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ABSTRACT

A model for optical potentials of composite particles is studied. Individual nucleon optical potentials are averaged over the internal motion of deuterons and tritons (or ^3He) with realistic wave functions. Analytic expressions are developed for form factors predicted. Results of some specific calculations with the model are presented.

I. INTRODUCTION

A model of optical potentials for deuterons was first suggested by Watanabe[1] and later generalized to ^{3}He and tritons by Abul-Magd and El-Nadi.[2] This model has stimulated the interest of many (see Refs. 3-9) in search of meaningful parameters in an optical model potential for composite particles. One assumes optical potentials for each of the nucleons in a composite particle and averages over the internal motion. After folding a Woods-Saxon potential with an appropriate wave function, one obtains a new shape for the optical potential. The nuclear radius, diffuseness, and well depth can usually be adjusted to approximate the new shape by a Woods-Saxon form.

II. THE MODEL FOR A TRITON (OR ^{3}He)

We assume that the total potential between the triton and target nucleus is the sum of the local, two-body potentials between each of the interacting particles. In this context, the target nucleus is treated as a single particle, but the triton is treated as the bound state of three particles (nucleons). The Hamiltonian can be written as

$$H = T + \sum_{k=1}^{3} T_k + \frac{1}{2} \sum_{\substack{i=1 \\ j=1 \\ i \neq j}}^{4} V_{ij} , \tag{1}$$

where the indices 1, 2, and 3 refer to the nucleons in the triton, and 4 refers to the target nucleus. The two-body potentials between particles i and j are written as V_{ij} and the internal kinetic energies of the nucleons within the triton are written as T_k. The kinetic energy of the center-of-mass coordinates of the triton is labeled T.

The Hamiltonian for the triton alone is

$$H_t = \sum_{k=1}^{3} T_k + \tfrac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{3} V_{ij} , \tag{2}$$

which defines the internal wave function, χ, of the triton. Thus,

$$H_t\ \chi(\vec{\rho},\vec{r}) = \varepsilon\ \chi(\vec{\rho},\vec{r}) \ , \tag{3}$$

where ε is the binding energy of the triton (see Fig. 1). The wave function for the total Hamiltonian is defined by

$$H\ \Psi(\vec{R},\vec{\rho},\vec{r}) = E\ \Psi(\vec{R},\vec{\rho},\vec{r}) \ . \tag{4}$$

Clearly, when $\vec{R}$ is large the triton is not under the influence of the force of the nucleus and Ψ is separable. One may write

$$\Psi(\vec{R},\vec{\rho},\vec{r}) = \Phi(\vec{R})\ \chi(\vec{\rho},\vec{r}) + T(\vec{R},\vec{\rho},\vec{r}) \ , \tag{5}$$

where F is zero for large $\vec{R}$ and represents the variation of Ψ from the simple product $\Phi\chi$ when the triton is in the proximity of the potential due to the target nucleus. It is therefore referred to as the "distortion term." Substituting Eq. (5) into Eq. (4), multiplying by $\chi^{\dagger}(\vec{\rho},\vec{r})$ and integrating over $d\vec{\rho}$ and $d\vec{r}$, one obtains

$$[T(\vec{R}) + U(\vec{R})]\ \Phi(\vec{R}) = E_o\ \Phi(\vec{R}) - \int d\vec{r}\ d\vec{\rho}\ \chi^{\dagger}(r)\ T(\vec{R},\vec{\rho},\vec{r}) \ , \tag{6}$$

where $E_o = E-\varepsilon$ and $U(\vec{R})$ has been identified as (see Fig. 1)

$$U(\vec{R}) = \iint d\vec{r}\ d\vec{\rho}\ \chi^{\dagger}(\vec{\rho},\vec{r})[V_{14}(\vec{r}_1-\vec{r}_4)+V_{24}(\vec{r}_2-\vec{r}_4)+V_{34}(\vec{r}_3-\vec{r}_4)]\ \chi(\vec{\rho},\vec{r}) \ . \tag{7}$$

To the extent that the distortion term is small, $U(\vec{R})$ is the first-order approximation to the triton-nucleus potential. Henceforth, calculations are made with $T(\vec{R},\vec{\rho},\vec{r}) \equiv 0$. Two triton wave functions will be used to calculate $U(\vec{R})$:

A. The Gaussian Triton Wave Function[10]

$$\chi(\vec{\rho},\vec{r}) = B\ e^{-\gamma\xi^2} \ , \tag{8}$$

where $B = \left(\frac{2\sqrt{3}\gamma}{\pi}\right)^{3/2}$ and $\gamma = 0.16\ \text{fm}^{-2}$ and

$$\xi^2 = |r_1-r_2|^2 + |r_1-r_3|^2 + |r_2-r_3|^2 = 2\rho^2 + \frac{3}{2}\,r^2 \ .$$

