-}r_{-}'L_{-}$
$\chi^{3/2}_{\frac{1}{2}}$	$2/\sqrt{3}$ $(3zz'-\underline{r}\cdot\underline{r}')L_{+}+3(zr_{+}'+r_{+}z')L_{z'}$	$(2\underline{r}\cdot\underline{r}'-5zz')L_{z'}$ $+(zr_{+}'+r_{+}z')L_{-}+4(zr_{-}'+r_{-}z')L_{+}$	$\frac{2}{3}(5\underline{r}\cdot\underline{r}'-12zz')L_{-}$ $12r_{-}r_{-}'L_{+}-6(r_{-}z'+zr_{-}')L_{z}$	$-4/\sqrt{3}$ $(zr_{-}'+r_{-}z')L_{-}+r_{-}r_{-}'L_{z}$
$\chi^{3/2}_{-\frac{1}{2}}$	$4/\sqrt{3}$ $(zr_{+}'+r_{+}z')L_{+}+r_{+}r_{+}'L_{z}$	$\frac{2}{3}(5\underline{r}\cdot\underline{r}'-12zz')L_{+}$ $12r_{+}r_{-}'L_{-}-6(r_{+}z'+zr_{+}')L_{z}$	$(5zz'-2\underline{r}\cdot\underline{r}')L_{z'}$ $+4(zr_{+}'+r_{+}z')L_{-}-4(zr_{-}'+r_{-}z')L_{+}$	$2/\sqrt{3}$ $(3zz'-\underline{r}\cdot\underline{r}')L_{+}+3(zr_{+}'+r_{+}z')L_{z'}$
$\chi^{3/2}_{-3/2}$	$24\,r_{+}r_{+}'L_{+}$	$-4/\sqrt{3}$ $(zr_{+}'+r_{+}z')L_{+}+r_{+}r_{+}'L_{z}$	$2/\sqrt{3}$ $(3zz'-\underline{r}\cdot\underline{r}')L_{+}+3(zr_{+}'+zr_{+}')L_{z'}$	$-(3zz'-\underline{r}\cdot\underline{r}')L_{z'}$

For the spherical harmonic integration the integrand again is a sum of products of three spherical harmonics. Finally we obtain

$$\int d\Omega\, d\Omega'\; e^{-\partial\,\underline{r}\cdot\underline{r}'} \langle S_{13}(\underline{r},\underline{r}')\,\underline{\sigma}_2\cdot\underline{L}_{r'}\rangle = \frac{4\pi}{\partial r r'}\, rr' \left[Q_{J[}\, \vartheta_{[+\frac{1}{2}}(\partial r r') \right]$$

where for $J \geq 3/2$, $\left[Q_{J[}\, \vartheta_{[+\frac{1}{2}}(\partial r r') \right]$

$$= \begin{pmatrix} -\frac{(2J-3)^2}{4J}\vartheta_{J-1} & 0 & \frac{2J-3}{4J}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}}\vartheta_{J} & 0 \\ 0 & \frac{20J^2+4J-43}{12(J+1)}\vartheta_{J} & 0 & -\frac{2J+5}{4J+4}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}}\vartheta_{J+1} \\ \frac{2J-3}{4J}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}}\vartheta_{J} & 0 & \frac{-20J^2-36J+27}{12J}\vartheta_{J+1} & 0 \\ 0 & -\frac{2J+5}{4J+4}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}}\vartheta_{J+1} & 0 & \frac{(2J+5)^2}{4(J+1)}\vartheta_{J+2} \end{pmatrix},$$

and for $J = \frac{1}{2}$,

$$\left[Q_{J\ell}\, \vartheta_{\ell+\frac{1}{2}}(\partial r r') \right] = \begin{bmatrix} \frac{-20J^2-36J+27}{12J}\,\vartheta_{J+1} \\ \frac{(2J+5)^2}{4(J+1)}\,\vartheta_{J+2} \end{bmatrix}$$

Using the foregoing results we obtain the integral for the indirect interaction thus:

$$\underset{S\text{-}D}{\overset{LS}{I}}(r) = -\left(\frac{4}{5}\right)^4 \frac{M}{\hbar^2}\left(\frac{2}{3}\right)^2 \frac{4\pi}{\delta} A_i A_j {}^{LS}U_k^{(2)} \int dr'\, e^{-ar^2-br'^2} \left[\quad\right]_{LS} \mathcal{F}(r')$$

where the terms in the bracket are given by

$$\begin{aligned}
\left[\quad\right]_{LS} = {} & \left[-\tfrac{3}{2}\frac{w'}{\delta}(4r^2+4rr'\beta_\delta+r'^2) - \frac{6w}{\delta^2} + \frac{21}{\delta}\right]\left[\tfrac{1}{2}A_{J\ell}\right]\left[\vartheta_{\ell+\frac{1}{2}}(\partial r r')\right] \\
& + \left[\tfrac{3}{2}w(4rr'\beta_\delta+2r'^2) - 6\right] r^2 \left[B_{J\ell}\right]\left[\vartheta_{\ell+\frac{1}{2}}(\partial r r')\right] \\
& + \left[-\tfrac{3}{2}w(2r^2+rr'\beta_\delta)+3\right] r'^2 \left[\vartheta_{\ell+\frac{1}{2}}\right]\left[B_{J\ell}\right] \\
& + \left[-\tfrac{3}{2}w(4r^2-r'^2)+3\right] rr' \left[P_{J\ell}\,\vartheta_{\ell+\frac{1}{2}}(\partial r r')\right] \\
& + \frac{6w}{\delta} r^2 \left[C_{J\ell}\right]\left[\vartheta_{\ell+\frac{1}{2}}(\partial r r')\right] + \tfrac{3}{2}\frac{w}{\delta} r'^2 \left[\vartheta_{\ell+\frac{1}{2}}(\partial r r')\right]\left[C_{J\ell}\right] \\
& + \frac{6w}{\delta}\left\{ rr' \left[Q_{J\ell}\,\vartheta_{\ell+\frac{1}{2}}(\partial r r')\right] - \frac{1}{\delta}\left[\tfrac{1}{2}A_{J\ell}\right]\left[\vartheta_{\ell+\frac{1}{2}}(\partial r r')\right] \right\} .
\end{aligned}$$

IX.3 REMARK

The spin-orbit force S-D terms do not add complexity to the integro-differential equations which has already been created by the inclusion of the quadratic spin-orbit forces. It is obvious that a new type of operators of the form $S_{23}(A^2)\,\underline{\sigma}_1 \cdot \underline{L}_B$ should occur in the integrals of both the direct and indirect interaction, but the evaluation of its matrix elements offers no difficulty. The direct interaction gives rise to a term involving the first derivative of the

radial function $f(r)$. However this term vanishes after the symmetrisation of the spin-orbit operator (Chapter XII).

CHAPTER X

THE TENSOR FORCE S-D TERMS

X.1. SPIN SIMPLIFICATION

The operator in the tensor force S-D terms occurs in the form of a double tensor operator . When applied to the three-body wave function it can be reduced to simple form.

X.1.1. THE DOUBLET CASE

In the direct and indirect interactions the spin matrix elements have the forms

$$\langle \chi^{\frac{1}{2}}(1) \mid S_{12}(\underline{A}^2) S_{23}(\underline{B}^2) \mid \chi^{\frac{1}{2}}(1) \rangle$$

and $$\langle \chi^{\frac{1}{2}}(1) \mid S_{12}(\underline{A}^2) S_{13}(\underline{B}^2) \mid \chi^{\frac{1}{2}}(2) \rangle \ .$$

These two matrices are the same, for if 1 and 2 are interchanged in one of them the matrices are equal provided

$$S_{12}(\underline{A}^2)\, \chi^{\frac{1}{2}}(1,\overline{23}) \equiv S_{12}(\underline{A}^2) \chi^{\frac{1}{2}}(2,\overline{13}) \quad \text{which is the case.}$$

By transforming the symmetrical doublet spin functions $\overline{\chi}^{\frac{1}{2}}$ into the antisymmetrical $\widetilde{\chi}^{\frac{1}{2}}$ as given in Appendix 3 then performing the spin products, the matrix elements are reduced to

$$\langle \overline{\chi}^{\frac{1}{2}}(1) \mid S_{12}(\underline{A}^2) S_{23}(\underline{B}^2) \mid \overline{\chi}^{\frac{1}{2}}(1) \rangle = \langle \widetilde{\chi}^{\frac{1}{2}}(1) \mid 2A^2B^2 - 6(\underline{A}\cdot\underline{B})^2 - 6i(\underline{A}\cdot\underline{B})(\underline{\sigma}_1 \underline{A} \underline{B}) \mid \widetilde{\chi}^{\frac{1}{2}}(1) \rangle \ .$$

X.1.2. THE QUARTET CASE

Because of the summetry of the spin function the matrix elements assume the form $\langle \chi^{3/2} \mid S_{12}(\underline{A}^2) S_{23}(\underline{B}^2) \mid \chi^{3/2} \rangle$ which can

be reduced to

$$\langle \chi^{3/2} | -A^2B^2 + 3(\underline{A}\cdot\underline{B})^2 + 3i(\underline{\sigma}_i \underline{A}\wedge\underline{B})(\underline{A}\cdot\underline{B}) - B^2 S_{23}(A^2) - A^2 S_{23}(B^2)$$
$$+ 3(\underline{A}\cdot\underline{B}) S_{23}(\underline{A},\underline{B}) + 3i(\underline{\sigma}_i \underline{A}\wedge\underline{B}) S_{23}(\underline{A},\underline{B}) | \chi^{3/2} \rangle \quad .$$

X.2. THE DIRECT INTERACTION

The tensor force S-D terms for both doublet and quartet cases are given by $T^{D}_{S\text{-}D}(T)$

$$= \frac{4}{3}\frac{M}{R^2} \int d\underline{R}\, d\Omega\, \psi^*(\Omega)\chi^*(1)\, \phi_S(23) \sum_\nu \tfrac{1}{4}(2w-h+2b-m)^\nu V_T(12)\, T(23)\, \phi_D(23)\, \chi(1)\psi(\Omega)\, \mathcal{F}^0(1).$$

Again the potential is the same as in the S-S terms given in section V.1. To evaluate the integral we put $\underline{A} = \underline{r}_{12} = \underline{r} - \frac{1}{2}\underline{R}$, and $\underline{B} = \underline{r}_{23} = \underline{R}$ in the operator identities quoted in sections X.1.1 and X.1.2. We consider the doublet and quartet cases seperately.

X.2.1. THE DOUBLET CASE

We perform the spin reduction and obtain for the matrix elements

$$\langle \bar{\chi}^{\frac{1}{2}} | S_{12}(r_{12}^2) S_{23}(r_{23}^2) | \bar{\chi}^{\frac{1}{2}} \rangle = \langle \tilde{\chi}^{\frac{1}{2}} | 2r^2R^2 - 6(\underline{r}\cdot\underline{R})^2 + 4(\underline{r}\cdot\underline{R})R^2 - R^4 + 6i(\underline{r}\cdot\underline{R} - \tfrac{1}{2}R^2)\, \underline{\sigma}_i \underline{I}_\wedge \underline{R} | \tilde{\chi}^{\frac{1}{2}} \rangle .$$

For the $d\underline{R}$ integration the various formulae given in Appendix 4 are used. After this integration (omitting exponential factors) we get

$$\left(\frac{\pi}{\lambda}\right)^{3/2} \langle \tilde{\chi}^{\frac{1}{2}} | 2(\gamma^2 r^4 + \tfrac{3}{2\lambda} r^2) - 6(\gamma^2 r^4 + \tfrac{1}{2\lambda} r^2) + 4(\gamma^3 r^4 + \tfrac{5}{2\lambda}\gamma r^2) - (\gamma^4 r^4 + \tfrac{5}{\lambda}\gamma^2 r^2 + \tfrac{15}{4\lambda^2}) | \tilde{\chi}^{\frac{1}{2}} \rangle$$
$$= \left(\frac{\pi}{\lambda}\right)^{3/2} \left[-\frac{15}{4\lambda^2} + \frac{10\gamma}{\lambda}\left(1-\tfrac{\gamma}{2}\right) r^2 - 4\gamma^2\left(1-\tfrac{\gamma}{2}\right)^2 r^4 \right] [\delta] \quad .$$

On integrating over $d\underline{R}$ we find that the term $(\underline{\sigma}_i \underline{I}_\wedge \underline{R})(\underline{r}\cdot\underline{R} - \frac{1}{2}R^2)$ is proportion to $\underline{\sigma}_i \cdot \underline{I}_\wedge \underline{r}$ and so it vanishes.

Hence it follows finally that

$$ {}^{T}_{S\text{-}D}D(r) = \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} A_i A_j' {}^{T}U^{(1)}_{K}\, e^{-(\mu-\lambda\gamma^2)r^2}\left[-\frac{15}{4\lambda^2}+\frac{10\gamma}{\lambda}\left(1-\frac{\gamma}{2}\right)r^2-4\gamma^2\left(1-\frac{\gamma}{2}\right)^2 r^4\right] \mathcal{F}^{e}(r). $$

X.2.2. THE QUARTET CASE

Following the procedure given in section X.2.1 we have the spin product identity:

$$ \langle \chi^{3/2} | S_{12}(r_{12}^2)\, S_{23}(r_{23}^2) | \chi^{3/2} \rangle $$

$$ = \langle \chi^{3/2} | -r^2R^2+3(\underline{r}\cdot\underline{R})^2-2(\underline{r}\cdot\underline{R})R^2+\tfrac{1}{2}R^4+3i(\underline{r}\cdot\underline{R}-\tfrac{1}{2}R^2)\,\underline{\sigma}_1\cdot\underline{r}\wedge\underline{R}-R^2S_{23}(r^2)+(3\underline{r}\cdot\underline{R}-\tfrac{1}{2}R^2)S_{23}(\underline{r},\underline{R}) $$

$$ -\left(r^2+\tfrac{1}{2}\underline{r}\cdot\underline{R}-\tfrac{1}{4}R^2\right)S_{23}(R^2)+3i\,\underline{\sigma}_1\cdot\underline{r}\wedge\underline{R}\left\{S_{23}(\underline{r},\underline{R})-\tfrac{1}{2}S_{23}(R^2)\right\} | \chi^{3/2} \rangle . $$

These terms, after $d\underline{R}$ integration, will become

$$ \left(\frac{\pi}{\lambda}\right)^{3/2} \langle \chi^{3/2} | \frac{15}{8\lambda^2}-\frac{5\gamma}{\lambda}\left(1-\frac{\gamma}{2}\right)r^2+2\gamma^2\left(1-\frac{\gamma}{2}\right)^2 r^4+\left[-\frac{7}{4}\frac{\gamma}{\lambda}\left(1-\frac{\gamma}{2}\right)+\gamma^2\left(1-\frac{\gamma}{2}\right)^2 r^2\right] S_{23}(r^2) | \chi^{3/2} \rangle . $$

Therefore we get the result

$$ {}^{T}_{S\text{-}D}D(r) = \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} A_i A_j' {}^{T}U^{(1)}_{K}\, e^{-(\mu-\lambda\gamma^2)r^2} \times $$

$$ \times\left\{\frac{15}{8\lambda^2}-\frac{5\gamma}{\lambda}\left(1-\frac{\gamma}{2}\right)r^2+2\gamma^2\left(1-\frac{\gamma}{2}\right)^2 r^4+\left[-\frac{7}{4}\frac{\gamma}{\lambda}\left(1-\frac{\gamma}{2}\right)+\gamma^2\left(1-\frac{\gamma}{2}\right)^2 r^2\right] r^2\left[B_{Jl}\right]\right\} \mathcal{F}^{e}(r). $$

X.3 THE INDIRECT INTERACTION

The integrals are given by

$$ {}^{T}_{S\text{-}D}I(r) $$

$$ = -\left(\frac{4}{3}\right)^{\dagger}\frac{M}{\hbar^2} r \int d\underline{r}'d\Omega\, y^{*}(\Omega)\chi^{*}(1)\,\phi_S(23)\sum_{\nu}\tfrac{1}{4}(w-2h+b-2m)_{\nu}\, {}^{\nu}_{T}V(12)\,T(13)\,\phi_D(13)\,\chi(2)\,y(\Omega')\,\tfrac{1}{r'}\,\mathcal{F}^{e}(r'). $$

X.3.1. THE DOUBLET CASE

Substituting for $\underline{A} = \underline{r}_{12} = \frac{2}{3}(\underline{r}-\underline{r}')$

and $\underline{B} = \underline{r}_{13} = \frac{2}{3}(2\underline{r}+\underline{r}')$ in the matrix elements

quoted in section X.1.1. we have the spin products

$$\left(\tfrac{3}{2}\right)^4 \langle \bar{\chi}^{\frac{1}{2}}(1) \mid S_{12}(r_{12}^2)\, S_{13}(r_{13}^2) \mid \bar{\chi}^{\frac{1}{2}}(2)\rangle$$

$$= \langle \tilde{\chi}^{\frac{1}{2}}(1) \mid -16r^4+34r^2r'^2-4r'^4+(16r^2-8r'^2)(\underline{r}\cdot\underline{r}')-22(\underline{r}\cdot\underline{r}')^2+18(-2r^2+\underline{r}\cdot\underline{r}'+r'^2)\tfrac{1}{i}(\underline{\sigma}_1\underline{r}'\wedge\underline{r}) \mid \tilde{\chi}^{\frac{1}{2}}(1)\rangle .$$

For the spherical harmonic integration we quote the result

$$\int d\Omega\, d\Omega'\; e^{-\partial\underline{r}\cdot\underline{r}'}\, Y^*_{lm}(\theta,\varphi)\,(\underline{r}\cdot\underline{r}')^n\, Y_{l'm'}(\theta'\varphi') = \delta_{ll'}\delta_{mm'}\frac{4\pi}{\partial r r'}(rr')^n\, p_\partial^{(n)}\, \vartheta_{l+\frac{1}{2}}(\partial r r') ,$$

~~from equation (6.7)~~ of section VI.3.1.

Thus the indirect interaction of the tensor force S-D terms is given by

$$I^{T}_{S\text{-}D}(r) = -\left(\tfrac{4}{3}\right)\frac{M}{\hbar^2}\left(\tfrac{2}{3}\right)^4\frac{4\pi}{\partial}A_i A'_j\, U^{T(2)}_k \int dr'\, e^{-ar^2-br'^2}\, [\;\;]_T\, \mathcal{F}^T(r')$$

where the terms in the bracket $[\;\;]_T$ are given by

$$[\;\;]_T = \left[(-16r'^4+34r^2r'^2-4r'^4)+(16r^2-8r'^2)rr'p_\partial-22r^2r'^2p_\partial^{(2)}\right]\left[\vartheta_{l+\frac{1}{2}}(\partial rr')\right]$$
$$+\left[\tfrac{18}{\partial}(-2r^2+rr'p_\partial+r'^2)+\tfrac{18}{\partial^2}\right]\left[3A_{jk}\right]\left[\vartheta_{l+\frac{1}{2}}(\partial rr')\right] .$$

X.3.2. THE QUARTET CASE

The spin products of the operator are given by

$$\left(\tfrac{3}{2}\right)^4 \langle \chi^{3/2} \mid S_{12}(r_{12}^2)\, S_{13}(r_{13}^2) \mid \chi^{3/2}\rangle$$

$$= \langle \chi^{3/2} \mid (8r^4-17r^2r'^2+2r'^4)-(8r^2-4r'^2)\underline{r}\cdot\underline{r}'+11(\underline{r}\cdot\underline{r}')+9(2r^2-\underline{r}\cdot\underline{r}'-r'^2)\tfrac{1}{i}\underline{\sigma}_2\underline{r}'\wedge\underline{r}+(4r^2-2\underline{r}\cdot\underline{r}'+11r'^2)S_{13}(r^2)$$
$$+(-2r^2+19\,\underline{r}\cdot\underline{r}'+r'^2)S_{13}(\underline{r},\underline{r}')+(-11r^2+\underline{r}\cdot\underline{r}'+r'^2)S_{13}(r'^2)+9\{2S_{13}(r^2)-S_{13}(\underline{r},\underline{r}')-S_{13}(r'^2)\}\tfrac{1}{i}\underline{\sigma}_2\underline{r}'\wedge\underline{r} \mid \chi^{3/2}\rangle .$$

The matrix elements of each of the above terms have already been evaluated

Therefore we can write down the indirect interaction in the quartet case as

$$ {}^{T}_{S=D}I(r) = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\left(\frac{2}{3}\right)^4 \frac{4\pi}{\delta} A_i A_j' \, {}^{T}U_k^{(2)} \int dr' \, e^{-ar^2-br'^2} \Big[\quad\Big]_T \mathcal{G}^{T}(r') $$

Where the terms in the bracket $\Big[\quad\Big]_T$ are given by

$$ \begin{aligned} \Big[\quad\Big]_T = {} & \left[(8r^4-17r^2r'^2+2r'^4)-(8r^2-4rr'+r'^2)\rho_\delta+11r^2r'^2\rho_\delta^{(2)}\right]\left[\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right] \\ & +\left[\frac{9}{\delta}(2r^2-rr'\rho_\delta-r'^2)+\frac{9}{\delta^2}\right]\frac{1}{2}\left[A_{JL}\right]\left[\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right] \\ & +(4r^2-2rr'\rho_\delta+11r'^2)\,r^2\left[B_{JL}\right]\left[\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right]+(-11r^2+rr'\rho_\delta+r'^2)\,r'^2\left[\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right]\left[B_{JL}\right] \\ & +(-2r^2+19rr'\rho_\delta+r'^2)\,rr'\left[P_{JL}\,\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right] \\ & +\frac{18}{\delta}r^2\left[C_{JL}\right]\left[\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right]-\frac{9}{\delta}r^2\left[\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right]\left[C_{JL}\right] \\ & -\frac{9}{\delta}rr'\left[Q_{JL}\,\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right]+\frac{9}{\delta^2}\left[\frac{1}{2}A_{JL}\right]\left[\mathcal{J}_{L+\frac{1}{2}}(\delta rr')\right] . \end{aligned} $$

CHAPTER XI

THE ENERGY S-D TERMS

XI.1. THE N-KERNELS

The energy dependent integrals are given by

$$N^{(1)}_{S\text{-}D} = (E_n - E_d)\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} r \int d\underline{r}' d\Omega \, \mathcal{Y}^*(\Omega) \chi^*(1) \phi_S(23) T(13) \phi_D(13) \chi(2) \mathcal{Y}(\Omega') \frac{1}{r'} F_e(r')$$

$$= (E_n - E_d)\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} A_i A_j' r \int d\underline{r}' d\Omega \, e^{-e'r^2 - f'r'^2 - w'\underline{r}\cdot\underline{r}'} \mathcal{Y}^*(\Omega) \chi^*(1) S_{13}(r_{13}^2) \chi(2) \mathcal{Y}(\Omega') \frac{1}{r'} F_e(r')$$

where $e'_{ij} = \frac{4}{9}(\alpha_i + 4\alpha_j')$,

$f'_{ij} = \frac{4}{9}(4\alpha_i + \alpha_j')$,

and $w'_{ij} = \frac{4}{9}(4\alpha_i + 4\alpha_j')$.

It is obvious that here is no contribution to the N-Kernel in the doublet case because of the tensor operator.

Hence the results of section V.2. we may write the integral for the quartet case as follows

$$N^{(1)}_{S\text{-}D} = (E_n - E_d)\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} \frac{4\pi}{w'} A_i A_j' \left(\frac{2}{3}\right)^2 \int dr' \, e^{-er^2 - fr'^2} \left[\ \right]_N F_e(r')$$

where $\left[\ \right]_N = 4r^2 \left[B_{J\ell}\right]\left[\mathcal{I}_{\ell+\frac{1}{2}}(w'rr')\right] + 4rr'\left[P_{J\ell}\mathcal{I}_{\ell+\frac{1}{2}}(w'rr')\right] + r'^2\left[\mathcal{I}_{\ell+\frac{1}{2}}(w'rr')\right]\left[B_{J\ell}\right]$.

XI.2 THE KINETIC ENERGY KERNELS

As in the N-Kernel the kinetic energy S-D terms are in the quartet case only.

We repeat the argument used in XII.2 and seperate the kinetic energy kernels into four components.

XI.2.1. THE KERNELS $P^{(1)}_{S\text{-}D}(r)$

Put $$P^{(1)}_{S\text{-}D}(r) = \tfrac{1}{2}\left[P^{'(1)}_{S\text{-}D}(r) + P^{''(1)}_{S\text{-}D}(r) \right]$$

where $$P^{'(1)}_{S\text{-}D}(r) = \left(\tfrac{4}{3}\right)^3 r \int d\underline{r}' d\Omega\, y^*(\Omega) x^*(1) \left[\nabla^2_{r'} \phi_S(23) T(13) \phi_D(13) \right] \chi(2) y(\Omega') \tfrac{1}{r'} \mathcal{H}(1')$$

$$P^{''(2)}_{S\text{-}D}(r) = \left(\tfrac{4}{3}\right)^3 r \int d\underline{r}' d\Omega\, y^*(\Omega) x^*(1) \left[\nabla^2_{r} \phi_S(23) T(13) \phi_D(13) \right] \chi(2) y(\Omega') \tfrac{1}{r'} \mathcal{H}(1').$$

The analytic forms of ϕ_S and ϕ_D are given by

$$\phi_S(23) = A_i \exp.[-\alpha_i r_{23}^2]$$

$$T(13)\phi_D(13) = A_j' S_{13}(r_{13}^2) \exp.[-\alpha_j' r_{13}^2] .$$

We also have $$\nabla^2_r uv = v\nabla^2_r u + 2\nabla_r u \cdot \nabla_r v + u \nabla^2_r v ,$$

and so we need the following results:

$$\nabla_{23} \phi_S(23) = -2\alpha_i \underline{r}_{23} A_i e^{-\alpha_i r_{23}^2} ,$$

$$\nabla^2_{23} \phi_S(23) = (4\alpha_i^2 r_{23}^2 - 6\alpha_i) A_i e^{-\alpha_i r_{23}^2} ,$$

$$\nabla_{13} T(13)\phi_D(13) = \left[-2\alpha_j' \underline{r}_{13} S_{13}(r_{13}^2) + 3(\underline{\sigma}_3 \underline{I}_{13})\underline{\sigma}_1 + 3(\underline{\sigma}_1 \underline{I}_{13})\underline{\sigma}_3 - 2(\underline{\sigma}_1 \underline{\sigma}_3)\underline{r}_{13}\right] A_j' e^{-\alpha_j' r_{13}^2} ,$$

$$\nabla^2_{13} T(13)\phi_D(13) = (4\alpha_j'^2 r_{13}^2 - 14\alpha_j') S_{13}(r_{13}^2) e^{-\alpha_j' r_{13}^2} .$$

From these we can derive the results

$$\tfrac{1}{2}(\nabla^2_{r'} + \nabla^2_r)\, \phi_S(23) T(13) \phi_D(13)$$

$$= \left[(10\alpha_i^2 r_{23}^2 + 10\alpha_j'^2 r_{13}^2 + 16\alpha_i\alpha_j' \underline{r}_{23}\underline{I}_{13} - 15\alpha_i - 35\alpha_j') S_{13}(r_{13}^2) - 16\alpha_i S_{13}(\underline{r}_{23}, \underline{I}_{13})\right] A_i A_j' e^{-\alpha_i r_{23}^2 - \alpha_j' r_{13}^2} .$$

Hence we obtain finally

$$P^{(1)}_{S\text{-}D}(r) = \left(\frac{4}{3}\right)^3\left(\frac{2}{3}\right)^2 A_i A_j' \, r \int d\underline{r}' d\Omega \, e^{-\alpha_i r_{23}^2 - \alpha_j' r_{13}^2} y^*(\Omega) x^*(1) \left[\ \right]_{P_1} \chi(2) y(\Omega') \perp_{r'} F(r')$$

where the terms in the square bracket are given by

$$\left[\ \right]_{P_1}$$

$$= \left(10\alpha_i^2 r_{23}^2 + 10\alpha_j'^2 r_{13}^2 + 16\alpha_i\alpha_j' I_{23} I_{13} - 15\alpha_i - 35\alpha_j'\right) S_{13}(r_{13}^2) - 16\alpha_i S_{13}(I_{23}, I_{13}) .$$

XI.2.2 THE KERNELS $P^{(2)}_{S\text{-}D}(r)$

By definition of $P^{(2)}_{S\text{-}D}(r)$ we may put

$$P^{(2)}_{S\text{-}D}(r) = \frac{1}{2}\left[P^{'(2)}_{S\text{-}D}(r) + P^{''(2)}_{S\text{-}D}(r)\right]$$

where

$$P^{'(2)}_{S\text{-}D}(r) = -\left(\frac{4}{3}\right)^4 r \int d\underline{r}' d\Omega \, y^*(\Omega) x^*(1) \left[\nabla^2_{23} \phi_S(23)\right] T(13) \phi_D(13) \chi(2) y(\Omega') \perp_{r'} F(r')$$

and

$$P^{''(2)}_{S\text{-}D}(r) = -\left(\frac{4}{3}\right)^4 r \int d\underline{r}' d\Omega \, y^*(\Omega) x^*(1) \, \phi_S(23) \left[\nabla^2_{13} T(13) \phi_D(13)\right] \chi(2) y(\Omega') \perp_{r'} F(r') .$$

Using the results of section XI.2.1 we get finally

$$P^{(2)}_{S\text{-}D}(r) = -\left(\frac{4}{3}\right)^4 A_i A_j' \, r \int d\underline{r}' d\Omega \, e^{-\alpha_i r_{23}^2 - \alpha_j' r_{13}^2} y^*(\Omega) x^*(1) \left[\ \right]_{P_2} \chi(2) y(\Omega') \perp_{r'} F(r')$$

where $\left[\ \right]_{P_2} = \left(2\alpha_i^2 r_{23}^2 + 2\alpha_j'^2 r_{13}^2 - 3\alpha_i - 7\alpha_j'\right) S_{13}(r_{13}^2)$.

XI.2.3 THE TOTAL KERNEL

Combining the two kernels given in XI.2.1 we obtain

$$P_{S\text{-}D}(r)$$

$$= \left(\frac{2}{3}\right)^2\left(\frac{4}{3}\right)^3 A_i A_j' r \int d\underline{r}' d\Omega \, e^{-\alpha_i r_{23}^2 - \alpha_j' r_{13}^2} y^*(\Omega) x^*(1) \left[\ \right]_P \chi(2) y(\Omega') \perp_{r'} F(r') ,$$

with the square bracket defined by

$$\begin{aligned}
\Big[\quad\Big]_P &= (4\alpha_i^2 T_{23}^2 + 4\alpha_j'^2 T_{13}^2 + 16\alpha_i\alpha_j' T_{23}\cdot T_{13} - 6\alpha_i - 14\alpha_j')S_{13}(r_{13}^2) - 16\alpha_i S_{13}(T_{23}, T_{13}) \\
&= \left(\frac{2}{3}\right)^2\Big[\left\{\frac{16}{9}\phi' r^2 + \frac{16}{9}\psi' r'^2 + \frac{64}{9}\chi' \underline{r}\cdot\underline{r}' - 6\alpha_i - 14\alpha_j'\right\}\left\{4S_{13}(r^2) + 4S_{13}(T,T') + S_{13}(r'^2)\right\} \\
&\qquad -16\alpha_i\left\{2S_{13}(r^2) + 5S_{13}(T,T') + 2S_{13}(r'^2)\right\}\Big]
\end{aligned}$$

where
$$\phi'_{ij} = \alpha_i^2 + 8\alpha_i\alpha_j' + 4\alpha_j'^2$$
$$\psi'_{ij} = 4\alpha_i^2 + 8\alpha_i\alpha_j' + \alpha_j'^2$$
and
$$\chi'_{ij} = \alpha_i^2 + 5\alpha_i\alpha_j + \alpha_j'^2 .$$

The matrix elements of the various terms are then worked out, and the expression obtained for the kinetic energy kernel is finally

$$P_{S\cdot D}(r) = \left(\frac{4}{3}\right)^3\left(\frac{2}{5}\right)^4 A_i A_j' \frac{4\pi}{w'}\int d\underline{r}'\, e^{-e'r^2 - f'r'^2}\Big[\quad\Big]_P \mathcal{F}^0(r') ,$$

where the terms in the square bracket are given by

$$\begin{aligned}
\Big[\quad\Big]_P &= \Big[\left(\frac{64}{9}\phi r^2 + \frac{64}{9}\psi r'^2 + \frac{256}{9}\chi rr' p_w\right) - 56\alpha_i - 58\alpha_j'\Big]\Big[B_{J\ell}\Big]\Big[\mathcal{I}_{\ell+\frac{1}{2}}(wrr')\Big] \\
&\quad + \Big[\left(\frac{16}{9}\phi r^2 + \frac{16}{9}\psi r'^2 + \frac{64}{9}\chi(rr') p_w\right) - 38\alpha_i - 14\alpha_j'\Big]\Big[\mathcal{I}_{\ell+\frac{1}{2}}(wrr')\Big]\Big[B_{J\ell}\Big] \\
&\quad + \Big[\left(\frac{64}{9}\phi r^2 + \frac{64}{9}\psi r'^2 + \frac{256}{9}\chi(rr' p_w\right) - 104\alpha_i - 56\alpha_j'\Big]\Big[P_{J\ell}\,\mathcal{I}_{\ell+\frac{1}{2}}(wrr')\Big] .
\end{aligned}$$

CHAPTER XII

THE D-S TERMS AND THE SYMMETRISATION OF THE SPIN-ORBIT TERMS

XII.1 THE D-S TERMS.