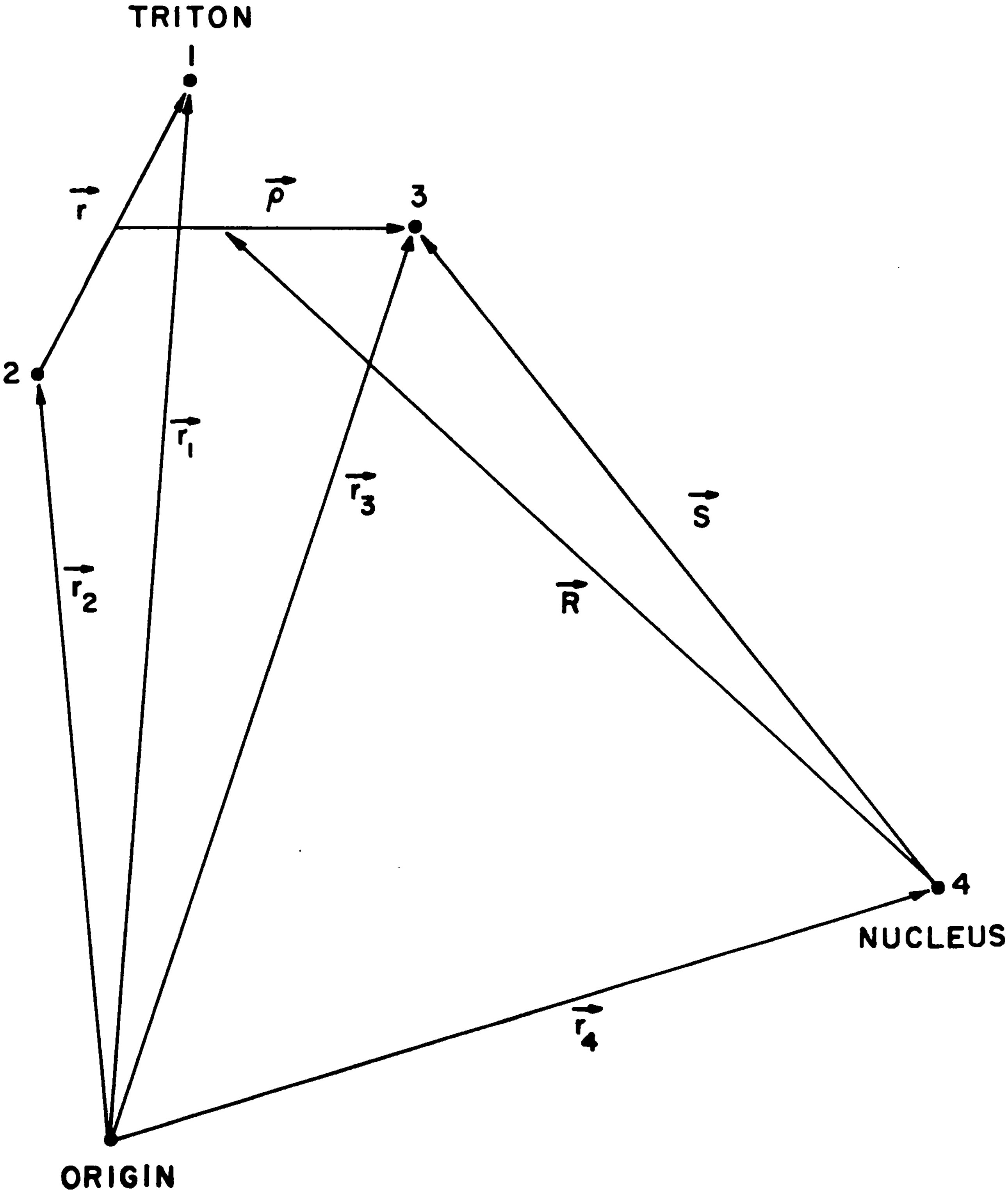


Fig. 1. Particles 1, 2, and 3 are assumed to be bound nucleons of a triton (or ^3He). Particle 4 is the scattering nucleus. Relevant coordinates for the calculation are indicated.

B. The Irving-Gunn Triton Wave Function[11] (see Appendix A)

$$\chi(\vec{\rho},\vec{r}) = A \frac{e^{-\frac{\alpha}{2}\xi}}{p} , \tag{9}$$

where $A = (\frac{\sqrt{3}}{2})^{\frac{1}{2}} \cdot \frac{\alpha^2}{\pi^{3/2}}$ and[12] $\alpha = 0.768\ \mathrm{fm}^{-1}$ and ξ is the same as for Eq. (8). In either case, χ depends explicitly on spatial coordinates through ξ, i.e., χ is spatially symmetric about the exchange of nucleons. An important result of this fact is the simplification of the calculation of $U(\vec{R})$ in Eq. (7). The integral is not changed if the triton coordinated system is reoriented each time so that the nucleon which is being folded lies along the vector $\vec{\rho}$. This allows Eq. (7) to be written

$$U(\vec{R}) = \iint d\vec{\rho}\ d\vec{r}\ \chi^{+}(\vec{\rho},\vec{r})[V_{14}(\vec{s}) + V_{24}(\vec{s}) + V_{34}(\vec{s})]\ \chi(\vec{\rho},\vec{r}) , \tag{10}$$

where $\vec{s} = \vec{R} + \frac{2}{3}\vec{\rho}$.

The potential $U(\vec{R})$ can be calculated by using a typical nucleon optical potential,[13]

$$V(\vec{s}) = -V_o\ f(s) - iW_o\ g(s) + \lambda_\pi^2\ V_{so}\ (\frac{1}{2}\frac{df}{ds})\ \vec{\sigma} \cdot \vec{L} , \tag{11}$$

where

$$f(s) = (1 + e^x)^{-1} \quad ; \quad x = \frac{s - r_o A^{1/3}}{a_o} \quad ; \tag{12}$$

$$g(s) = -4a \frac{d}{ds} f(s) . \tag{13}$$

The calculation of the central term is straightforward and the spin-orbit term is only slightly more complicated. Substituting Eq. (11) into Eq. (10), the spin-orbit part of $U(\vec{R})$ becomes

$$U'_{so}(R) = \lambda_\pi^2\ V_{so} \iint d\vec{\rho}\ d\vec{r}\ \chi \cdot (\frac{1}{s}\frac{df}{ds}) \cdot (\sigma_1 + \sigma_2 + \sigma_3) \cdot \vec{L}\ \chi . \tag{14}$$

Neglecting any d state, the spin of the triton is the sum of the spins of the three nucleons. In particular, of course, the two neutrons are antialigned and the triton has spin 1/2. This can be represented also by Pauli spin matrices, and Eq. (14) becomes

$$U'_{so}(R) = \lambda_\pi^2 V_{so}\, \sigma \cdot \iint d\vec{\rho}\, d\vec{r}\, \chi \left(\frac{1}{s}\frac{df}{ds}\right) \cdot \frac{\vec{s}\times\vec{\nabla}_s}{i} \chi , \tag{15}$$

where the substitution $\vec{L} = \frac{1}{i}\vec{s}\times\vec{\nabla}_s$ has been made. Since $\vec{s} = \vec{R} + \frac{2}{3}\vec{\rho}$, $\vec{\nabla}_s = \frac{1}{3}\vec{\nabla}_R + \vec{\nabla}_\rho$, and because wave functions which depend only on the magnitude of $\vec{\rho}$ are considered, i.e.,

$$\vec{\nabla}_\rho\, \chi(\rho,r) = \frac{\vec{\rho}}{\rho}\frac{d\chi}{d\rho} ,$$

the term

$$\iint d\vec{\rho}\, d\vec{r}\, \chi(\rho,r) \left(\frac{1}{s}\frac{df}{ds}\right) (\vec{R} + \frac{2}{3}\vec{\rho}) \times \vec{\nabla}_\rho\, \chi(\rho,r)$$

vanishes because the nonzero portion of the integral is oriented along $\vec{R}$. The same reasoning shows that the only contribution to the $\vec{\rho}\times\vec{\nabla}_R$ term in Eq. (15) is from that portion of $\vec{\rho}$ which lies along $\vec{R}$. Therefore, Eq. (15) can be written

$$U'_{so}(R) = \lambda_\pi^2 \frac{V_{so}}{3} \iint d\vec{\rho}\, d\vec{r} |\chi|^2 \left(\frac{1}{s}\frac{df}{ds}\right) \left(1 + \frac{2}{3}\frac{\vec{\rho}\cdot R}{R^2}\right) \vec{\sigma}\cdot\vec{L} , \tag{16}$$

where $\vec{L} = \frac{1}{i}\vec{R}\times\vec{\nabla}_R$. Lastly, it can be seen that Eq. (16) is of the Thomas form, since

$$s = (R^2 + \frac{4}{9}\rho^2 + \frac{4}{3}\vec{R}\cdot\vec{\rho})^{1/2} ,$$

$$\frac{1}{R}\frac{\partial f(s)}{\partial R} = \frac{1}{R}\frac{\partial f(s)}{\partial s}\cdot\frac{\partial s}{\partial R} = \frac{\partial f}{\partial s}\cdot\frac{1 + \frac{2}{3}\frac{\vec{R}\cdot\vec{\rho}}{R^2}}{s} ,$$

and Eq. (16) can be written (taking $U_{so}(\vec{R})\vec{\sigma}\cdot\vec{L} = U'_{so}(R)$)

$$U_{so}(R) = \lambda_\pi^2 \frac{V_{so}}{3}\cdot\frac{1}{R}\frac{\partial}{\partial R}\iint d\vec{\rho}\, d\vec{r}\, \chi^\dagger f(s)\, \chi . \tag{17}$$

Therefore, U can be written

$$U(\vec{R}) = -U_o\ F(R) - iY_o\ G(R) + \lambda_\pi^2 \frac{V_{so}}{3} \frac{1}{R} \frac{dF}{dR} \vec{\sigma} \cdot \vec{L} , \tag{18}$$

where

$$F(R) = \iint d\vec{\rho}\ d\vec{r}\ \chi^\dagger(\vec{\rho},\vec{r})\ [f(s)]\ \chi(\vec{\rho},\vec{r}) \tag{19}$$

$$G(R) = \iint d\vec{\rho}\ d\vec{r}\ \chi^\dagger(\vec{\rho},\vec{r})\ [g(s)]\ \chi(\vec{\rho},\vec{r}) \tag{20}$$

$$U_o = [V_o^p + 2V_o^n] \tag{21}$$

$$Y_o = [W_o^p + 2W_o^n] , \tag{22}$$

where, for simplicity, it has been assumed the neutrons and protons have the same well shapes but not necessarily the same well depths.

Specific calculations of $U(\vec{R})$ are discussed in Sec. IV. However, many of the important effects of this model can be extracted from Eq. (18) if the triton wave function is replaced by a delta function. For Eqs. (19-22) we make the simplifying assumption that $|\chi(\rho,r)|^2 = \delta(\rho)\ \delta(r)$ and $V_o^p = V_o^n = V_o$. Then Eq. (18) becomes

$$U(\vec{R}) = -3V_o\ f(R) - 3W_o\ g(R) + \lambda_\pi^2 \frac{V_{so}}{3} \frac{1}{R} \frac{df(R)}{dR} \vec{\sigma} \cdot \vec{L} . \tag{23}$$

Equation (23) is a standard-shaped nucleon optical potential as in Eq. (11), except that it is three times deeper and the spin-orbit effect is one-third as deep. An important consequence of this result is the prediction that triton polarization should be small in the elastic scattering process. This is easily seen from the Born approximation which predicts that the magnitude of polarization scales as the ratio of the spin-orbit term to the well depth (see Appendix B). Therefore,

$$P_t \propto \frac{U_{so}}{U_o} = \frac{\frac{1}{3} V_{so}}{3V^N} \quad ; \qquad P_t \approx \frac{1}{9} P_N ,$$

where P_t, the triton polarization, is estimated to be 1/9 of P_N, the nucleon polarization. At present, attempts to measure polarization of tritons elastically scattered from intermediate weight nuclei have indicated small values.[14,15]

One last point should be mentioned. The nucleon optical potentials which are inserted into the integrals of Eq. (18) to calculate $U(\vec{R})$ are known to be energy-dependent. Each nucleon of a triton at energy E shares one-third of that bombarding energy. However, each nucleon also possesses an internal kinetic energy within the triton itself. It is shown in Appendix A, Eq. (A-9), that this value is 20.6 MeV/nucleon. Therefore, the nucleon optical model parameters which are to be inserted into Eq. (18) perhaps should be evaluated at

$$(20.6 + \frac{E}{3}) \text{ MeV} ,$$

where E is the triton bombarding energy. However, an elementary calculation indicates that a nucleon traverses the triton several times during the time a 20-MeV triton traverses, say a nickel nucleus. This, coupled with the fact that the triton is certainly distorted during this interval of time, makes a clear recommendation difficult. An empirical approach to the solution is in progress.

III. A MODEL FOR DEUTERON OPTICAL POTENTIALS

The general methods used in Sec. II for a spin-1/2 composite particle can also be applied to a spin-one composite particle. However, if the spin-1 composite particle contains a significant amount of $\ell = 2$ orbital angular momentum (as, of course, does the deuteron), the calculation is considerably more tedious. The first exact calculation for such a case was published by Raynal.[4] A similar calculation appears in Appendix C. An outline of the results of the calculation is now presented.

The Hamiltonian for a deuteron is written as $H_d = T_{pn} + V_{pn}$ where T_{pn} is the kinetic energy of the relative motion of the proton and neutron, and V_{pn} is the potential between them. This Hamiltonian defines the deuteron wave function χ_d, where

$$H_d \chi_d = \varepsilon_d \chi_d , \tag{24}$$

and ε_d is the binding energy of the deuteron.

The interaction of the deuteron with a "core" can be described by a total Hamiltonian, H, where

$$H \Psi = E \Psi ,$$

and we seek the total wave function Ψ. The total Hamiltonian can be written $H = H_{dc} + H_d$, where the Hamiltonian H_{dc} describes the interaction of the deuteron with the core, i.e.,

$$H_{dc} = T_{dc} + U_{dc} = T_{dc} + V_{pc} + V_{nc} . \tag{25}$$

T_{dc} is the relative kinetic energy between the center of mass of the deuteron and the core, and V_{pc} and V_{nc} describe the individual potentials between the nucleons in the deuteron and the core. It is our purpose to find an optical potential for the deuteron which will allow us to calculate the wave function Φ_{dc} which describes the elastic interaction of the deuteron with the core. That is,

$$H_{dc} \Phi_{dc} = E_{dc} \Phi_{dc} . \tag{26}$$

We will neglect the distortion term $T_d(\vec{R},\vec{r})$ as was done in Sec. II. In this approximation we can combine Eqs. (24), (25), and (26) to write (dropping subscripts)

$$\Psi(\vec{R},\vec{r}) = \Phi(\vec{R}) \chi(\vec{r})$$

$$[H_d(\vec{r}) + T_{dc}(\vec{R}) + V_{pc}(\vec{s}_p) + V_{nc}(\vec{s}_n)]\Phi(\vec{R})\chi(\vec{r}) = (\varepsilon_d+E_{dc}) \Phi(\vec{R})\chi(\vec{r}) . \tag{27}$$