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 deuteron D-state wave function are in reverse order. Since these operators are Hermitian the results have exactly the same form as those of the S-D terms with only the suffices i and j interchanged, and in addition, r and r' in the kernels of the indirect interactions interchanged.

As an example we consider the tensor force terms. The D-S direct interaction is given by $^{T}_{D\text{-}S}D(r)$

$$= \frac{4}{3}\frac{M}{\hbar^2}\int d\underline{R}\,d\Omega\left[T(23)\,\phi_D(23)\,\chi(1)\,y(\Omega)\right]^*\sum_{\nu}\frac{1}{4}(2w-h+2b-m)_{\nu}\,{}^{\nu}_{T}V(12)\,\phi_S(23)\,\chi(1)\,y(\Omega)\,\mathcal{F}(r)$$

$$= \frac{4}{3}\frac{M}{\hbar^2}A_i'A_j\,{}^{T}U_K^{(1)}\,e^{-(\mu-\lambda\gamma^2)r^2}\int d\underline{R}\,d\Omega\,e^{-\lambda(\underline{R}-\gamma\underline{r})^2}\,y^*(\Omega)\,\chi^*(1)\,S_{23}(r_{23}^2)\,S_{13}(r_{12}^2)\,\chi(1)\,y(\Omega)\,\mathcal{F}(r)$$

where the parameters λ and γ in the D-S term calculations are given by

$$\lambda = \lambda''_{ijk} = \alpha_i'+\alpha_j+\tfrac{1}{4}\mu_k = \lambda'_{jik}\,,$$

$$\gamma = \gamma''_{ijk} = \tfrac{1}{2}\mu_k/\lambda''_{ijk} = \gamma'_{jik}\,.$$

The corresponding direct interaction in the doublet case gives

$$^{T}_{D\text{-}S}D(r)$$

$$= \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2}A_i'A_j\,{}^{T}U_K^{(1)}\,e^{-(\mu-\lambda\gamma^2)r^2}\left[-\frac{15}{4\lambda^2}+\frac{10\gamma}{\lambda}\left(1-\frac{\gamma}{2}\right)r^2-4\gamma^2\left(1-\frac{\gamma}{2}\right)^2r^4\right]\mathcal{F}(r)\,,$$

where λ and γ are defined as before in terms of double primed symbols.

Similarly the indirect interaction of the tensor force D-S terms, in the doublet case may be written as

$$ {}^{T}I^{(1)}_{D\text{-}S} = -\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2}\left(\frac{2}{3}\right)^4 \frac{4\pi}{\delta} A_i' A_j \, {}^{T}U_K^{(2)} \int dr' \, e^{-br^2-ar'^2} \; [\;\;]_T \; \mathcal{F}(r') $$

where the terms in the square bracket are given by

$$ [\;\;]_T = \left[(-4r^4+34r^2r'^2-16r'^4)+(-8r^2+16r'^2)\,rr'\mathcal{P}_\delta - 22r^2r'^2\mathcal{P}_\delta^{(2)}\right]\left[\mathcal{I}_{l+\frac{1}{2}}(\delta rr')\right] $$

$$ + \left[\frac{18}{\delta}(r^2+rr'\mathcal{P}_\delta-2r'^2)+\frac{18}{\delta^2}\right]\left[3A_{jl}\right]\left[\mathcal{I}_{l+\frac{1}{2}}(\delta rr')\right] . $$

Again the parameters a, b, δ are defined in terms of doubly primed ones thus:

$$ a = a''_{ijk} = \tfrac{4}{9}(\alpha_i'+4\alpha_j+\mu_K) = b'_{jik} , $$

$$ b = b''_{ijk} = \tfrac{4}{9}(4\alpha_i'+\alpha_j+\mu_K) = a'_{jik} , $$

$$ \delta = \delta''_{ijk} = \tfrac{4}{9}(4\alpha_i'+4\alpha_j-2\mu_K) = \delta'_{jik} . $$

The central force D-S and the energy D-S terms were obtained in the same way.

XII.2 THE SYMMETRISATION OF THE SPIN-ORBIT TERMS

The results of the last section stem from the fact that operators such as $S_{23}(r_{23}^2)\,S_{12}(r_{12}^2)$, although not being Hermitian themselves, however when applied to the n-d system give the same eigen values as their Hermitian adjoints ,

$$ \left[S_{23}(r_{23}^2)\,S_{12}(r_{12}^2)\right]^* . $$

This is not true when we consider the direct interaction of the spin-orbit S-D terms with the spin-orbit operator defined as $\frac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}$. With this definition we have operators appearing such as

$\frac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\ S_{23}(r_{23}^2)$ in the S-D term

and $S_{23}(r_{23}^2)\ \frac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}$ in the D-S term.

It is clear that one is not a Hermitian adjoint of the other. But in fact only one factor of the operator causes this trouble, the other factors do not because the difference between the two operators vanishes when applied to the eigen functions xy of the system. The significance lies in the term C resulting from the factorisation of the operator $\frac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\underline{L}_{12}\,S_{23}(r_{23}^2)$ (see section IX.1).

This term C in the S-D calculation gives

$$\left(\frac{\pi}{\lambda}\right)^{3/2} 3i\left[3\gamma^2\left(1-\frac{\gamma}{2}\right)\left\{r^2(\underline{\sigma}_3\cdot\underline{r})(\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}})-(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_3\cdot\underline{r})(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right\}+\frac{\gamma\alpha_i}{\lambda}S_{23}(r^2)-\frac{3\gamma}{8\lambda}S_{23}(\underline{r},\frac{\partial}{\partial\underline{r}})\right],$$

while the corresponding part in the D-S calculation is

$$\left(\frac{\pi}{\lambda}\right)^{3/2} 3i\left[-3\gamma^2\left(1-\frac{\gamma}{2}\right)\left\{r^2(\underline{\sigma}_3\cdot\underline{r})(\underline{\sigma}_2\cdot\frac{\partial}{\partial\underline{r}})-(\underline{\sigma}_2\cdot\underline{r})(\underline{\sigma}_3\cdot\underline{r})(\underline{r}\cdot\frac{\partial}{\partial\underline{r}})\right\}+\frac{\gamma\alpha_j}{\lambda}S_{23}(r^2)+\frac{3\gamma}{8\lambda}S_{23}(\underline{r},\frac{\partial}{\partial\underline{r}})\right].$$

The difference in signs is due to the factor $i\ (=\sqrt{-1})$ in the definition of $\underline{L}_{12}$.

Hence to symmetrise the integrals we may re-define the spin-orbit operator as

$$\frac{1}{2}\left[\frac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\overrightarrow{\underline{L}_{12}}-\frac{1}{2}(\underline{\sigma}_1+\underline{\sigma}_2)\cdot\overleftarrow{\underline{L}_{12}}\right],$$

so that both the S-D and the D-S terms are the same.

With such a definition, contributions of the term C to the S-D and the D-S terms are both now

$$\left(\frac{\pi}{\lambda}\right)^{3/2} \frac{3}{4} i \frac{\gamma}{\lambda}(\sigma_i+\sigma_j)\, S_{23}(r^2) \ .$$

It follows that the direct interaction of the spin-orbit S-D terms, in the quartet case is given by

$$D^{LS}_{S\text{-}D}(r)$$

$$= \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} A_i A_j' \, {}^{LS}U_K^{(1)} \exp.\left[-(\mu-\lambda\gamma^2)r^2\right] .x$$

$$\times\left\{\left[\frac{21\gamma}{32\lambda}-\frac{3}{8}\left(1-\frac{\gamma}{2}\right)\gamma^2 r^2\right]\left[A_{J\ell}\right]+\frac{3}{4}\frac{\gamma}{\lambda}(\sigma_i+\sigma_j)\left[B_{J\ell}\right]+\frac{3}{4}\left(1-\frac{\gamma}{2}\right)\gamma^2 r^2\left[C_{J\ell}\right]\right\} F_\ell(r)$$

and that of the D-S terms is of the same form with indices i and j interchanged.

The results in the doublet case, and also in the S-S term calculations are not altered by this definition of the spin-orbit operator.

The need for a symmetrisation of the operator in the indirect interaction calculations does not arise. This is due to the integration by parts performed during the derivation and the differences cancel out.

XII.3. THE SYMMETRISATION OF THE QUADRATIC SPIN-ORBIT TERMS

Similar to the case of the spin-orbit S-D terms, the quadratic spin-orbit operator should be defined in the Hermitian form as

$$\tfrac{1}{2}\left(\vec{Q}_{12} + \overleftarrow{Q}_{12}\right) .$$

This operator gives the same results for the direct and the indirect interaction, except that in the direct interaction the matrix elements $[D_{Jl}]$ and $[E_{Jl}]$ are now symmetrical, being defined by

$$[D_{Jl}] = \tfrac{1}{2}\left\langle \tfrac{1}{2}\left\{(\underline{\sigma}_1 \underline{I})(\underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{I}}) + (\underline{\sigma}_2 \underline{I})(\underline{\sigma}_1 \cdot \frac{\partial}{\partial \underline{I}})\right\} + \tfrac{1}{2}\left\{(\underline{\sigma}_1 \cdot \frac{\partial}{\partial \underline{I}})(\underline{\sigma}_2 \underline{I}) + (\underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{I}})(\underline{\sigma}_1 \underline{I})\right\}\right\rangle$$

and

$$\frac{1}{\gamma^2}[E_{Jl}] = \tfrac{1}{2}\left\langle \tfrac{1}{2}\left\{(\underline{\sigma}_1 \cdot \frac{\partial}{\partial \underline{I}})(\underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{I}}) + (\underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{I}})(\underline{\sigma}_1 \cdot \frac{\partial}{\partial \underline{I}})\right\} + \tfrac{1}{2}\left\{(\underline{\sigma}_1 \cdot \frac{\partial}{\partial \underline{I}})(\underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{I}}) + (\underline{\sigma}_2 \cdot \frac{\partial}{\partial \underline{I}})(\underline{\sigma}_1 \cdot \frac{\partial}{\partial \underline{I}})\right\}\right\rangle .$$

Thus the re-defined $[D_{Jl}]$ and $[E_{Jl}]$ are given by

$$[D_{Jl}] = \begin{pmatrix} -\frac{2J-3}{4J} & 0 & \frac{1}{4J}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} & 0 \\ 0 & \frac{2J+5}{4(J+1)} & 0 & \frac{1}{4(J+1)}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} \\ \frac{1}{4J}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} & 0 & \frac{2J-3}{4J} & 0 \\ 0 & \frac{1}{4(J+1)}\left[3(2J-1)(2J+3)\right]^{\frac{1}{2}} & 0 & -\frac{2J+5}{4(J+1)} \end{pmatrix} \quad \ldots\ldots(12.1)$$

and

$$[E_{Jl}] = \begin{pmatrix} -\frac{(2J+1)(2J-3)}{8J} & 0 & \frac{4J^2+3}{8J}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} & 0 \\ 0 & \frac{-16J^3-28J^2+16J+37}{24(J+1)} & 0 & \frac{(4J^2+8J+7)}{8(J+1)}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} \\ \frac{4J^2+3}{8J}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} & 0 & \frac{-16J^3-20J^2+24J-9}{24J} & 0 \\ 0 & \frac{(4J^2+8J+7)}{8(J+1)}\left[\frac{(2J-1)(2J+3)}{3}\right]^{\frac{1}{2}} & 0 & \frac{(2J+1)(2J+5)}{8(J+1)} \end{pmatrix} \quad \ldots(12.2)$$

with the usual exception for $J = \frac{1}{2}$.

CHAPTER XIII

THE COMPLETE INTEGRO-DIFFERENTIAL EQUATIONS

In writing down the full integro-differential equations for the radial wave functions we collect the results obtained in Chapter III-XII and regroup the terms in a way that is convenient for numerical calculations.

XIII.1 THE DOUBLET CASE

We write down the integro-differential equations in the doublet case in the form of single equations and they are given by

$$\mathcal{D}_l^2 f_l(r) + \tau_l(r) \frac{1}{r^2} f_l(r) + \mathcal{U}_l(r) f_l(r) + \mathcal{V}_l(r) \frac{1}{r} \frac{d}{dr} f_l(r) + W_l(r) \frac{d^2}{dr^2} f_l(r)$$

$$+ \int_0^\infty dr' \left[P_l(r,r') + N_l(r,r') + K_l(r,r') \right] f_l(r') = 0 \qquad \ldots\ldots \quad (13.1)$$

for $l = J - \frac{1}{2}$ and $l = J + \frac{1}{2}$,

where $\mathcal{D}_l^2 = \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2$, with $k^2 = \frac{4}{3} \frac{M}{\hbar^2} E_n$,

and

$$\tau_l(r) = {}^{Q}t_l(r) ,$$

$$\mathcal{U}_l(r) = {}^{C}u(r) + {}^{LS}u_l(r) + {}^{Q}u_l(r) + {}^{LS}u_l'(r) + {}^{LS}u_l''(r) + {}^{T}u_l'(r) + {}^{T}u_l''(r) ,$$

$$\mathcal{V}_l(r) = {}^{Q}v(r) ,$$

$$W_l(r) = {}^{Q}w(r) ,$$

$$K_l(r,r') = {}^{C}k_l(r,r') + {}^{LS}k_l(r,r') + {}^{Q}k_l(r,r')$$
$$+ {}^{LS}k_l'(r,r') + {}^{LS}k_l''(r,r') + {}^{T}k_l'(r,r') + {}^{T}k_l''(r,r') .$$

These terms represent the contributions from various interactions indicated by the symbols attached. The prime and the double prime symbols denote the S-D and the D-S interactions respectively. Again 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 terms in equation (13.1) are given by

$$ {}^{Q}t_{l}(r) = {}^{Q}t_{l}^{(1)}(r) + {}^{Q}t_{l}^{(3)}(r) \quad , \quad \text{where} $$

$$ {}^{Q}t_{l}^{(1)}(r) = -\frac{3}{4\lambda}\,[(l+1)\,{}^{Q}G_{S\text{-}S}^{(1)} \quad , $$

$$ {}^{Q}t_{l}^{(3)}(r) = \frac{27}{16\lambda}\,[(l+1)\,{}^{Q}G_{S\text{-}S}^{(3)} \quad , $$

and

$$ {}^{C}u(r) = {}^{C}G_{S\text{-}S}^{(1)} \quad , $$

$$ {}^{LS}u_{l}(r) = \tfrac{1}{4}(1-\tfrac{\gamma}{2})\,\Lambda_{Jl}\,{}^{LS}G_{S\text{-}S}^{(1)} \quad , $$

$$ {}^{Q}u_{l}(r) = {}^{Q}u_{l}^{(1)}(r) + {}^{Q}u_{l}^{(3)}(r) \quad , \quad \text{where} $$

$$ {}^{Q}u_{l}^{(1)}(r) = \left[\frac{6\alpha}{\lambda} - 3(1-\tfrac{\gamma}{2})^{2}\left[(l+1) + \tfrac{8}{3}\nu + \tfrac{8}{3}\sigma r^{2}\right]\right] {}^{Q}G_{S\text{-}S}^{(1)} \quad , $$

$$ {}^{Q}u_{l}^{(3)}(r) = \left[-\frac{27}{2}\frac{\alpha}{\lambda} + \frac{27}{4}(1-\tfrac{\gamma}{2})^{2}\left[(l+1) - 6\nu - 6\sigma r^{2}\right]\right] {}^{Q}G_{S\text{-}S}^{(3)} \quad , $$

and

$$ {}^{Q}v(r) = {}^{Q}v^{(1)}(r) + {}^{Q}v^{(3)}(r) \quad , \quad \text{where} $$

$$ {}^{Q}v^{(1)}(r) = -\tfrac{8}{3}\nu r^{2}\,{}^{Q}G_{S\text{-}S}^{(1)} \quad , $$

$$ {}^{Q}v^{(3)}(r) = 6\nu r^{2}\,{}^{Q}G_{S\text{-}S}^{(3)} \quad , $$

and

$$ {}^{Q}w(r) = {}^{Q}w^{(1)}(r) + {}^{Q}w^{(3)}(r) , $$

$$ {}^{Q}w^{(1)}(r) = \frac{3}{4\lambda}\, {}^{Q}G^{(1)}_{S\text{-}S} , $$

$$ {}^{Q}w^{(3)}(r) = -\frac{27}{16\lambda}\, {}^{Q}G^{(3)}_{S\text{-}S} , $$

and

$$ N_l(r,r') = -\tfrac{1}{2}\cdot\tfrac{4}{3}\frac{M}{\hbar^2}\, Z_{S\text{-}S}\,(E_n - E_d)\, \mathcal{I}_{[l+\frac{1}{2}]}(wrr') , $$

$$ P_l(r,r') = Z_{S\text{-}S}\left[-\tfrac{3}{2}w + \frac{64}{81}(\phi r^2 + \psi r'^2 + 4\chi rr' p_w)\right] \mathcal{I}_{[l+\frac{1}{2}]}(wrr') , $$

$$ {}^{C}k_l(r,r') = {}^{C}H^{(2)}_{S\text{-}S}\, \mathcal{I}_{[l+\frac{1}{2}]}(\partial rr') , $$

$$ {}^{LS}k_l(r,r') = {}^{LS}H^{(2)}_{S\text{-}S}\, \frac{w}{2\delta}\, \Lambda_{Jl}\, \mathcal{I}_{[l+\frac{1}{2}]}(\partial rr') , $$

$$ {}^{Q}k_l(r,r') = {}^{Q}k_l^{(2)}(r,r') + {}^{Q}k_l^{(4)}(r,r') , $$

$$ {}^{Q}k_l^{(2)}(r,r') = -\tfrac{4}{3}\, {}^{Q}H^{(2)}_{S\text{-}S}\left[9w^2r^2r'^2 - 2\zeta(r^2+r'^2) + 6 + 4\zeta rr' p_\delta - 9w^2r^2r'^2 p^{(2)}_\delta\right] \mathcal{I}_{[l+\frac{1}{2}]}(\partial rr') , $$

$$ {}^{Q}k_l^{(4)}(r,r') = 3\, {}^{Q}H^{(4)}_{S\text{-}S}\left[9w^2r^2r'^2 - 2\zeta(r^2+r'^2) + 6 + 4\zeta rr' p_\delta - 9w^2r^2r'^2 p^{(2)}_\delta\right] \mathcal{I}_{[l+\frac{1}{2}]}(\partial rr') , $$

and for the S-D and D-S terms

$$ {}^{LS}u'_l(r) = \left[\tfrac{\gamma^2}{2}(1-\tfrac{\gamma}{2})r^2 - \frac{5\gamma}{8\lambda}\right] \Lambda_{Jl}\, {}^{LS}G^{(1)}_{S\text{-}D} , $$

$$ {}^{LS}u''_l(r) = \left[\tfrac{\gamma^2}{2}(1-\tfrac{\gamma}{2})r^2 - \frac{5\gamma}{8\lambda}\right] \Lambda_{Jl}\, {}^{LS}G^{(1)}_{D\text{-}S} , $$

$$ {}^{T}u'(r) = \left[-\frac{15}{4\lambda^2} + \frac{10\gamma}{\lambda}(1-\tfrac{\gamma}{2})r^2 - 4\gamma^2(1-\tfrac{\gamma}{2})^2 r^4\right] {}^{T}G^{(1)}_{S\text{-}D} , $$

$$ {}^{T}u''(r) = \left[-\frac{15}{4\lambda^2} + \frac{10\gamma}{\lambda}(1-\tfrac{\gamma}{2})r^2 - 4\gamma^2(1-\tfrac{\gamma}{2})^2 r^4\right] {}^{T}G^{(1)}_{D\text{-}S} , $$

$$ {}^{LS}k'_{l}(r,r') = \frac{4}{9}\,{}^{LS}H^{(2)}_{S\text{-}D}\,\Lambda_{Jl}\left[\tfrac{1}{4}w(4r^2+r'^2+4rr'\beta_\delta)-\tfrac{5}{2}\right]\vartheta_{l+\frac{1}{2}}(\delta rr'), $$

$$ {}^{LS}k''_{l}(r,r') = \frac{4}{9}\,{}^{LS}H^{(2)}_{D\text{-}S}\,\Lambda_{Jl}\left[\tfrac{1}{4}w(r^2+4r'^2+4rr'\beta_\delta)-\tfrac{5}{2}\right]\vartheta_{l+\frac{1}{2}}(\delta rr'), $$

$$ {}^{T}k'_{l}(r,r') = \frac{16}{81}\,{}^{T}H^{(2)}_{S\text{-}D}\times $$

$$ \times\left[8r^4-34r^2r'^2+4r'^4+(-16r^2+8r'^2)rr'\beta_\delta+22r^2r'^2\beta^{(2)}_\delta+\frac{18}{\delta}(2r^2-r'^2-rr'\beta_\delta)\Lambda_{Jl}\right]\vartheta_{l+\frac{1}{2}}(\delta rr'), $$

$$ {}^{T}k''_{l}(r,r') = \frac{16}{81}\,{}^{T}H^{(2)}_{D\text{-}S}\times $$

$$ \times\left[4r^4-34r^2r'^2+8r'^4+(8r^2-16r'^2)rr'\beta_\delta+22r^2r'^2\beta^{(2)}_\delta+\frac{18}{\delta}(-r^2+2r'^2-rr'\beta_\delta)\Lambda_{Jl}\right]\vartheta_{l+\frac{1}{2}}(\delta rr') $$

where $\Lambda_{Jl} = l$ for $l = J-\frac{1}{2}$

$= -(l+1)$ for $l = J+\frac{1}{2}$,

and

$$ {}^{\xi}G^{(\eta)}_{S\text{-}S}(r) = -\frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2}A_iA_j\,{}^{\xi}U^{(\eta)}_k\,e^{-(\mu-\lambda\delta^2)r^2}, $$

$$ {}^{\xi}G^{(\eta)}_{S\text{-}D}(r) = -\frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2}A_iA'_j\,{}^{\xi}U^{(\eta)}_k\,e^{-(\mu-\lambda\delta^2)r^2}, $$

$$ Z_{S\text{-}S}(r,r') = -\left(\frac{4}{3}\right)^3\frac{4\pi}{w}A_iA_j\,e^{-er^2-fr'^2}, $$

$$ {}^{\xi}H^{(\eta)}_{S\text{-}S}(r,r') = +\frac{4}{3}\frac{M}{\hbar^2}\left(\frac{4}{3}\right)^3\frac{4\pi}{\delta}A_iA_j\,{}^{\xi}U^{(\eta)}_k\,e^{-ar^2-br'^2}, $$

$$ {}^{\xi}H^{(\eta)}_{S\text{-}D}(r,r') = +\frac{4}{3}\frac{M}{\hbar^2}\left(\frac{4}{3}\right)^3\frac{4\pi}{\delta'}A_iA'_j\,{}^{\xi}U^{(\eta)}_k\,e^{-a'r^2-b'r'^2}, $$

$$ {}^{\xi}H^{(\eta)}_{D\text{-}S}(r,r') = +\frac{4}{3}\frac{M}{\hbar^2}\left(\frac{4}{3}\right)^3\frac{4\pi}{\delta''}A'_iA_j\,{}^{\xi}U^{(\eta)}_k\,e^{-a''r^2-b''r'^2}. $$

The definitions of all the parameters are given in Appendix 5.

XIII.2 THE QUARTET CASE

The integro-differential equations are written in matrix form as

$$\mathcal{D}^2 \mathcal{F}(r) + \mathcal{T} \frac{1}{r^2} \mathcal{F}(r) + \mathcal{U} \mathcal{F}(r) + \mathcal{V} \frac{1}{r} \frac{d}{dr} \mathcal{F}(r) + \mathcal{W} \frac{d^2}{dr^2} \mathcal{F}(r)$$

$$+ \int_0^\infty dr' \left[\mathcal{N}(r,r') + \mathcal{P}(r,r') + \mathcal{K}(r,r') \right] \mathcal{F}(r') = 0 \qquad \ldots\ldots (13.2)$$

where

$$\mathcal{F}(r) = \begin{bmatrix} f_{J-3/2}(r) \\ f_{J-\frac{1}{2}}(r) \\ f_{J+\frac{1}{2}}(r) \\ f_{J+3/2}(r) \end{bmatrix} \qquad \text{for} \quad J \geq 3/2 ,$$

$$= \begin{bmatrix} f_{J+\frac{1}{2}}(r) \\ f_{J+3/2}(r) \end{bmatrix} \qquad \text{for} \quad J = \tfrac{1}{2} ,$$

and

$$\mathcal{D}^2 = \begin{bmatrix} \mathcal{D}^2_{J-3/2} & & & \\ & \mathcal{D}^2_{J-\frac{1}{2}} & & \\ & & \mathcal{D}^2_{J+\frac{1}{2}} & \\ & & & \mathcal{D}^2_{J+3/2} \end{bmatrix} \qquad \text{for} \quad J \geq 3/2 ,$$

$$= \begin{bmatrix} \mathcal{D}^2_{J+\frac{1}{2}} & \\ & \mathcal{D}^2_{J+3/2} \end{bmatrix} \qquad \text{for} \quad J = \tfrac{1}{2} .$$

$\mathcal{T}$, $\mathcal{U}$, $\mathcal{V}$ and $\mathcal{W}$ denote 4X4 matrices for $J \geq 3/2$ and 2X2 matrices for $J = \frac{1}{2}$,

and so do $\mathcal{N}(r,r')$, $\mathcal{P}(r,r')$ and $\mathcal{K}(r,r')$.

Similar to the doublet case we have

$$\mathcal{D}_l^2 = \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_l^2 \quad \text{with} \quad k_l^2 = \frac{4}{3}\frac{M}{\hbar^2}E_n ,$$

and

$$\mathcal{T} = {}^{Q}t(r) ,$$

$$\mathcal{U} = {}^{C}u(r) + {}^{LS}u(r) + {}^{T}u(r) + {}^{Q}u(r) + {}^{C}u'(r) + {}^{C}u''(r) + {}^{LS}u'(r) + {}^{LS}u''(r) + {}^{T}u'(r) + {}^{T}u''(r) ,$$

$$\mathcal{V} = {}^{Q}v(r) ,$$

$$\mathcal{W} = {}^{Q}w(r) ,$$

$$\mathcal{N}(r,r') = n(r,r') + n'(r,r') + n''(r,r') ,$$

$$\mathcal{P}(r,r') = p(r,r') + p'(r,r') + p''(r,r') ,$$

$$\mathcal{K}(r,r') = {}^{C}k(r,r') + {}^{LS}k(r,r') + {}^{T}k(r,r') + {}^{Q}k(r,r') + {}^{C}k'(r,r') + {}^{C}k''(r,r') + {}^{LS}k'(r,r') + {}^{LS}k''(r,r') + {}^{T}k'(r,r') + {}^{T}k''(r,r') .$$

These matrices are explicitly given by

$${}^{Q}t(r) = \left\{ \frac{9}{16\lambda}[\delta] + \frac{9}{32\lambda}[(l+1)[\delta] - \frac{9}{32\lambda}[B_{Jl}] + \frac{9}{16\lambda}[D_{Jl}] - \frac{9}{32\lambda}[E_{Jl}] \right\} {}^{Q}G_{S\text{-}S}^{(1)} ,$$

$${}^{C}u(r) = {}^{C}G_{S\text{-}S}^{(3)}[\delta] ,$$

$${}^{LS}u(r) = \frac{3}{4}(1-\frac{\gamma}{2})[A_{Jl}]\,{}^{LS}G_{S\text{-}S}^{(1)} ,$$

$$
\begin{aligned}
{}^{T}u(r) &= \left(1-\tfrac{\gamma}{2}\right)^{2} r^{2}\left[B_{Jl}\right]\,{}^{T}G^{(1)}_{S\text{-}S}\,, \\
{}^{Q}u(r) &= \left\{-\left(\tfrac{4}{3}\sigma r^{2}+\tfrac{4}{3}\nu+3\tfrac{\alpha}{\lambda}\right)-\left(\tfrac{8}{3}r^{2}+\tfrac{1}{3}\nu\right)\left[B_{Jl}\right]+\nu\left[D_{Jl}\right]+\tfrac{9}{4}\left(1-\tfrac{\gamma}{2}\right)^{2}\left(\left[\Omega_{Jl}\right]-\left[F_{Jl}\right]\right)\right\}{}^{Q}G^{(1)}_{S\text{-}S}\,, \\
{}^{Q}v(r) &= \left\{\left(\tfrac{4}{3}\nu r^{2}-\tfrac{9}{16\lambda}\right)+\left(\tfrac{1}{3}\nu r^{2}+\tfrac{9}{32\lambda}\right)\left[B_{Jl}\right]-\tfrac{9}{16\lambda}\left[D_{Jl}\right]\right\}{}^{Q}G^{(1)}_{S\text{-}S}\,, \\
{}^{Q}w(r) &= \left\{-\tfrac{3}{8\lambda}-\tfrac{3}{32\lambda}\left[B_{Jl}\right]\right\}{}^{Q}G^{(1)}_{S\text{-}S}\,,
\end{aligned}
$$

and

$$
\begin{aligned}
n(r,r') &= \tfrac{4}{3}\tfrac{M}{\hbar^{2}}\,Z_{S\text{-}S}\,(E_{n}-E_{d})\left[\mathcal{J}_{l+\frac{1}{2}}(wrr')\right]\,, \\
p(r,r') &= Z_{S\text{-}S}\left[-\tfrac{3}{2}w+\tfrac{64}{81}\left(\phi r^{2}+\psi r'^{2}+4\chi rr'p_{w}\right)\right]\left[\mathcal{J}_{l+\frac{1}{2}}(wrr')\right]\,, \\
{}^{C}k(r,r') &= {}^{C}H^{(4)}_{S\text{-}S}\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]\,, \\
{}^{LS}k(r,r') &= {}^{LS}H^{(2)}_{S\text{-}S}\;\tfrac{w}{2\delta}\left[A_{Jl}\right]\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]\,, \\
{}^{T}k(r,r') &= {}^{T}H^{(2)}_{S\text{-}S}\;\tfrac{4}{9}\left\{r^{2}\left[B_{Jl}\right]\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]+r'^{2}\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]\left[B_{Jl}\right]-2rr'\left[P_{Jl}\,\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]\right\}, \\
{}^{Q}k(r,r') &= {}^{Q}H^{(2)}_{S\text{-}S}\;\times \\
&\quad\times\left\{\left[8-\tfrac{8}{3}\zeta\left(r^{2}+r'^{2}\right)+9w^{2}r^{2}r'^{2}\right]\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]\right. \\
&\quad+\left[-\left(6\tfrac{w^{2}}{\delta^{2}}-\tfrac{16}{3}\zeta\right)rr'p_{\delta}-9w^{2}r^{2}r'^{2}p^{(2)}_{\delta}\right]\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right] \\
&\quad+\tfrac{1}{3}\zeta r^{2}\left[B_{Jl}\right]\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]+\tfrac{1}{3}\zeta r'^{2}\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]\left[B_{Jl}\right] \\
&\quad\left.+\tfrac{1}{3}\left(9\tfrac{w^{2}}{\delta^{2}}-2\zeta\right)rr'\left[P_{Jl}\,\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]-9\tfrac{w^{2}}{\delta^{2}}\left[F_{Jl}\right]\left[\mathcal{J}_{l+\frac{1}{2}}(\delta rr')\right]\right\}\,,
\end{aligned}
$$

and

$$ {}^{c}u'(r) = \gamma^2 r^2 \, {}^{c}G^{(3)}_{S\text{-}D}\,[B_{Jl}], $$

$$ {}^{c}u''(r) = \gamma^2 r^2 \, {}^{c}G^{(3)}_{D\text{-}S}\,[B_{Jl}], $$

$$ {}^{LS}u'(r) = {}^{LS}G^{(1)}_{S\text{-}D}\left\{\left[\frac{21\gamma}{32\lambda} - \frac{3}{8}(1-\tfrac{\gamma}{2})\gamma^2 r^2\right]\left[\tfrac{1}{2}A_{Jl}\right] + \frac{3}{4}\frac{\gamma}{\lambda}(\alpha_i+\alpha_j)\left[B_{Jl}\right] + \frac{3}{4}(1-\tfrac{\gamma}{2})\gamma^2 r^2\left[C_{Jl}\right]\right\}, $$

$$ {}^{LS}u''(r) = {}^{LS}G^{(1)}_{D\text{-}S}\left\{\left[\frac{21\gamma}{32\lambda} - \frac{3}{8}(1-\tfrac{\gamma}{2})\gamma^2 r^2\right]\left[\tfrac{1}{2}A_{Jl}\right] + \frac{3}{4}\frac{\gamma}{\lambda}(\alpha_i+\alpha_j)\left[B_{Jl}\right] + \frac{3}{4}(1-\tfrac{\gamma}{2})\gamma^2 r^2\left[C_{Jl}\right]\right\}, $$