Multiplying Eq. (27) from the left by $\chi^{\dagger}(\vec{r})$ and integrating over $d\vec{r}$, we have

$$[T_{dc}(\vec{R}) + U(\vec{R})]\, \Phi(\vec{R}) = E_{dc}\, \Phi(\vec{R}) \quad , \tag{28}$$

where a potential for the center of mass of the deuteron has been identified as

$$U(\vec{R}) = \int \chi^{\dagger}(\vec{r})\, [V_{pc}(\vec{s}_p) + V_{nc}(\vec{s}_n)]\, \chi(\vec{r})\, d\vec{r} \ . \tag{29}$$

We now substitute a specific value for V_{pc} and V_{nc} to calculate $U(\vec{R})$. Although it is not necessary, it will be convenient to assume that the proton and neutron potentials are identical (see Fig. 2). Therefore,

$$V_{pc}(\vec{s}) = V_{nc}(\vec{s}) = V_c(s) + V_{so}(s)\, \vec{\sigma} \cdot \vec{L} \ , \tag{30}$$

where $V_c(s)$ is a central term (in general complex) and $V_{so}(s)$ is a functional coefficient of $\vec{\sigma} \cdot \vec{L}$, the spin-orbit term. $\vec{L}(\vec{s})$ is the angular momentum operator which is replaced by $\frac{1}{i}\, \vec{s}\times\vec{\nabla}_s$ in the calculations. Using Eq. (30) in Eq. (29), the calculation of $U(\vec{R}) = U_1(\vec{R}) + U_2(\vec{R})$ becomes

$$U_1(\vec{R}) = \int d\vec{r}\, \chi^{\dagger}(\vec{r})\, [2V_c(s)]\, \chi(\vec{r}) \tag{31}$$

and

$$U_2(\vec{R}) = \int d\vec{r}\, \chi^{\dagger}(\vec{r})\, [V_{so}(s)\cdot(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{s} \times \frac{\vec{\nabla}_s}{i}]\, \chi(\vec{r}) \ , \tag{32}$$

where $\vec{s} = \vec{R} + \frac{\vec{r}}{2}$ and $\vec{\nabla}_s = \frac{1}{2}\vec{\nabla}_R + \vec{\nabla}_r$.

The deuteron wave function will be taken as a Hulthen wave function.[16]

$$\chi(\vec{r}) = \frac{1}{\sqrt{4\pi}} \left[\frac{u(r)}{r} + \frac{w(r)}{r\sqrt{8}}\, S_{12}(\theta,\phi)\right] \ , \tag{33}$$

where

$$S_{12} = 3(\vec{\sigma}_1\cdot\vec{r})\,(\vec{\sigma}_2\cdot\vec{r}) - \vec{\sigma}_1\cdot\vec{\sigma}_2 \ .$$

We can always replace $\vec{\sigma}_1\cdot\vec{\sigma}_2$ by 1 in this calculation because the deuteron may always be found in a triplet state y_1^m, and $\vec{\sigma}_1\cdot\vec{\sigma}_2\, y_1^m = y_1^m$. Substituting Eq. (33) into Eq. (31), we see that $U_1(\vec{R})$ can be written as the sum of a

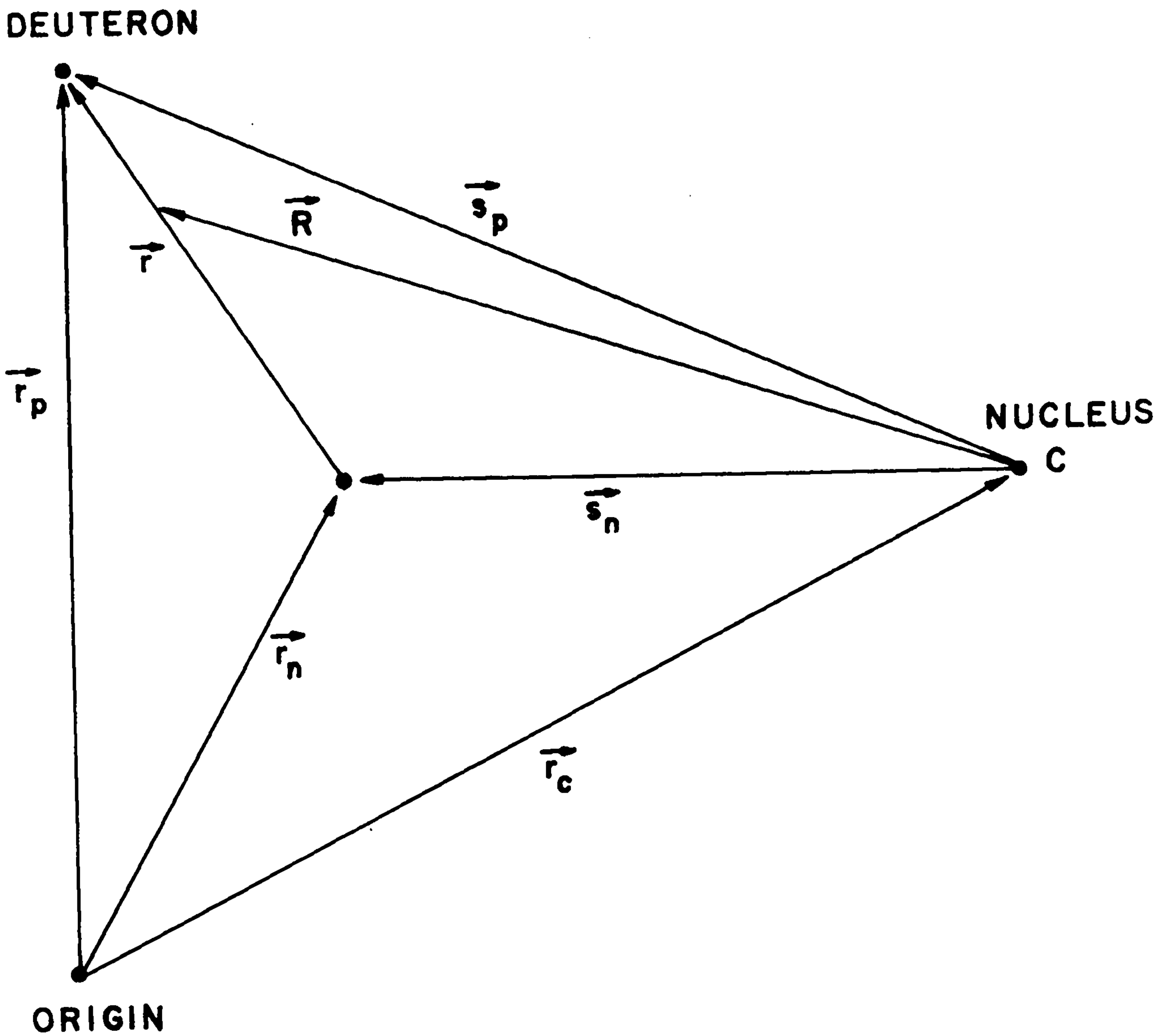


Fig. 2. The deuteron contains a proton (p) and neutron (n). The nucleus (core) is represented by c. Relevant coordinates for the calculation are indicated.