$$ {}^{T}u'(r) = {}^{T}G^{(1)}_{S\text{-}D}\left[\left\{\frac{15}{4\lambda^2} - \frac{5\gamma}{\lambda}(1-\tfrac{\gamma}{2})r^2 + 2\gamma^2(1-\tfrac{\gamma}{2})^2 r^4\right\}[\delta] + \left\{-\frac{7\gamma}{4\lambda}(1-\tfrac{\gamma}{2})r^2 + \gamma^2(1-\tfrac{\gamma}{2})^2 r^4\right\}[B_{Jl}]\right], $$

$$ {}^{T}u''(r) = {}^{T}G^{(1)}_{D\text{-}S}\left[\left\{\frac{15}{4\lambda^2} - \frac{5\gamma}{\lambda}(1-\tfrac{\gamma}{2})r^2 + 2\gamma^2(1-\tfrac{\gamma}{2})^2 r^4\right\}[\delta] + \left\{-\frac{7\gamma}{4\lambda}(1-\tfrac{\gamma}{2})r^2 + \gamma^2(1-\tfrac{\gamma}{2})^2 r^4\right\}[B_{Jl}]\right], $$

and

$$ n'(r,r') = \frac{4}{3}\frac{M}{\hbar^2} Z_{S\text{-}D} \left(\frac{4}{3}\right)(E_n - E_d) \times $$

$$ \times\left[4r^2[B_{Jl}][\mathcal{J}_{[+\frac{1}{2}}(wrr')] + r'^2[\mathcal{J}_{[+\frac{1}{2}}(wrr')][B_{Jl}] + 4rr'[P_{Jl}\mathcal{J}_{[+\frac{1}{2}}(wrr')]\right], $$

$$ n''(r,r') = \frac{4}{3}\frac{M}{\hbar^2} Z_{D\text{-}S} \left(\frac{4}{3}\right)(E_n - E_d) \times $$

$$ \times\left[r^2[B_{Jl}][\mathcal{J}_{[+\frac{1}{2}}(wrr')] + 4r'^2[\mathcal{J}_{[+\frac{1}{2}}(wrr')][B_{Jl}] + 4rr'[P_{Jl}\mathcal{J}_{[+\frac{1}{2}}(wrr')]\right], $$

$$ p'(r,r') = \frac{16}{81} Z_{S\text{-}D}\left[\left(\frac{64}{9}\phi r^2 + \frac{64}{9}\psi r'^2 + \frac{256}{9}\chi rr' p_w - 56\alpha_i - 56\alpha_j'\right) r^2[B_{Jl}][\mathcal{J}_{[+\frac{1}{2}}(wrr')]\right. $$

$$ + \left(\frac{16}{9}\phi r^2 + \frac{16}{9}\psi r'^2 + \frac{64}{9}\chi rr' p_w - 38\alpha_i - 14\alpha_j'\right) r'^2[\mathcal{J}_{[+\frac{1}{2}}(wrr')][B_{Jl}] $$

$$ \left. + \left(\frac{64}{9}\phi r^2 + \frac{64}{9}\psi r'^2 + \frac{256}{9}\chi rr' p_w - 104\alpha_i - 56\alpha_j'\right) rr'[P_{Jl}\mathcal{J}_{[+\frac{1}{2}}(wrr')]\right], $$

$$ p''(r,r') = \frac{16}{81} Z_{D\text{-}S}\left[\left(\frac{16}{9}\phi r^2 + \frac{16}{9}\psi r'^2 + \frac{64}{9}\chi rr' p_w - 14\alpha_i' - 38\alpha_j\right) r^2[B_{Jl}][\mathcal{J}_{[+\frac{1}{2}}(wrr')]\right. $$

$$ + \left(\frac{64}{9}\phi r^2 + \frac{64}{9}\psi r'^2 + \frac{256}{9}\chi rr' p_w - 56\alpha_i' - 56\alpha_j\right) r'^2[\mathcal{J}_{[+\frac{1}{2}}(wrr')][B_{Jl}] $$

$$ \left. + \left(\frac{64}{9}\phi r^2 + \frac{64}{9}\psi r'^2 + \frac{256}{9}\chi rr' p_w - 56\alpha_i' - 104\alpha_j\right) rr'[P_{Jl}\mathcal{J}_{[+\frac{1}{2}}(wrr')]\right], $$

$$ {}^{c}k'(r,r') = \frac{4}{9}\,{}^{c}\mathcal{H}^{(4)}_{S\text{-}D} \times $$

$$ \times \left[4r^2 [B_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] + r'^2 [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] [B_{Jl}] + 4rr' [P_{Jl} \mathcal{J}_{l+\frac{1}{2}}(\partial rr')] \right], $$

$$ {}^{c}k''(r,r') = \frac{4}{9}\,{}^{c}\mathcal{H}^{(4)}_{D\text{-}S} \times $$

$$ \times \left[r^2 [B_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] + 4r'^2 [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] [B_{Jl}] + 4rr' [P_{Jl} \mathcal{J}_{l+\frac{1}{2}}(\partial rr')] \right], $$

$$ {}^{LS}k'(r,r') = \frac{4}{9}\,{}^{LS}\mathcal{H}^{(2)}_{S\text{-}D} \times $$

$$ \Big[\left\{ -\frac{3}{2}\frac{w}{\delta}(4r^2+r'^2) - 6\frac{w}{\delta} rr' p_\delta - 12\frac{w}{\delta^2} + \frac{21}{\delta} \right\} [\tfrac{1}{2}A_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] $$

$$ + \frac{3}{2}\frac{w}{\delta} \left\{ 4r^2 [C_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] + r'^2 [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] [C_{Jl}] + 4rr' [Q_{Jl} \mathcal{J}_{l+\frac{1}{2}}(\partial rr')] \right\} $$

$$ + (-6+3wr'^2+6wrr'p_\delta) r^2 [B_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] + (3-3wr^2-\tfrac{3}{2}wrr'p_\delta) r'^2 [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] [B_{Jl}] $$

$$ + \left\{ 3 + \tfrac{3}{2}w(-4r^2+r'^2) \right\} [P_{Jl} \mathcal{J}_{l+\frac{1}{2}}(\partial rr')] \Big], $$

$$ {}^{LS}k''(r,r') = \frac{4}{9}\,{}^{LS}\mathcal{H}^{(2)}_{D\text{-}S} \times $$

$$ \Big[\left\{ -\frac{3}{2}\frac{w}{\delta}(r^2+4r'^2) - 6\frac{w}{\delta} rr' p_\delta - 12\frac{w}{\delta^2} + \frac{21}{\delta} \right\} [\tfrac{1}{2}A_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] $$

$$ + \frac{3}{2}\frac{w}{\delta} \left\{ r^2 [C_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] + 4r'^2 [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] [C_{Jl}] + 4rr' [Q_{Jl} \mathcal{J}_{l+\frac{1}{2}}(\partial rr')] \right\} $$

$$ + (3-3wr'^2-\tfrac{3}{2}wrr'p_\delta) r^2 [B_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] + (-6+3wr'^2+6wrr'p_\delta) r'^2 [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] [B_{Jl}] $$

$$ + \left\{ 3 + \tfrac{3}{2}w(r^2-4r'^2) \right\} [P_{Jl} \mathcal{J}_{l+\frac{1}{2}}(\partial rr')] \Big], $$

$$ {}^{T}k'(r,r') = \frac{16}{81}\,{}^{T}\mathcal{H}^{(2)}_{S\text{-}D} \times $$

$$ \Big[\left\{ 8r^4 - 17r^2r'^2 + 2r'^4 + (-8r^2+4r'^2) rr' p_\delta + 11r^2r'^2 p_\delta^{(2)} + \frac{9}{\delta}(2r^2-r'^2-rr'p_\delta) [\tfrac{1}{2}A_{Jl}] \right\} [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] $$

$$ + \frac{9}{\delta} \left\{ 2r^2 [C_{Jl}] [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] - r'^2 [\mathcal{J}_{l+\frac{1}{2}}(\partial rr')] [C_{Jl}] - rr' [Q_{Jl} \mathcal{J}_{l+\frac{1}{2}}(\partial rr')] \right\} + $$

$$+ (4r^2-11r'^2-2rr'p_\delta)\, r^2[B_{JL}][\vartheta_{L+\frac{1}{2}}(\delta rr')] + (-11r^2+r'^2+rr'p_\delta)\, r'^2[\vartheta_{L+\frac{1}{2}}(\delta rr')][B_{JL}]$$

$$+ (-2r^2+r'^2+19rr'p_\delta)\, rr'[P_{JL}\,\vartheta_{L+\frac{1}{2}}(\delta rr')]\ \Big] \ ,$$

$${}^{T}k''(r,r') = \frac{16}{81}\,{}^{T}H^{(2)}_{D\cdot S} \times$$

$$\Big[\{(2r^4-17r^2r'^2+8r'^4)+(4r^2-8r'^2)rr'p_\delta+11r^2r'^2p^{(2)}_\delta+\frac{2}{\delta}(-r^2+2r'^2-rr'p_\delta)\,[\tfrac{1}{2}A_{JL}]\}[\vartheta_{L+\frac{1}{2}}(\delta rr')]$$

$$+\frac{2}{\delta}\{-r^2[C_{JL}][\vartheta_{L+\frac{1}{2}}(\delta rr')]+2r'^2[\vartheta_{L+\frac{1}{2}}(\delta rr')][C_{JL}]-rr'[Q_{JL}\,\vartheta_{L+\frac{1}{2}}(\delta rr')]\}$$

$$+ (r^2-11r'^2+rr'p_\delta)\, r^2[B_{JL}][\vartheta_{L+\frac{1}{2}}(\delta rr')] + (-11r^2+4r'^2-2rr'p_\delta)\, r'^2[\vartheta_{L+\frac{1}{2}}(\delta rr')][B_{JL}]$$

$$+ (r^2-2r'^2+19rr'p_\delta)\, rr'[P_{JL}\,\vartheta_{L+\frac{1}{2}}(\delta rr')]\ \Big]$$

where $$Z_{S\cdot D}(r,r') = -\left(\frac{4}{3}\right)^3 \frac{4\pi}{w'}\, A_i' A_j'\, e^{-e'r^2-f'r'^2}$$

$$Z_{D\cdot S}(r,r') = -\left(\frac{4}{3}\right)^3 \frac{4\pi}{w''}\, A_i' A_j\, e^{-e''r^2-f''r'^2}$$

and $G(r)$, $H(r,r')$ are as defined in the doublet case

We are using the notation

$$r^n r'^n p^{(n)}_\varepsilon [\vartheta_{L+\frac{1}{2}}(\varepsilon rr')] = (-1)^n \varepsilon \frac{d^n}{d\varepsilon^n}\left[\frac{1}{\varepsilon}\,\vartheta_{L+\frac{1}{2}}(\varepsilon rr')\right] .$$

The matrix elements are given by equations in various sections with the following references :

$[A_{JL}]$ ..... (4.1.a) , (4.1.b) ; $[B_{JL}]$ ..... (5.1)

$[C_{JL}]$ ..... (9.1) ; $[D_{JL}]$ ..... (12.1)

$[E_{JL}]$ ..... (12.2) ; $[F_{JL}]$ ..... (6.3.a)

$[\Omega_{JL}]$ ..... (6.3)

$[P_{JL}\,\vartheta_{L+\frac{1}{2}}(\varepsilon rr')]$ ..... (5.2) ; $[Q_{JL}\,\vartheta_{L+\frac{1}{2}}(\varepsilon rr')]$ ..... (9.2)

CHAPTER XIV

MODIFICATION DUE TO HARD CORE EFFECT

The Gaussian form of the deuteron wave function is

$$r^2 A_i e^{-\alpha_i r^2} = -\frac{\partial}{\partial \alpha_i} A_i e^{-\alpha_i r^2} .$$

Thus before the expressions in equations (13.1), (13.2) can be evaluated, each has to be differentiated, twice if it is an S-S term, and once if an S-D or D-S term.

Let the expressions be denoted by $E_{S\cdot S}(\alpha_i, \alpha_j)$, $E_{S\cdot D}(\alpha_i, \alpha_j')$ and $E_{D\cdot S}(\alpha_i', \alpha_j)$ then the modified expressions are

$$\frac{\partial^2}{\partial \alpha_i \partial \alpha_j} E_{S\cdot S}(\alpha_i, \alpha_j) ,$$

$\frac{\partial}{\partial \alpha_i} E_{S\cdot D}(\alpha_i, \alpha_j')$ and $\frac{\partial}{\partial \alpha_j} E_{D\cdot S}(\alpha_i', \alpha_j)$ respectively.

We are now quoting a few examples of this procedure.

In the direct interaction we take the central S-S term $E_{S\cdot S}$, where

$$E_{S\cdot S} = \frac{4}{3}\frac{M}{\hbar^2}\left(\frac{\pi}{\lambda}\right)^{3/2} A_i A_j U_X e^{-(\mu-\lambda\gamma^2)r^2} .$$

Puting $\varepsilon = \frac{1}{\lambda}$,

$K = \frac{1}{2}\mu$,

and $B = \frac{4}{3}\frac{M}{\hbar^2} A A U \pi^{3/2}$, we have

$$E_{S\cdot S} = B\varepsilon^{3/2} e^{-(2K-K^2\varepsilon)r^2} .$$

Thus the modified expression for $E_{S\cdot S}$ is given by

$$\frac{\partial^2}{\partial \alpha_i \partial \alpha_j} E_{S\cdot S} = \left(\frac{15}{4}\varepsilon^2 + 5\varepsilon^3 K^2 r^2 + \varepsilon^4 K^4 r^4\right) B\varepsilon^{3/2} e^{-(2K-K^2\varepsilon)r^2} .$$

As an example of the indirect interaction, the N-or the P-kernels can be written as

$$k(r,r') = cu\, e^{-er^2-fr'^2}\, \mathcal{J}_{l+\frac{1}{2}}(wrr')$$

in which c is independent of α_i and α_j,

and u is a function of α_i and α_j.

We have

$$\frac{\partial^2}{\partial\alpha_i\partial\alpha_j} k(r,r')$$

$$= \left(\frac{2}{3}\right)^4 \exp.[-er^2-fr'^2] \cdot \Big[16r^2r'^2 u\, \mathcal{J}''_{l+\frac{1}{2}} + rr'\Big\{9\Big(\frac{\partial u}{\partial\alpha_i}+\frac{\partial u}{\partial\alpha_j}\Big) - 20(r^2+r'^2)u\Big\}\mathcal{J}'_{l+\frac{1}{2}}$$

$$+\Big\{\frac{81}{16}\frac{\partial^2 u}{\partial\alpha_i\partial\alpha_j} - \frac{45}{4}(r^2+r'^2)\Big(\frac{\partial u}{\partial\alpha_i}+\frac{\partial u}{\partial\alpha_j}\Big) + (4r^2+r'^2)(r^2+4r'^2)\, u\Big\}\mathcal{J}_{l+\frac{1}{2}}\Big].$$

In the case of the N-kernel (S-S term) $u = \frac{1}{w}$.

From Appendix 4,

$$r^2r'^2\, \mathcal{J}''_{l+\frac{1}{2}}(wrr') = \Big[\frac{l(l+1)}{w^2} + r^2r'^2\Big]\mathcal{J}_{l+\frac{1}{2}}(wrr').$$

Hence the modified N-kernel, is given by

$$\frac{\partial^2}{\partial\alpha_i\partial\alpha_j} k(r,r') = \frac{16}{81} C\, e^{-er^2-fr'^2} \times$$

$$\times\Big[\Big\{16\Big[\frac{l(l+1)}{w^3}+\frac{32}{w^3}+\frac{20}{w^2}(r^2+r'^2)+4\frac{(r^4+r'^4)}{w}+33\frac{r^2r'^2}{w}\Big]\mathcal{J}_{l+\frac{1}{2}} + \Big\{-\frac{32}{w^2}rr' - \frac{20}{w}(r^3r'+rr'^3)\Big\}\mathcal{J}'_{l+\frac{1}{2}}\Big].$$

The modified kernels are best left in terms of a Spherical Bessel Function and its first derivative in order that the preparation of data for the kernel evaluations should not be lengthened.

(see next Chapter).

CHAPTER XV

NUMERICAL ANALYSIS AND COMPUTATION

XV.1 THE NUMERICAL METHOD

The equations for the radial wave functions to be numerically solved are simultaneous equations of the form

$$\frac{d^2}{dr^2} y^p(r) + \sum_{q=1}^{m} \frac{1}{r^2} \tau^{pq}(r) y^p(r) + \sum_{q=1}^{m} U^{pq}(r) y^q(r)$$
$$+ \sum_{q=1}^{m} \frac{1}{r} V^{pq}(r) \frac{d}{dr} y^q(r) + \sum_{q=1}^{m} W^{pq}(r) \frac{d^2}{dr^2} y^q(r)$$
$$+ \sum_{q=1}^{m} \int K^{pq}(r,r') y^q(r') \, dr' = 0 \qquad \ldots\ldots (15.1)$$

for $p = 1, 2, \ldots\ldots m$.