central term and a tensor term,

$$U_1(\vec{R}) = U_{1c}(R) + U_{1T}(R) \cdot [(\vec{S}\cdot\hat{R})^2 - \tfrac{2}{3}] \ , \tag{34}$$

where

$$U_{1c}(R) = \frac{2}{4\pi}\int d\vec{r}\ V_c(s) \left\{[\frac{u(r)}{r}]^2 + [\frac{w(r)}{r}]^2\right\} \tag{35}$$

$$U_{1T}(R) = \frac{12}{4\pi}\int d\vec{r}\ V_c(s)\ P_2(\theta) \left\{\frac{u(r)w(r)}{r^2\sqrt{2}} - [\frac{w(r)}{2r}]^2\right\} \tag{36}$$

$$[(\vec{S}\cdot\hat{R})^2 - \tfrac{2}{3}] = \frac{1}{6}\,[3(\vec{\sigma}_1\cdot\hat{R})(\vec{\sigma}_2\cdot\hat{R}) - 1] = \frac{1}{6}\,S_{12}(\hat{R}) \ , \tag{37}$$

in which $\vec{S} = \frac{1}{2}(\vec{\sigma}_1+\vec{\sigma}_2)$ and $P_2(\theta)$ is the Legendre polynomial for $\ell = 2$.

Returning to the calculation of $U_2(\vec{R})$ in Eq. (32), we see that it can be written as the sum of a central term, a spin-orbit term, and a tensor term. That is,

$$U_2(\vec{R}) = U_{2c}(R) + U_{2so}(R)\ \vec{S}\cdot\vec{L} + U_{2T}(R)\ [(\vec{S}\cdot\hat{R})^2 - \tfrac{2}{3}] \ , \tag{38}$$

where

$$U_{2c}(R) = \frac{-3}{4\pi}\int d\vec{r}\ V_{so}(s) \left\{[\frac{w}{r}]^2 + 2\cdot(\frac{R}{r})[\frac{w}{r}]^2\right\} \tag{39}$$

$$U_{2so}(R) = \frac{1}{4\pi}\int d\vec{r}\ \frac{V_{so}(s)}{r^2} \left\{\left[U^2 - \frac{uw}{\sqrt{2}} - w^2\right](1 + \frac{\vec{r}\cdot\vec{R}}{2R^2}) + \frac{3}{\sqrt{8}}\,[uw + \frac{w^2}{2}]\sin^2\theta\right\} \tag{40}$$

$$U_{2T}(R) = \frac{9R}{4\pi}\int d\vec{r}\ V_{so}(s)\ \frac{\sin^2\theta\cos\theta}{r\sqrt{2}} \left[\frac{(wu'-uw')}{r} + \frac{2uw}{r^2} - \frac{4w^2}{\sqrt{2}r^2}\right]$$
$$- \frac{18R}{4\pi}\int d\vec{r}\ V_{so}(s)\ \frac{w}{r^3\sqrt{2}} \left[u - \frac{w}{\sqrt{2}}\right] \ . \tag{41}$$

Section V will consider specific calculations of $U(\vec{R})$. However, just as in the case of the triton, some general observations can be made at this point. Satchler has shown[17] that a consequence of parity conservation and time reversal invariance is that $U(\vec{R})$ can, in principle, contain three irreducible tensor terms. They are

$$(\vec{S}\cdot\hat{R})^2 - \frac{2}{3}$$

$$(\vec{S}\cdot\vec{P})^2 - \frac{2}{3}P^2 \tag{42}$$

$$(\vec{S}\cdot\vec{L})^2 + \frac{1}{2}(\vec{S}\cdot\vec{L}) - \frac{2}{3}L^2 .$$

If the present model is valid, only the term $[(\vec{S}\cdot\hat{R})^2 - \frac{2}{3}]$ appears in the tensor optical potential for deuterons.

It is interesting to note that if one sets w = 0 in the Hulthen wave function, then all terms of $[(\vec{S}\cdot\hat{R})^2 - \frac{2}{3}]$ which appear in $U(\vec{R})$ vanish. That is, the existence of a tensor potential in this model is the consequence of the D state of the deuteron.

Taking U(r) as a delta function $\delta(r)$, and setting $w(r) = 0$, the deuteron potential reduces to

$$U(\vec{R}) = 2V_c(R) + V_{so}(R)\,\vec{S}\cdot\vec{L} \tag{43}$$

or

$$U(\vec{R}) = 2V_c(R) + \frac{1}{2}V_{so}(R)\,(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{L} . \tag{44}$$

Equation (44) is written in a form which emphasizes that just as the triton spin-orbit potential is one-third the nucleon spin-orbit potential, so the deuteron spin-orbit potential is one-half the nucleon spin-orbit potential. This point is less obvious in Eq. (43), where $\vec{S} = \frac{1}{2}(\vec{\sigma}_1+\vec{\sigma}_2)$.

It should also be mentioned that there is no a priori reason to exclude the Coulomb term from V_c when calculating U(R). A study of this problem revealed that the effect on the central part is negligible, in the sense that the new "shape" for the Coulomb potential is of the same form but with the Coulomb radius, r_c, changed by less than 1%. Optical model fits are very insensitive to such a change in r_c. One point we have not investigated is that the Coulomb potential contributes to the tensor part of the deuteron potential as can be seen in Eq. (36).

Again, just as in the case of the triton, one may include the internal kinetic energy of the nucleons. This is calculated in Appendix D [Eq. (D-29)] to be 25.6 MeV. Therefore, the nucleon optical potential parameters which are to be used in Eq. (29) perhaps should be evaluated at $(25.6 + \frac{E}{2})$ MeV, where E is the deuteron bombarding energy (see, however, the last paragraph of Sec. II).

IV. EMPIRICAL FITS TO THE TRITON OPTICAL POTENTIAL

The formulas for $U(\vec{R})$ in Eqs. (18) through (22) have been calculated in a computer program for both the Gaussian triton wave function [Eq. (8)] and the Irving-Gunn triton wave function (Eq. (9) and Appendix A). The results of some preliminary studies will be presented.

It was found that when a Woods-Saxon shaped potential is used to calculate $U(\vec{R})$, the result appears close to a Woods-Saxon shape. That is, with a new choice of diffuseness, radius, and sometimes well depth, one can find empirically a new Woods-Saxon shape that is close to that calculated for $U(\vec{R})$. Optical model computer programs usually are written with these shapes (including derivatives of Woods-Saxon, etc.) as options. This avoids having a table lookup form factor.

We have devised a computer program (RHOS-T) which calculates the integrals and determines "best values" for a modified Woods-Saxon shape. The triton optical potential that is calculated by RHOS-T is [Eq. (18)]

$$U(\vec{R}) = -U_o\, F(R) - iY_o\, G(R) + \lambda_\pi^2 \frac{V_{so}}{3} \cdot \frac{1}{R}\frac{dF}{dR}\, \vec{\sigma} \cdot \vec{L} \,, \qquad (45)$$

where

$$F(R) = \iint d\vec{\rho}\; d\vec{r}\; \chi^\dagger(\rho,r)\; [f(s)]\; \chi(\rho,r) \;,$$

or

$$F(R) = 8\pi^2 \int_0^\infty \rho^2 \, d\rho \int_{-1}^{1} f(s) \, d\mu \int_0^\infty [\chi(\rho,r)]^2 \, r^2 \, dr \, , \tag{46}$$

where $\mu = \cos\theta$, $s = \sqrt{R^2 + \frac{4}{9} P^2 + \frac{4}{3} R\rho\mu}$, and

$$f(x_o) = \frac{1}{(1+e^{x_o})} \quad ; \qquad x_o = \frac{s-r_o A^{1/3}}{a_o} \, . \tag{47}$$

Adjustments were then made to find r_o' and a_o' such that

$$\frac{F(R)}{F(0)} = f(x_o') \quad ; \qquad x_o' = \frac{R-r_o' A^{1/3}}{a_o'} \, . \tag{48}$$

Likewise, for the imaginary part,

$$G(R) = \iint d\vec{\rho} \, d\vec{r} \, \chi^\dagger(\rho,r) \, [g(s)] \, \chi(\rho,r) \, ,$$

or

$$G(R) = 8\pi^2 \int_0^\infty \rho^2 \, d\rho \int_{-1}^{1} g(s) \, d\mu \int_0^\infty [\chi(\rho,r)]^2 \, r^2 \, dr \, , \tag{49}$$

where $g(s)$ might be a volume term,

$$g(x_i) = f(x_i) \quad ; \qquad x_i = \frac{s-r_i A^{1/3}}{a_i} \, , \tag{50}$$

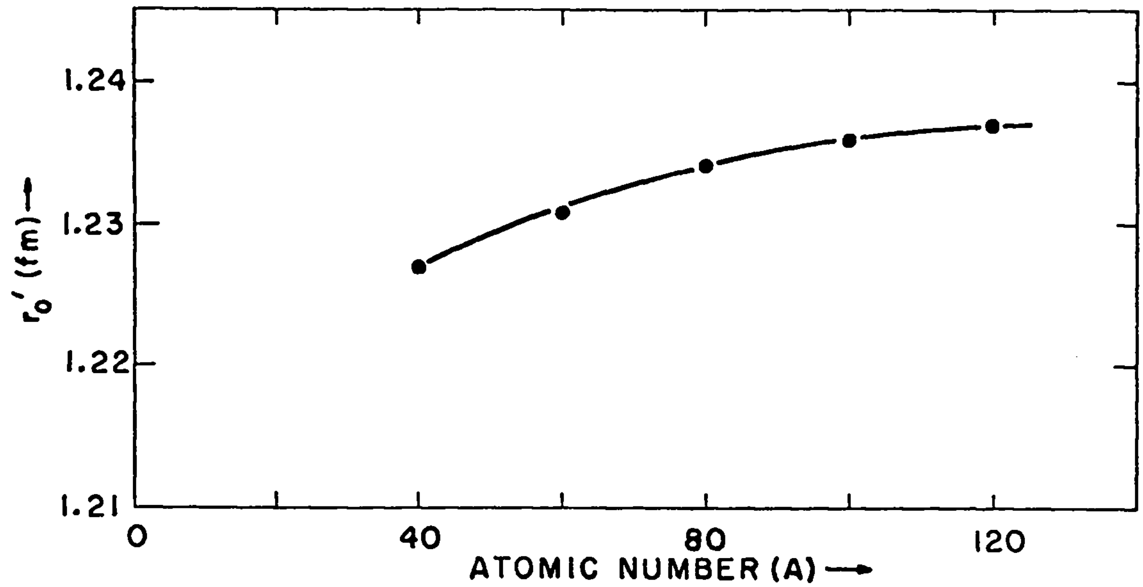
or a surface term,

$$g(x_i) = \frac{d}{dx_i} f(x_i) \, . \tag{51}$$

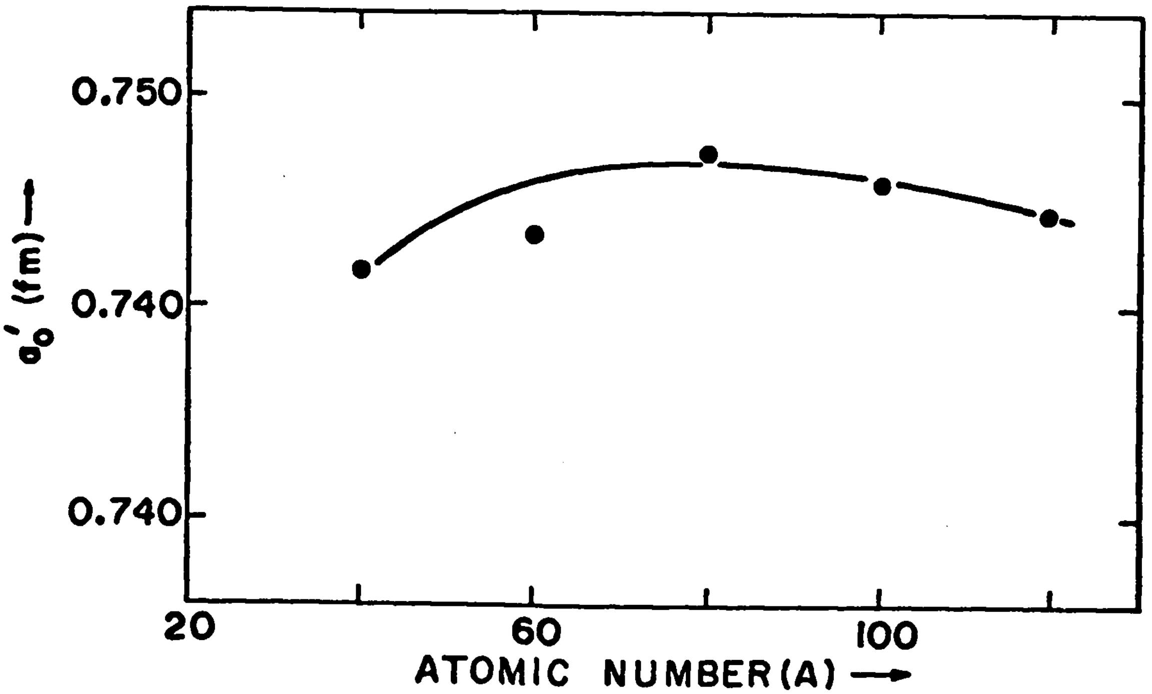
For the surface term, a_i and r_i were determined such that