The functions τ, U, K, etc. have the following properties:

$$K^{pq}(r,0) = K^{pq}(0,r') = 0 ,$$

$\frac{1}{r^2}\tau^{pq}(r)$, $U^{pq}(r)$, $\frac{1}{r} V^{pq}(r)$, $W^{pq}(r)$ and $K^{pq}(r,r')$ vanish at sufficiently large r and/or r'.

Also $\tau^{pq}(r)$, $U^{pq}(r)$, $V^{pq}(r)$, $W^{pq}(r)$ have no poles at the origin.

Further the expressions $\tau^{pq}(r)$ and $U^{pq}(r)$ are given by

$$\tau^{pq}(r) = l_p(l_p+1)\delta^{pq} + F^{pq}(r)$$

and

$$U^{pq}(r) = -k_p^2 \delta^{pq} + G^{pq}(r)$$

where δ^{pq} is the Krönecker delta.

The boundary conditions of $y^p(r)$ are

$$y^p(0) = 0 \qquad \text{and} \qquad y^p(h) = \text{a constant,}$$

where h is the interval of integration chosen to give small error terms.

The numerical method for the solutions of the equations in which the first derivative is absent was suggested by Fox and Goodwin, 1949, and the details of its application to the nuclear scattering problems were given by Robertson, 1956. We shall follow very closely the work of Robertson and add modifications to include the first derivative term in the equations.

We choose to divide the range of integration into two parts so that near the origin the expressions in the equations are tabulated at a small interval and in the asymptotic region at a large interval. The pivotal points are taken to be $0, h, 2h, \ldots\ldots n_1 h, \overline{n_1+2}\,h, \ldots\ldots n_2 \cdot 2h$.

Equations (15.1) can then be reduced to a system of linear difference equations in unknowns $y^p(2h), y^p(3h) \ldots\ldots y^p(n_1 h), y^p(\overline{n_1+2}\,h), \ldots\ldots y^p(n_2 \cdot 2h)$, by using the central difference formulae for derivatives given by

$$h^2 \frac{d^2}{dr^2} y(r) = (\delta^2 - \tfrac{1}{12}\delta^4 + \tfrac{1}{90}\delta^6 - \ldots\ldots)\, y(r)$$

and

$$h \frac{d}{dr} y(r) = \mu(\delta - \tfrac{1}{6}\delta^3 + \tfrac{1}{30}\delta^5 - \ldots\ldots)\, y(r)$$

where δ and μ have usual definitions (cf. Buckingham, 1962, p.146)

Therefore the equations (15.1) are replaced by

$$\sum_{q=1}^{m} \left[\delta^{pq} + W^{pq}(r)\right](\delta^2 - \tfrac{1}{12}\delta^4 + \tfrac{1}{90}\delta^6 - \ldots\ldots)\, y^q(r) + h^2 \sum_{q=1}^{m} \tfrac{1}{r^2} \tau^{pq}(r)\, y^q(r)$$

$$+ h^2 \sum_{q=1}^{m} U^{pq}(r)\, y^q(r) + h \sum_{q=1}^{m} \tfrac{1}{r} V^{pq}(r)\, \mu(\delta - \tfrac{1}{6}\delta^3 + \tfrac{1}{30}\delta^5 - \ldots\ldots)\, y^q(r)$$

$$+ h^2 \sum_{q=1}^{m} \sum_{s=0}^{n+1} h\, T_s\, K^{pq}(r, sh)\, y^q(sh) = 0 \,, \qquad \ldots\ldots (15.2)$$

where $h' = h$ for $0 \le s \le n_1$

$= 2h$ for $n_1 < s \le n_2$

$n = \frac{1}{2}n_1 + n_2 - 1$,

and T_s are the integration coefficients.

Here the method of Fox and Goodwin to reduce the errors in the difference formulae is not applicable. To keep the errors as small as practicable we include the terms in δ^4 and $\mu\delta^3$ and neglect those of higher orders.

The following notations are used :

$$y^p(th') = y^p_t ,$$

$$\delta^{pq} + w^{pq}(th') = x^{pq}(th') = x^{pq}_t ,$$

and $$h T_s K^{pq}(th', sh') = K^{pq}_{ts} .$$

Equations (15.2) are now written as

$$\sum_{q=1}^{m} x^{pq}_t \left(-\tfrac{1}{12}y^q_{t-2} + \tfrac{4}{3}y^q_{t-1} - \tfrac{5}{2}y^q_t + \tfrac{4}{3}y^q_{t+1} - \tfrac{1}{12}y^q_{t+2}\right)$$

$$+ h' \sum_{q=1}^{m} \frac{1}{th'} v^{pq}_t \left(-\tfrac{1}{12}y^q_{t-2} + \tfrac{2}{3}y^q_{t-1} - \tfrac{2}{3}y^q_{t+1} + \tfrac{1}{12}y^q_{t+2}\right)$$

$$+ h'^2 \sum_{q=1}^{m} \left[\frac{1}{(th')^2}\left\{ l_p(l_p+1)\delta^{pq} + F^{pq}_t \right\} + \left\{ -k_p^2\delta^{pq} + G^{pq}_t \right\} \right] y^q_t$$

$$+ h'^2 \sum_{q=1}^{m} \sum_{s=0}^{n+1} K^{pq}_{ts}\, y^q_s = 0 , \qquad \ldots\ldots (15.3)$$

for $t = 2, 3, \ldots\ldots (n-1)$.

Equations (15.3) are a system of $(n-2)$ simultaneous equations with n unknowns. The reduction in the number of equations is due to the use of the five-point difference formulae for the derivatives. The additional

equations may be obtained by applying a forward difference formula to the euqations at the point where $t=1$ and a backward difference formula where $t=n$, and the formulae are chosen so that they carry errors of the same order as the other formulae used.

By specifying the boundary conditions for each y^p the equations (15.1) give m linearly independent sets of solutions, so the equations (15.3) may be written in short as

$$Ay = B$$

where A and B are matrices of dimensions $(mn)\times(mn)$ and $(mn)\times m$ respectively.

and y is an $(mn)\times(mn)$ matrix given, for each p, by

$$y = \begin{pmatrix} {}^{(1)}y^1 & {}^{(2)}y^1 & \cdots & {}^{(m)}y^1 \\ {}^{(1)}y^2 & {}^{(2)}y^2 & \cdots & {}^{(m)}y^2 \\ \vdots & \vdots & & \vdots \\ {}^{(1)}y^m & {}^{(2)}y^m & \cdots & {}^{(m)}y^m \end{pmatrix}$$

where each ${}^{(q)}y^p$ $(p, q = 1, 2, \ldots\ldots m)$ is a $(n-1)\times 1$ column vector,

$${}^{(q)}y^p = \begin{pmatrix} {}^{(q)}y^p_2 \\ {}^{(q)}y^p_3 \\ \vdots \\ {}^{(q)}y^p_{n+1} \end{pmatrix} .$$

Hence it remains to evaluate and combine the contributions of all the terms in equation (2.6) to the matrices A and B at each pivotal point, and then the radial wave functions given by y are obtained by matrix inversion.

XV.2 PROGRAMMING FOR COMPUTATION

The numerical process of solving the integro-differential equations which occur in the nuclear scattering problems has always been a long and tedious one. With the help of electronic computers we are now able to extend the calculations so as to improve the accuracy but the programmes for presentation to the machines can become rather complicated. In this section we give brief details of the process used with the London University Atlas computer, starting with the numerical data and resulting in the solutions of the equation..

The range of integration in our problem was chosen as

$$n_1 h + (n_2 - \tfrac{1}{2} n_1)\, 2h$$

where

$$h = 0{\cdot}2 \times 10^{-13} \text{ cm.}$$

and $n_1 = 16$ and $n_2 = 32$.

The various expressions in the equations were evaluated to six decimal places and the asymptotic regions starts at $12{\cdot}8 \times 10^{-13}$ cm.

XV.2.1 PREPARING THE DATA

The preliminary step is to compute the constants in all the terms given in euations (13.1), (13.2) which are functions of the parameters, for each of the eight Gaussian terms. This is necessary for the tabulation of the kernels (indirect interaction) because the programme for the kernels is itself very long.

For example, we take the term ${}^{LS}K_l(r,r')$ of equation (13.1) which is given by

$$ {}^{LS}K_l(r,r') = +\left(\frac{4}{3}\right)^4 \frac{M}{\hbar^2} \frac{4\pi}{\delta} A_i A_j \, {}^{LS}U^{(2)}_{K\, 2\delta} \frac{w}{} \Lambda_{Jl} \, \mathcal{J}_{L+\frac{1}{2}}(\delta r r') \, e^{-ar^2 - br'^2} $$

The parameters and the constants to be evaluated for each ℓ are

$$a_{ijk},\ b_{ijk},\ \delta_{ijk} \quad \text{and} \quad +\left(+\frac{4}{3}\right)^{4} \frac{M}{\hbar^2} 4\pi A_i A_j \overset{LS}{U}{}^{(2)}_{k} \frac{w_{ij}}{2\delta^2_{ijk}} \Lambda_{J\ell},$$

for each $i,j,k = 1,2$.

XV.2.2. EVALUATION OF THE DIRECT TERMS

There are four types of the direct terms in the equations, and are classified as $\tau^{pq}(r)$, $u^{pq}(r)$, $v^{pq}(r)$ and $w^{pq}(r)$. In the actual computation it is the expressions $F^{pq}(r)$, $G^{pq}(r)$, $V^{pq}(r)$ and $X^{pq}(r)$ which are tabulated at the following 40 points, $h, 2h, 3h, \ldots 16h, 18h, \ldots 64h$.

The computer programmes can easily be written to evaluate these terms as well as all the parameters and constants. It is convenient to seperate the programmes for the doublet and the quartet case because some of the data in the two cases are different.

If we use

p to denote the four different types of the direct terms, e.g. a $u(r)$,

q to represent the cases, e.g. a doublet case with $\ell = 1$,

s to distinguish the interaction terms, e.g. the quadratic spin-orbit S-S term with $\frac{1}{4}(2b-m)_\nu {}^{\nu}V_Q$ potential.

and t to number the Gaussian terms (t takes eight values),

then for each p and q the general form of the direct term is given by

$$D_{pq} = \sum_{s,t} K^{st}_{pq} \Phi^{st}_{pq} e^{-a_{st}r^2}.$$

An outline of the programme for the evaluation of the direct terms is given in Table 6.

XV.2.3. THE EVALUATION OF THE KERNELS.

Burke (1959) wrote a programme (for the Mercury computer) for the tabulation of kernels of a given type with changes of interval lengths. The programme is adjusted for our purpose with an additional part to include the evaluation of kernels which contain first order derivatives of the Spherical Bessel functions.

The general form of the kernels may be written

$$K(r,r') = \sum_s A_s \sum_t \phi_{st}(r,r') e^{-a_{st}r^2 - b_{st}r'^2} j_{l_{st}+\frac{1}{2}}(c_{st}rr')$$

where s counts the number of kernels in each case,

t counts the number of expressions in each kernel,

$\phi_{st}(r,r')$ is a polynomial form given by

$$\phi_{st}(r,r') = \sum_{n_t(p,q)} B_{pq}^{st} r^p r'^q ,$$

where n_t represents the number of terms in each $\phi_{st}(r,r')$.

An outline of the 'kernel programme' is given in Table 7.

In the actual programme the settings of r and r' are divided into parts so as to take care of the changes of interval in r and r' and the kernels are tabulated in the corresponding regions of the (r,r') plane.

The programme for the kernels containing the function $j'_{l+\frac{1}{2}}(x)$ involves the same sequence of computation. The functions $j_{l+\frac{1}{2}}(x)$ and $j'_{l+\frac{1}{2}}(x)$ are calculated by using their analytical forms for $l = 0, 1, 2, 3$ and 4.

The tabulated kernels will now consists of two types, the energy-dependent called the N-kernels and the energy-independent called the non- N kernels.

XV.2.4 SOLUTIONS OF THE INTEGRO-DIFFERENTIAL EQUATIONS

The computer programme for the solutions of the integro-differential equations has the same structure as that of Burke's with the modification in the numerical method illustrated in section XV.1. The direct terms and the kernels which are thus tabulated and stores as output in a suitable form are now used as part of the data in the 'equation programme' outlined in Table 8. In the programme which is written in Mercury Autocode language the contributions of the various elements of the kernels and the direct terms to the matrices A and B are computed row by row, and at some points owing to changes in interval length interpolations are necessary. These changes in the interval of tabulation make it more difficult to specify the storage addresses in the computer of the elements of the kernels and the matrix elements. This difficulty may be eliminated if the programme is written in a language such as FORTRAN or ALGOL in which specifications of matrix elements can be done in simple ways. The dimension of the matrices to be inverted in the calculation is 39×39 for single equations and 78×78 for coupled equations.

TABLE 6. PROGRAMME TO EVALUATE THE DIRECT TERMS.

```
Set s
        read data
        store data in order of s and t
repeat for s
set q
        clear store for results
        set p
                set s
                    set t
                        evaluate parameters and constants
                        set r
                            evaluate expressions
                            store results
                        repeat for r
                    repeat for t
                repeat for s
        repeat for p
        output results
repeat for q
end
```

TABLE 7. PROGRAMME TO EVALUATE THE KERNELS

read s

set s read n_t

set n_t

read pairs of (p,q)

repeat for n_t

read t

set t

read coefficients a_{st}, b_{st}, c_{st}, Γ_{st} and B_{pq}^{st}

repeat for t

read A_s

set r'

set r

evaluate $r^p r'^q$ for all pairs of (p,q)

set t

evaluate $\Phi_{st}(r,r')$

evaluate $exp.[-a_{st}r^2 - b_{st}r'^2]$

compute $\mathcal{J}_{\Gamma_{st}+\frac{1}{2}}(c_{st}rr')$

put $K_s(r,r') = \Phi_{st}(r,r')\, e^{-a_{st}r^2 - b_{st}r'^2}\, \mathcal{J}_{\Gamma_{st}+\frac{1}{2}}(c_{st}rr')$

add $K_s(r,r')$ together

repeat for t

repeat for r

repeat for r'

repeat for s

output

TABLE 8 THE 'EQUATION PROGRAMME'

```
begin
read data
read kernels
read direct terms
set cycle for energy
      clear store for result
      set cycle for terms in coupled equations
            add elements of N and non-N kernels
            compute contributions to matrices A and B
            (for each region of kernels)
            set cycle for direct terms
                  compute cobtributions to A and B
            repeat for all direct terms
      repeat for all terms in coupled equations
      manipulation
      matrix inversion
      output
repeat for all energy levels
end.
```

CHAPTER XVI.

PHASE SHIFTS ANALYSIS AND CROSS SECTIONS

XVI.1. PHASE SHIFT ANALYSIS

As mentioned in section I.3. the inclusion of the non-central forces has introduced couplings of states with different values of the orbital angular momentum ℓ, thus the phases of the scattered wave are split into components depending on ℓ and the total angular momentum J. Blatt and Biedenharn, 1952 have given a detailed discussion on reactions which involve more than one channel of collision between two particles. Further analyses specialised to the elastic n-d scattering process are given by Bransden, Tate and Smith, 1959, and Hamda, 1959. In all these papers the procedure of the parametrisation of the scattering matrix was used to identify the'phase shifts' and to derive general formulae for cross-sections. Here we propose to obtain the phase shifts in a straight forward way. In Table 9 we list the radial wave functions and the phase shifts corresponding to the substates of each pair of (J, P) with $J = \frac{1}{2}$ and $3/2$, and P defined by

$$P = (-1)^{J-\frac{1}{2}+\ell} .$$

The two pairs of coupled states (when $s = 3/2$ only) are specified by

$(J, P) = (\frac{3}{2}, -)$ corresponding to $(\ell, s) = (0, 3/2)$ and $(2, 3/2)$

and $(J, P) = (\frac{3}{2}, +)$ corresponding to $(\ell, s) = (1, 3/2)$ and $(3, 3/2)$.