$$\frac{G(R)}{G(r_o' A^{1/3})} = g(x_i') \quad , \text{ where } \quad x_i' = \frac{R-r_i' A^{1/3}}{a_i'} \, . \tag{52}$$

The resulting modified parameters are indicated in Fig. 3. The nucleon parameters were taken as[18] $r_o = 1.25$ F, $a_o = 0.65$ F, $r_i = 1.25$ F, and $a_i = 0.47$ F.

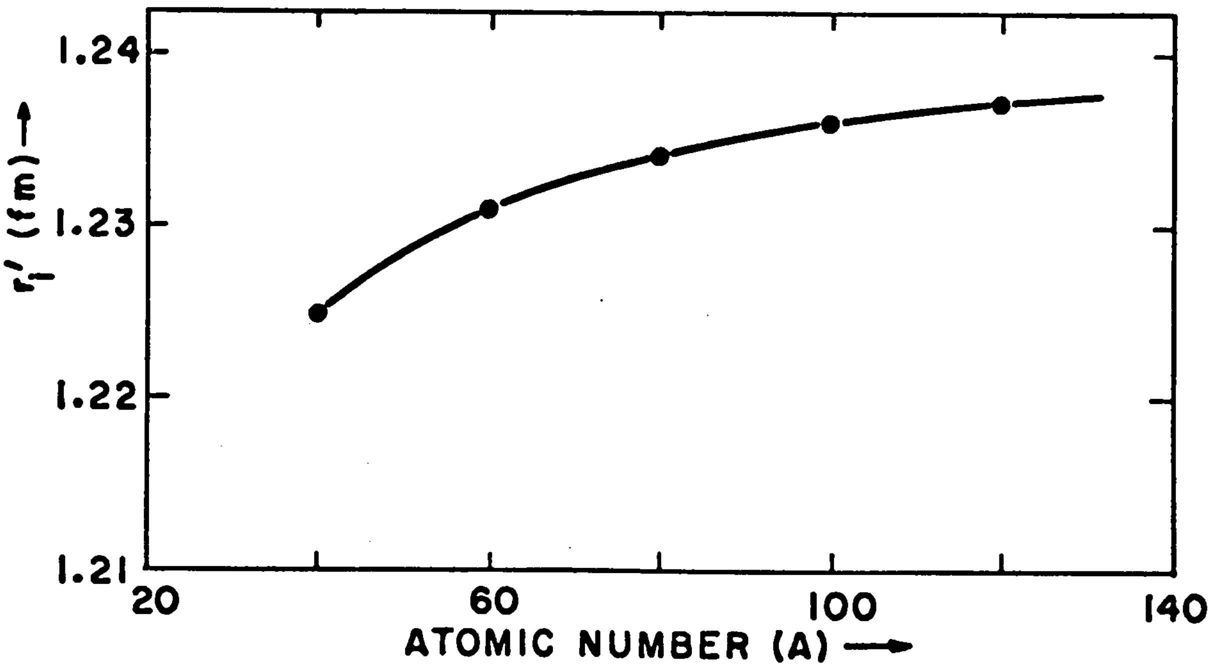


(a)

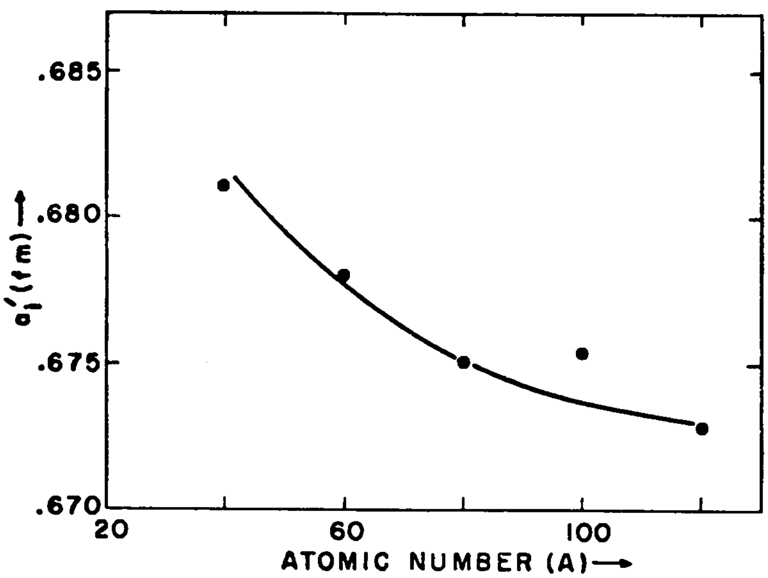


(b)

Fig. 3. Woods-Saxon parameters for triton (or ^{3}He) optical potential form factors plotted as a function of atomic number. The calculations were made with the following nucleon parameters: r_o = 1.25 fm, a_o = 0.65 fm, r_i = 1.25 fm, a_i = 0.47 fm.


1.24
1.23
1.22
1.21
r_I' (fm)
20
60
100
140
ATOMIC NUMBER (A)

(c)


.685
.680
.675
.670
a_I' (fm)
20
60
100
ATOMIC NUMBER (A)

(d)

Fig. 3 (cont.)

A Gaussian wave function [Eq. (8)] was used. A plot of the effects on $U(\vec{R})$ as a function of atomic number, i.e., nuclear "size," is indicated by showing modified parameters. F(0) did not vary by more than 1% from 1 in the range from A = 27 to A = 120. $G[(r_i'/a_i')A^{1/3}]$ was also essentially constant, not varying from the value 0.77 by more than 1% over the same range.