TABLE 9

	(l,s)	(J,P)	wave function	phase shifts
Doublet case	$0,\frac{1}{2}$	$\frac{1}{2},+$	$^2f_0^+$	$^2\eta_0^+$
	$1,\frac{1}{2}$	$\frac{1}{2},-$	$^2f_1^-$	$^2\eta_1^-$
	$1,\frac{1}{2}$	$\frac{3}{2},+$	$^2f_1^+$	$^2\eta_1^+$
	$2,\frac{1}{2}$	$\frac{3}{2},-$	$^2f_2^-$	$^2\eta_2^-$
Quartet case	$1,\frac{3}{2}$	$\frac{1}{2},-$	$^4f_1^-$	$^4\eta_1^-$
	$2,\frac{3}{2}$	$\frac{1}{2},+$	$^4f_2^+$	$^4\eta_2^+$
Coupled	$0,\frac{3}{2}$	$\frac{3}{2},-$	$^4f_0^-$	$^4\eta_0^-$
Coupled	$2,\frac{3}{2}$	$\frac{3}{2},-$	$^4f_2^-$	$^4\eta_2^-$
	$1,\frac{3}{2}$	$\frac{3}{2},+$	$^4f_1^+$	$^4\eta_1^+$
	$3,\frac{3}{2}$	$\frac{3}{2},+$	$^4f_3^+$	$^4\eta_3^+$

XVI.1.1 Single states

The calculation of phase shifts in uncoupled states is straight forward. The asymptotic form of any of the wave functions has the form (e.g. Mott and Massey, 1949, p.35)

$$f_l(r) = K_l\left[\sqrt{kr}\cos\eta_l J_{l+\frac{1}{2}}(kr) + \sqrt{kr}\sin\eta_l J_{-l-\frac{1}{2}}(kr)\right] \quad \ldots\ldots(16.1)$$

where K_l is the constant amplitude,

$J_{l+\frac{1}{2}}(kr)$, $J_{-l-\frac{1}{2}}(kr)$ are the Bessel functions of half integer order, and k is the wave number of the incident neutron given by

$$k = \frac{4}{3}\frac{M}{\hbar^2}E_n .$$

By applying the formula at two neighbouring points r_1 and r_2 we thus obtain

$$\tan \eta_\ell = - \frac{f_\ell(r_2)\sqrt{kr_1}\, J_{\ell+\frac{1}{2}}(kr_1) - f_\ell(r_1)\sqrt{kr_2}\, J_{\ell+\frac{1}{2}}(kr_2)}{f_\ell(r_2)\sqrt{kr_1}\, J_{-\ell-\frac{1}{2}}(kr_1) - f_\ell(r_1)\sqrt{kr_2}\, J_{-\ell-\frac{1}{2}}(kr_2)} .$$

The phase shifts η_ℓ are calculated using two pairs of the agrument r as a check. Their numerical values at each energy are given in Tables 10.-13.

XVI.1.2 Coupled states

If we distinguish the two independent solution of the integro-differential equation given in section XIII.2 by the suffices (i), $i = 1,2$ then the pairs of the radial wave functions can be denoted by

$$\left[{}^4f_\ell^{(1)}, {}^4f_{\ell+2}^{(1)} \right] \quad \text{and} \quad \left[{}^4f_\ell^{(2)}, {}^4f_{\ell+2}^{(2)} \right]$$

for $\ell = 0, 1$.

Thus arbitrary solutions of the integro-differential equations are given by

$$ {}^4f_\ell = a\, {}^4f_\ell^{(1)} + b\, {}^4f_\ell^{(2)}$$

and

$$ {}^4f_{\ell+2} = a\, {}^4f_{\ell+2}^{(1)} + b\, {}^4f_{\ell+2}^{(2)}$$

where a and b are constants.

The phase shifts ${}^4\eta_\ell^{(i)}$, ${}^4\eta_{\ell+2}^{(i)}$ and the corresponding ampolitudes $K_\ell^{(i)}$, $K_{\ell+2}^{(i)}$ can now be calculated using the same formula (16.1) for each ${}^4f_\ell^{(i)}$, ${}^4f_{\ell+2}^{(i)}$. In order to define the solutions uniquely we have to impose some relation between the amplitudes of the incidental waves. We take ${}^4K_\ell = {}^4K_{\ell+2}$ so that the scattered wave is unpolarized. This corresponds to the situation where the incident neutron beam is unpolarized because the interaction due to the non-central forces is symmetrical.

Equating the coefficients of the Bessel functions in the general asymptotic solutions given above we get

$$K \cos \eta_\ell = a K_\ell^{(1)} \cos \eta_\ell^{(1)} + b K_\ell^{(2)} \cos \eta_\ell^{(2)}$$

$$K \sin \eta_\ell = a K_\ell^{(1)} \sin \eta_\ell^{(1)} + b K_\ell^{(2)} \sin \eta_\ell^{(2)}$$

and

$$K \cos \eta_{\ell+2} = a K_{\ell+2}^{(1)} \cos \eta_{\ell+2}^{(1)} + b K_{\ell+2}^{(2)} \cos \eta_{\ell+2}^{(2)}$$

$$K \sin \eta_{\ell+2} = a K_{\ell+2}^{(1)} \sin \eta_{\ell+2}^{(1)} + b K_{\ell+2}^{(2)} \sin \eta_{\ell+2}^{(2)}$$

where η_ℓ , $\eta_{\ell+2}$ are the required phase shifts

K is the common amplitude of the required solution.

and a , b are the constants which have to be determined.

By eliminating η_ℓ , $\eta_{\ell+2}$ and K from these equations we obtain a quadratic equation for a/b :

$$a^2 \left[(K_\ell^{(1)})^2 - (K_{\ell+2}^{(1)})^2 \right] + 2ab \left[K_\ell^{(1)} K_\ell^{(2)} - K_{\ell+2}^{(1)} K_{\ell+2}^{(2)} \right] + b^2 \left[(K_\ell^{(2)})^2 - (K_{\ell+2}^{(2)})^2 \right] = 0 .$$

The two solution of the equation correspond to $K_\ell = \pm K_{\ell+2}$,

and on examination of the numerical results it is possible to choose the value of a/b which corresponds to $K_\ell = K_{\ell+2}$.

Finally the phase shifts are given by

$$\tan \eta_\ell = \frac{a K_\ell^{(1)} \sin \eta_\ell^{(1)} + b K_\ell^{(2)} \sin \eta_\ell^{(2)}}{a K_\ell^{(1)} \cos \eta_\ell^{(1)} + b K_\ell^{(2)} \cos \eta_\ell^{(2)}}$$

and similarly for $\eta_{\ell+2}$.

XVI.2 THE TOTAL CROSS SECTIONS.

From the general formula given by Blatt and Biedenharn, 1952, we may explicitly write down the total cross-section S for the n-d collision in our notation as

$$S = \frac{2\pi}{3k^2} \times$$

$$\times \left[2 \left\{ \sin^2\left({}^2\eta_0^+\right) + \sin^2\left({}^2\eta_1^-\right) + \sin^2\left({}^4\eta_1^-\right) + \sin^2\left({}^4\eta_2^+\right) \right\} \right.$$

$$\left. + 4 \left\{ \sin^2\left({}^2\eta_1^+\right) + \sin^2\left({}^2\eta_2^-\right) + \sin^2\left({}^4\eta_0^-\right) + \sin^2\left({}^4\eta_1^+\right) + \sin^2\left({}^4\eta_2^-\right) + \sin^2\left({}^4\eta_3^+\right) \right\} \right].$$

TABLE 10 The ${}^2\eta_0^+$ phases

k	E_n	${}^2\eta_0^+$	BHM	CG	BR
0·075	0·26	0·701	-0·30		-0·227
0·104	0·5	0·807	-0·42*	-0·177*	
0·147	1·0	0·871	-0·58*	-0·285*	
0·205	1·95	0·852	-0·81*	-0·431*	
0·265	3·29	0·763			
0·4	7·45	0·444	-1·40		-1·322
0·548	14	0·040			
0·6	16·77	-0·098	-1·81		
0·803	30	-0·579			
1·036	50	-1·002			

TABLE 11 : The $^2\eta_1$ phases

k	E_n	$^2\eta_1^-$	$^2\eta_1^+$	BHM	CG	BR
0.075	0.26	-0.007	-0.007			
0.104	0.5	-0.018	-0.018	-0.02 †	-0.04 †	
0.147	1.0	-0.045	-0.046	-0.04 †	-0.07 †	
0.205	1.95	-0.095	-0.098	-0.09 †	-0.11 †	
0.265	3.29	-0.137	-0.143			
0.4	7.45	-0.084	-0.093	-0.25	-0.25 *	-0.253
0.548	14.0	0.172	0.158	-0.20 *	-0.26 *	
0.6	16.77	0.281	0.266	-0.19	-0.19 *	-0.238
0.803	30	0.704	0.679			
1.036	50	1.114	1.071			

TABLE 12 : The $^4\eta_1$ phases

k	E_n	$^4\eta_1^-$	BHM	CG	BR
0.075	0.26	0.016			
0.104	0.5	0.039	0.065 †	0.09 †	
0.147	1.0	0.098	0.135 †	0.17 †	
0.205	1.95	0.225	0.27 †	0.295 †	
0.265	3.29	0.405			
0.4	7.45	0.926	0.55	0.39 *	0.417
0.548	14.0	-1.547	0.39 *	0.36 *	
0.6	16.77	-1.360	0.30	0.34 *	0.322
0.803	30	-0.350			
1.036	50	0.71			

TABLE 13: The D-Phases.

k	E_n	$^2\eta_2$			$^4\eta_2$		
		$^2\eta_2^-$	BHM	CG	$^4\eta_2^+$	BHM	CG
0.075	0.26						
0.104	0.5	-0.0003	0.0045†	0.004†		-0.014†	-0.008†
0.147	1.0	-0.0016	0.0095†	0.009†	0.026	-0.027†	-0.0185†
0.205	1.95	-0.0074	0.02†	0.025†	0.193	-0.0515†	-0.046†
0.265	3.29	-0.0216			1.232		
0.4	7.45		-0.085		-1.074	-0.177	
0.548	14.0	-0.175			-1.231		
0.6	16.77		-0.100		-1.256	-0.177	
0.803	30	-0.209			-1.139		
1.036	50	-0.288			-1.236		

The phases are given in radians between the range

$$-\pi/2 \leq \eta \leq \pi/2 .$$

The previous results are taken from

BHM - Buckingham, Hubbard and Massey, 1955, (MHWB force)

CG - Christian and Gammel, 1953,

BR - Burke and Robertson, 1957, (MHWB force) with $\mu = 0.3 \times 10^{26}$ cm.$^{-2}$)

† - from Elwyn, Lane and Lansdorf, 1962,

* - from de Borde and Massey, 1955.

CONCLUSION

The theoretical consideration of the n - d scattering problem using the resonating group method for three-body wave functions and the nucleon-nucleon interaction derived by Hamada and Johnston (1962) presents difficulties and we sum up the attempts to overcome these.

1. The presence of non-central force operators necessitates the use of the potential wells in Gaussian form in order to simplify the analysis. This is not in line with the results of recent field theory and even though two Gaussian terms were used, the interaction still appears to give a smaller contribution than the Yukawa form at large distances. The similar representation of the deuteron radial wave functions is more satisfactory.

2. The hard cores of the potentials present a difficulty in the analysis of scattering problems of more than two particles. Their presence causes the M -dependence of the eigen functions and this has to be overcome. Although the modification of the deuteron wave function is to take care of the hard core effecr, it has not fully been accounted for because the core radius is taken to be zero.

3. The complexity of the algebra is mainly due to the quadratic spin-orbit operator. It introduces new typesof matrix elements and terms which involve first and second order derivatives of the unknown radial wave functions in the integro-differential equations. The difference formulae used in the numerical method to solve this type of equations gave results accurate to five decimal places.

4. The symmetrisations of the quadratic spin-orbit and the S-D, D-S spin-orbit direct terms were necessary because we had used the more compact forms of the respective operators instead of the fully Hermitian ones.

We have so far obtained the solutions and the phase shifts for the uncoupled equations but the coupled equations present considerable

difficulties. The results of the coupled equations (with corresponding phases, ${}^4\eta_0^-$, ${}^4\eta_2^-$, ${}^4\eta_1^+$, ${}^4\eta_3^+$) will be reported in a future publication.

It should be noted that the phases in our case are split into components depending on ℓ and J whereas the phases calculated by other authors depend on ℓ only. The only direct comparision which can be made is in the ${}^2\eta_0^+$ phases and our values are much larger in magnitude. At low incident neutron energies, the S- and D - phasesof our calculation have opposite sign to the corresponding phases obtained by the others, but the P - phases have the same sign and at energies up to about 3 Mev. they differ only slightly. Our values of the P - phases for $J = \frac{1}{2}$ and $J = 3/2$ for the doublet case are nearly the same. The large discrepensies in the phases may be due entirely to the completely different nature of the nuclear interaction used.

It remains to be seen whether these discrepensies will reflect in the differential and the total cross-sections and also whether the interaction which fits the nucleon-nucleon data will give the correct triton binding energy. A significant difference will prove that there are other phenomenae to be considered when applying the nucleon-nucleon interaction to many-body problems.

APPENDIX 1.

COORDINATES AND TRANSFORMATION

The incident neutron is labelled as the particle 1 and has the position vector $\underline{r}_1$. The other neutron is labelled 2 and the proton, 3 with respective position vectors $\underline{r}_2$ and $\underline{r}_3$.

We define $\underline{r}$ as the co-ordinates of particle 1 relative to the centre of mass of the other two, thus

$$\underline{r} = \underline{r}_1 - \tfrac{1}{2}(\underline{r}_2 + \underline{r}_3) .$$

We usually write $(1\text{-}23) = (1) = \underline{r} = (r, \theta, \varphi)$

Similarly $\underline{r}'$ is defined as

$$\underline{r}' = \underline{r}_2 - \tfrac{1}{2}(\underline{r}_3 + \underline{r}_1) ,$$

and we write $(2\text{-}13) = (2) = \underline{r}' = (r', \theta', \varphi')$

Other co-ordinates are defined by

$$(23) = \underline{r}_{23} = \underline{r}_2 - \underline{r}_3 = \underline{R} ,$$

$$(12) = \underline{r}_{12} = \underline{r}_1 - \underline{r}_2 = \underline{r} - \tfrac{1}{2}\underline{R} .$$

If $\underline{p}_1$ and $\underline{p}_2$ are the momentum vectors of the particles 1 and 2 respectively referred to a fixed origin then

$$i\underline{p}_1 = \frac{\partial}{\partial \underline{r}_1} = \frac{\partial}{\partial \underline{r}}$$

$$i\underline{p}_2 = \frac{\partial}{\partial \underline{r}_2} = -\tfrac{1}{2}\frac{\partial}{\partial \underline{r}} + \frac{\partial}{\partial \underline{R}} .$$

Hence it follows that

$$i\underline{L}_{12} = (\underline{r}_1 - \underline{r}_2) \wedge (\underline{p}_1 - \underline{p}_2)$$

$$= (\underline{r} - \tfrac{1}{2}\underline{R}) \wedge \left(\tfrac{3}{2}\frac{\partial}{\partial \underline{r}} - \frac{\partial}{\partial \underline{R}}\right) .$$

In the calculation for the indirect interaction, the following co-ordinates are used:

$$\underline{r}_{23} = \tfrac{2}{3}(\underline{r}+2\underline{r}') ,$$

$$\underline{r}_{13} = \tfrac{2}{3}(2\underline{r}+\underline{r}') ,$$

$$\underline{r}_{12} = \tfrac{2}{3}(\underline{r}-\underline{r}') .$$

and the momentum operators,

$$i\underline{p}_1 = \frac{\partial}{\partial \underline{r}} - \tfrac{1}{2}\frac{\partial}{\partial \underline{r}'} ,$$

$$i\underline{p}_2 = -\tfrac{1}{2}\frac{\partial}{\partial \underline{r}} + \frac{\partial}{\partial \underline{r}'} .$$

Hence we obtain

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

The transformation used for the volume integration is

$$d\underline{r}_{23} = \left(\tfrac{4}{3}\right)^3 d\underline{r}'$$

with $$d\underline{r}' = r'^2\, d\Omega' dr' ,$$

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

APPENDIX 2

NUMERICAL CONSTANTS

A. THE DEUTERON RADIAL WAVE FUNCTIONS

The S- and D- state deuteron radial wave functions are interpolated from Hamada and Johnston's data into the following Gaussian form:

$$\phi(r) = r^2 \sum_{i=1}^{2} A_i e^{-\alpha_i r^2}$$

The numerical values of the constants are listed below :

S-state $A_1 = 0.174285$, $\alpha_1 = 0.7330$,

$A_2 = 0.022563$, $\alpha_2 = 0.1651$.

D-state $A_1' = 0.042822$, $\alpha_1' = 1.1140$,

$A_2' = 0.005500$, $\alpha_2' = 0.2864$.

Both A and α have the same unit of 10^{26} $cm.^{-2}$

The wave functions are normalised such that

$$\int (\phi_S^2 + B\phi_D^2)\, d\tau = 1 .$$

B. THE NUCLEAR INTERACTION

The interactions defined in various Chapters are degined in general by

$$\sum_{K=1}^{2} {}^{\lambda}U_K^{(\gamma)} e^{-{}^{\lambda}\mu_K^{(\gamma)} r^2}$$

and in the case of the tensor force only, by

$$r^2 \sum_{K=1}^{2} {}^{T}U_K^{(\gamma)} e^{-{}^{T}\mu_K^{(\gamma)} r^2} .$$

The numerical values of U_K and μ_K are given in Table 14.

TABLE 14

λ	(ν)	$U_1 =$	$\mu_1 =$	$U_2 =$	$\mu_2 =$
Central	Direct 1	1712·9610	6·2499	60·4330	1·0834
	Direct 3	929·4136	14·3418	−41·6698	1·6348
	Indirect 2	−510·9348	4·8030	−66·5970	0·9926
	Indirect 4	−108·7694	2·0638	−11·6857	0·5419
spin-orbit	Direct 1	−13055·3858	7·3379	−546·8303	2·1088
	Indirect 2	−15822·9438	8·5581	−848·1197	2·3607
Tensor	Direct 1	33421·5771	11·7651	124·1191	1·5351
	Indirect 2	148602·1967	22·4051	4·4024	0·2849
Quadratic spin-orbit	Direct 1	−86082·9505	16·4675	74·2121	2·2038
	Direct 3	8692·9506	9·3852	92·8297	2·6856
	Indirect 2	−7120·5038	8·6826	−16·0719	1·8611
	Indirect 4	11194·6159	11·7960	164·9214	3·6515

U_k are given in Mev.

and μ_k in 10^{26} $cm.^{-2}$

APPENDIX 3.

SPIN FUNCTIONS

We indicate the incident neutron, the other neutron and the proton in the system by suffices $1, 2$ and 3 respectively. If α_i and β_i are the usual spin functions of the nucleon i, then we can write the three-body spin functions, $\chi^S_{m_S}$ in the following way (see e.g. Schiff, 1955 p. 235).

DOUBLET CASE:

With $S = \frac{1}{2}$, $m_S = \frac{1}{2}$ and $-\frac{1}{2}$, the spin functions are

$$\chi^{\frac{1}{2}}_{\frac{1}{2}}(1,\bar{23}) = \frac{1}{\sqrt{6}}(\alpha_1\alpha_2\beta_3 + \alpha_1\beta_2\alpha_3 - 2\beta_1\alpha_2\alpha_3),$$

$$\chi^{\frac{1}{2}}_{-\frac{1}{2}}(1,\bar{23}) = \frac{1}{\sqrt{6}}(\beta_1\alpha_2\beta_3 + \beta_1\beta_2\alpha_3 - 2\alpha_1\beta_2\beta_3)$$

and they are symmetrical in 2 and 3.

It is often very useful in the doublet case to use the anti-symmetrical spin functions in the simplification of spin products. These functions are given by

$$\chi^{\frac{1}{2}}_{\frac{1}{2}}(1,\tilde{23}) = \frac{1}{\sqrt{2}}\alpha_1(\alpha_2\beta_3 - \alpha_3\beta_2)$$

and

$$\chi^{\frac{1}{2}}_{-\frac{1}{2}}(1,\tilde{23}) = \frac{1}{\sqrt{2}}\beta_1(\alpha_2\beta_3 - \alpha_3\beta_2).$$

They have the following properties:

$$\chi^{\frac{1}{2}}_{m_S}(1,\tilde{23})\,\underline{\sigma}_i\,\chi^{\frac{1}{2}}_{m_S}(1,\tilde{23}) = 0 \qquad \text{for } i = 2 \text{ and } 3,$$

and

$$f(\underline{\sigma}_2,\underline{\sigma}_3)(\underline{\sigma}_2+\underline{\sigma}_3)\chi^{\frac{1}{2}}_{m_S}(1,\tilde{23}) = 0 \qquad \text{for any function } f.$$

Vectors of the Spin functions which we often use in the derivation of the integro-differential equations are defined as

$$\chi^{\frac{1}{2}} \equiv \bar{\chi}^{\frac{1}{2}} \equiv \bar{\chi}^{\frac{1}{2}}(1) = \left[\bar{\chi}^{\frac{1}{2}}_{\frac{1}{2}}(1,\bar{23}),\ \bar{\chi}^{\frac{1}{2}}_{-\frac{1}{2}}(1,\bar{23})\right],$$

and $$\tilde{\chi}^{\frac{1}{2}} \equiv \tilde{\chi}^{\frac{1}{2}}(1) = \left[\tilde{\chi}^{\frac{1}{2}}_{\frac{1}{2}}(1,2\tilde{3}) , \tilde{\chi}^{\frac{1}{2}}_{-\frac{1}{2}}(1,2\tilde{3}) \right] .$$

Some of the transformations used before spin summations are

$$\bar{\chi}^{\frac{1}{2}}(1) = \frac{1}{\sqrt{3}} \underline{\sigma}_1 \cdot \underline{\sigma}_2 \, \tilde{\chi}^{\frac{1}{2}}(1)$$

$$\bar{\chi}^{\frac{1}{2}}(2) = \frac{1}{2\sqrt{6}} (3 - \underline{\sigma}_1 \cdot \underline{\sigma}_2) \, \tilde{\chi}^{\frac{1}{2}}(1) .$$

The following is an example to illustrate the simplification of spin products.

Consider $$\chi^{*\frac{1}{2}} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L} \; \chi^{\frac{1}{2}}(2) .$$

By the transformation

$$\chi^{*\frac{1}{2}} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L} \; \chi^{\frac{1}{2}}(2) = \left[\frac{1}{\sqrt{3}} \underline{\sigma}_1 \cdot \underline{\sigma}_2 \, \tilde{\chi}^{\frac{1}{2}} \right]^* (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L} \left[\frac{1}{2\sqrt{3}} (3 - \underline{\sigma}_1 \cdot \underline{\sigma}_2) \, \tilde{\chi}^{\frac{1}{2}}(1) \right]$$

$$= \frac{1}{6} \, \tilde{\chi}^{*\frac{1}{2}} \, \underline{\sigma}_1 \cdot \underline{\sigma}_2 \, (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L} \, (3 - \underline{\sigma}_1 \cdot \underline{\sigma}_2) \, \tilde{\chi}^{\frac{1}{2}}$$

Now $$\underline{\sigma}_1 \cdot \underline{\sigma}_2 \, (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L} \, (3 - \underline{\sigma}_1 \cdot \underline{\sigma}_2) = \underline{\sigma}_1 \cdot \underline{\sigma}_2 \left[3 (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L} - \left\{ \underline{\sigma}_2 \cdot \underline{L} + i \, \underline{\sigma}_1 \cdot \underline{L} \wedge \underline{\sigma}_2 + \underline{\sigma}_1 \cdot \underline{L} + i \, \underline{\sigma}_2 \cdot \underline{L} \wedge \underline{\sigma}_1 \right\} \right]$$

$$= 2 \, \underline{\sigma}_1 \cdot \underline{\sigma}_2 \left[\underline{\sigma}_1 \cdot \underline{L} + \underline{\sigma}_2 \cdot \underline{L} \right]$$

$$= 2 \, (\underline{\sigma}_2 \cdot \underline{L} + \underline{\sigma}_1 \cdot \underline{L}) .$$

The term $\underline{\sigma}_2 \cdot \underline{L}$ gives zero elements,

so $$\chi^{*\frac{1}{2}} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot \underline{L} \; \chi^{\frac{1}{2}}(2) = \frac{1}{3} \, \tilde{\chi}^{*\frac{1}{2}} \, \underline{\sigma}_1 \cdot \underline{L} \, \tilde{\chi}^{\frac{1}{2}}$$

which can be easily evaluated .

QUARTET CASE :

The eigen values of the total spin and its $\hat{z}$-components in the quartet case are given by

$$S = 3/2 , \quad m_s = \tfrac{3}{2} , \tfrac{1}{2} , -\tfrac{1}{2} \text{ and } -\tfrac{3}{2} .$$

Thus we have

$$\chi^{3/2}_{3/2}(1.23) = \alpha_1\alpha_2\alpha_3 ,$$

$$\chi^{3/2}_{\frac{1}{2}}(1.23) = \frac{1}{\sqrt{3}}(\alpha_1\alpha_2\beta_3 + \alpha_1\beta_2\alpha_3 + \beta_1\alpha_2\alpha_3) ,$$

$$\chi^{3/2}_{-\frac{1}{2}}(1.23) = \frac{1}{\sqrt{3}}(\beta_1\alpha_2\beta_3 + \beta_1\beta_2\alpha_3 + \alpha_1\beta_2\beta_3) ,$$

$$\chi^{3/2}_{-3/2}(1.23) = \beta_1\beta_2\beta_3 .$$

The spin functions are symmetrical in 1, 2 and 3 and there can be no confusion if they are written as $\chi^{3/2}_{m_s}$.

APPENDIX 4

INTEGRATION FORMULAE AND SPHERICAL BESSEL FUNCTIONS

A. THE DIRECT INTERACTION

In the calculation of the direct interactions, the following formulae are used:

$$\mathcal{K}\int e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = 1 ,$$

$$\mathcal{K}\int \underline{R}\, e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \gamma\underline{I} ,$$

$$\mathcal{K}\int R^2 e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \frac{3}{2\lambda}+\gamma^2 I^2 ,$$

$$\mathcal{K}\int \underline{R}^3 e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \left(\frac{5}{2\lambda}+\gamma^2 I^2\right)\gamma\underline{I} ,$$

$$\mathcal{K}\int R^4 e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \frac{15}{4\lambda^2}+\frac{5}{\lambda}\gamma^2 I^2+\gamma^4 I^4 ,$$

$$\mathcal{K}\int S_{23}(R^2)\, e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \gamma^2 S_{23}(I^2) ,$$

$$\mathcal{K}\int (\underline{A}\cdot\underline{R})\, S_{23}(R^2)\, e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \gamma^3(\underline{A}\cdot\underline{I})\, S_{23}(I^2)+\frac{\gamma}{\lambda} S_{23}(\underline{A},\underline{I}) ,$$

$$\mathcal{K}\int R^2 S_{23}(R^2)\, e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \left(\frac{7}{2\lambda}+\gamma^2 I^2\right)\gamma^2 S_{23}(I^2) ,$$

$$\mathcal{K}\int (\underline{A}\cdot\underline{R})(\underline{B}\cdot\underline{R})\, e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \gamma^2(\underline{A}\cdot\underline{I})(\underline{B}\cdot\underline{I})+\frac{1}{2\lambda}\underline{A}\cdot\underline{B} ,$$

$$\mathcal{K}\int (\underline{A}\cdot\underline{R})(\underline{B}\cdot\underline{R})(\underline{C}\cdot\underline{R})\, e^{-\lambda(\underline{R}-\gamma\underline{I})^2}\,d\underline{R} = \gamma^3(\underline{A}\cdot\underline{I})(\underline{B}\cdot\underline{I})(\underline{C}\cdot\underline{I})+\frac{\gamma}{2\lambda}\left[(\underline{B}\cdot\underline{C})(\underline{A}\cdot\underline{I})+(\underline{C}\cdot\underline{A})(\underline{B}\cdot\underline{I})+(\underline{A}\cdot\underline{B})(\underline{C}\cdot\underline{I})\right] ,$$

where $\mathcal{K} = \left(\frac{\lambda}{\pi}\right)^{3/2}$ and $S_{23}(\underline{A},\underline{B}) = S_{23}(\underline{B},\underline{A}) = 3(\underline{\sigma}_2\cdot\underline{A})(\underline{\sigma}_3\cdot\underline{B})-\underline{\sigma}_2\cdot\underline{\sigma}_3(\underline{A}\cdot\underline{B})$.

B. THE INDIRECT INTERACTION

The integrations over spherical harmonics in the indirect interaction calculation depend on the use of the well known formula

$$\int Y_{lm}(\theta,\varphi)\, e^{-\partial \underline{r}\cdot\underline{r}'}\, d\Omega = \frac{4\pi}{\partial r r'}\, Y_{lm}(\theta',\varphi')\, \mathcal{J}_{l+\frac{1}{2}}(\partial r r')$$

where

$$\underline{r} = (r,\Omega) = (r,\theta,\varphi) ,$$

$$\underline{r}' = (r',\Omega') = (r',\theta',\varphi')$$

and $$d\Omega = \sin\theta\, d\theta\, d\phi .$$

The Spherical Bessel function is defined by

$$\mathcal{J}_{l+\frac{1}{2}}(x) = i^{l-\frac{1}{2}} \left(\frac{\pi x}{2}\right)^{\frac{1}{2}} J_{l+\frac{1}{2}}(ix) ,$$

the first few values being

$$\mathcal{J}_{\frac{1}{2}}(x) = \sinh x ,$$

$$\mathcal{J}_{\frac{3}{2}}(x) = \frac{\sinh x}{x} - \cosh x .$$

The recurrence relations between the functions are (from e.g. Whittaker and Watson, 1952)

$$\frac{(2l+1)}{x}\, \mathcal{J}_{l+\frac{1}{2}}(x) = \mathcal{J}_{l+\frac{3}{2}}(x) - \mathcal{J}_{l-\frac{1}{2}}(x)$$

and

$$\mathcal{J}'_{l+\frac{1}{2}}(x) = \frac{(l+1)}{x}\, \mathcal{J}_{l+\frac{1}{2}}(x) - \mathcal{J}_{l+\frac{3}{2}}(x) .$$

From these two formulae we may further derive the result

$$\mathcal{J}''_{l+\frac{1}{2}}(x) = \left[\frac{l(l+1)}{x^2} + 1\right] \mathcal{J}_{l+\frac{1}{2}}(x) .$$

APPENDIX 5

COLLECTION OF PARAMETERS

The parameters defined in the direct interaction calculation are as follows:

S-S	S-D	D-S
$\lambda_{ijk} = \alpha_i+\alpha_j+\frac{1}{4}\mu_k$,	$\lambda'_{ijk} = \alpha_i+\alpha'_j+\frac{1}{4}\mu_k$	$= \lambda''_{jik}$,
$\gamma_{ijk} = \frac{1}{2}\mu_k/\lambda_{ijk}$,	$\gamma'_{ijk} = \frac{1}{2}\mu_k/\lambda'_{ijk}$	$= \gamma''_{jik}$,

$$\nu = \frac{3}{2}\left[\frac{1}{2}(1-\frac{\gamma}{2})(1+3\frac{\gamma}{2}) - \frac{\alpha_i}{\lambda}\right] ,$$

$$\sigma = -2\alpha_i\left[(1-\frac{\gamma}{2})(1+3\frac{\gamma}{2}) - \frac{\alpha_i}{\lambda}\right] .$$

In the indirect interaction calcutation, the following parameters are defined:

S-S	S-D	D-S
$a_{ijk} = \frac{4}{9}(\alpha_i+4\alpha_j+\mu_k)$,	$a'_{ijk} = \frac{4}{9}(\alpha_i+4\alpha'_j+\mu_k)$	$= b''_{jik}$,
$b_{ijk} = \frac{4}{9}(4\alpha_i+\alpha_j+\mu_k)$,	$b'_{ijk} = \frac{4}{9}(4\alpha_i+\alpha'_j+\mu_k)$	$= a''_{jik}$,
$e_{ij} = \frac{4}{9}(\alpha_i+4\alpha_j)$,	$e'_{ij} = \frac{4}{9}(\alpha_i+4\alpha'_j)$	$= f''_{ji}$,
$f_{ij} = \frac{4}{9}(4\alpha_i+\alpha_j)$,	$f'_{ij} = \frac{4}{9}(4\alpha_i+\alpha'_j)$	$= e''_{ji}$,
$\delta_{ijk} = \frac{4}{9}(4\alpha_i+4\alpha_j-2\mu_k)$,	$\delta'_{ijk} = \frac{4}{9}(4\alpha_i+4\alpha'_j-2\mu_k)$	$= \delta''_{jik}$,
$w_{ij} = \frac{4}{9}(4\alpha_i+4\alpha_j)$,	$w'_{ij} = \frac{4}{9}(4\alpha_i+4\alpha'_j)$	$= w''_{ji}$,
$\phi_{ij} = \alpha_i^2+8\alpha_i\alpha_j+4\alpha_j^2$,	$\phi'_{ij} = \alpha_i^2+8\alpha_i\alpha'_j+4\alpha_j'^2$	$= \phi''_{ji}$,
$\psi_{ij} = 4\alpha_i^2+8\alpha_i\alpha_j+\alpha_j^2$,	$\psi'_{ij} = 4\alpha_i^2+8\alpha_i\alpha'_j+\alpha_j'^2$	$= \psi''_{ji}$,
$\chi_{ij} = \alpha_i^2+5\alpha_i\alpha_j+\alpha_j^2$,	$\chi'_{ij} = \alpha_i^2+5\alpha_i\alpha'_j+\alpha_j'^2$	$= \chi''_{ji}$,

$$\zeta = \frac{8}{9}(4\alpha_i+4\alpha_j+\mu_k) ,$$

$$a''_{ijk} = \frac{4}{9}(\alpha'_i+4\alpha_j+\mu_k) \quad \text{etc.}$$

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