We have used the geometry in Fig. 3 and obtained reasonable fits to triton elastic scattering data for nuclei in the region of A = 60 by allowing U_o and Y_o to vary. However, we have not attempted a systematic study pending our polarization measurements of tritons elastically scattered from nuclei in that mass region. We anticipate that triton polarization measurements, which are in progress,[15] will expedite such a study.

V. EMPIRICAL FITS TO THE DEUTERON OPTICAL POTENTIAL

We have also devised a computer program (RHOS-D) to calculate the deuteron optical potential $U(\vec{R})$ of Eq. (29). To date, we have calculated only the zeroth-order terms as indicated in Appendix C (Sec. VIII, part C). Keeping only the large terms,

$$U(\vec{R}) = U_c^{(0)}(R) + U_{so}^{(0)}(R)\ \vec{S}\cdot\vec{L} + U_T^{(0)}(R)\ [(\vec{S}\cdot\hat{R})^2 - \tfrac{2}{3}] \ ,$$

where

$$U_c^{(0)}(R) = \frac{2}{4\pi}\int d\vec{r}\ V_c(s)\ (\frac{u}{r})^2$$

$$U_{so}^{(0)}(R) = \frac{1}{4\pi}\int d\vec{r}\ \frac{V_{so}(s)}{r^2}\left\{[u^2 - \frac{uw}{\sqrt{2}}]\ (1 - \frac{\vec{r}\cdot\vec{R}}{2R^2}) + \frac{3uw}{\sqrt{8}}\sin^2\theta\right\}$$

$$U_T^{(0)}(R) = \frac{6\sqrt{2}}{4\pi}\int d\vec{r}\ V_c(s)\ \frac{uw}{r^2}\ P_2(\theta)\ . \tag{53}$$

Assuming that the proton and neutron optical potential shapes are the same (which in practice is not true) we take as the nucleon optical potential

$$V(s) = -V_o\, f(s) - iW_o\, g(s) - \lambda_\pi^2\, V_{so}\, h(s)\, \vec{\sigma} \cdot \vec{L} , \tag{54}$$

where f(s) is given in Eq. (47) and g(s) is given in Eqs. (50) and (51). The term h(s) is defined as

$$h(s) = \frac{1}{s} \frac{df(s)}{ds} . \tag{55}$$

Substituting Eq. (54) into Eq. (53),

$$\begin{aligned} U(R) = & -[U_o\, F(R) + iY_o\, G(R)] \\ & -[\lambda_\pi^2\, U_{so}\, H(R)]\, \vec{S}\cdot\vec{L} \\ & -[\lambda_\pi^2\, U_T\, M(R) + i\lambda_\pi^2\, Y_T\, N(R)] , \end{aligned} \tag{56}$$

where the central part is

$$F(R) = \frac{1}{2} \int_o^\infty dr \int_{-1}^{1} d\mu\; f(s)\, u^2(r)$$

$$G(R) = \frac{1}{2} \int_o^\infty dr \int_{-1}^{1} d\mu\; g(s)\, u^2(r)$$

$$s = \sqrt{R^2 + \frac{r^2}{4} + Rr\mu} \quad ; \qquad \mu = \cos\theta ,$$

and

$$\begin{aligned} U_o &= V_o^p + V_o^n \\ Y_o &= W_o^p + W_o^n . \end{aligned} \tag{57}$$

The spin-orbit term contains

$$H(R) = \frac{1}{2} \int_o^\infty dr \int_{-1}^{1} d\mu\; h(s) \left\{ [u^2 - \frac{uw}{\sqrt{2}}](1 + \frac{\mu r}{2R}) + \frac{3uw}{\sqrt{8}}(1 - \mu^2) \right\}$$

$$U_{so} = V_{so} \quad , \qquad \lambda_\pi^2 = 2.0 \text{ fm}^2 . \tag{58}$$

The tensor terms are written

$$M(R) = \frac{3}{\sqrt{2}} \int_0^\infty dr \int_{-1}^{1} d\mu\ f(s)\ u(r)\ w(r)\ P_2(\mu)$$

$$N(R) = \frac{3}{\sqrt{2}} \int_0^\infty dr \int_{-1}^{1} d\mu\ g(s)\ u(r)\ w(r)\ P_2(\mu)$$

$$P_2(\mu) = (\frac{3}{2}\mu^2 - 1)$$

$$U_T = V_o^P + V_o^n$$

$$Y_T = W_o^P + W_o^n \ . \qquad (59)$$

Each of the form factors F, G, H, M, and N has been calculated for various values of atomic number, A, with RHOS-D and a characteristic shape has been determined. By trial and error, we were able to find form factors that approximate the integrals in Eq. (56) (see, however, Ref. 19). These form factors are defined below:

$$f_d(R) \equiv F_o\ f(R) \simeq F(R) \quad ; \quad f(R) \text{ is Woods-Saxon shaped ;}$$

$$g_d(R) \equiv G_o\ g(R) \simeq G(R)$$

$$h_d(R) \equiv \frac{H_o}{R} \frac{d}{dR} \left(\frac{f_d(R)}{F_o}\right) \simeq H(R)$$

$$m_d(R) \equiv -R \cdot M_o \frac{d}{dR} \left(\frac{h_d(R)}{H_o}\right) \simeq M(R)$$

$$n_d(R) \equiv R \cdot N_o \frac{d}{dR} \left[\frac{1}{R} \frac{d}{dR} \left(\frac{g_d}{G_o}\right)\right] \simeq N(R) \ . \qquad (60)$$

The constants F_o, G_o, H_o, M_o, and N_o must be adjusted to fit each integral. The specific form factors that have been calculated are listed below.

$$f_d(x) = \frac{F_o}{(1+e^x)}$$

$$g_d(x) = -4a_i' \, G_o \frac{d}{dR} \left(\frac{f_d}{F_o}\right) = \frac{4G_o e^x}{(1+e^x)^2}$$

$$h_d(x) = -\frac{H_o}{R} \frac{d}{dR} \left(\frac{f_d}{F_o}\right) = \frac{H_o}{Ra_o'} \frac{e^x}{(1+e^x)^2}$$

$$m_d(x) = -RM_o \frac{d}{dR} \left(\frac{h_d}{H_o}\right) = \frac{M_o}{(a_o')^2} \left(\frac{e^x}{(1+e^x)^2}\right) \left(\frac{a_o}{R} - \frac{1-e^x}{1+e^x}\right)$$

$$n_d(x) = RN_o \frac{d}{dR} \left(\frac{1}{R} \frac{d}{dR} \left(\frac{g_d}{G_o}\right)\right) = \frac{4N_o}{Ra_i'} \left(\frac{e^x}{(1+e^x)^4}\right) \left(\frac{R}{a_i} (1-4e^x+e^{2x})-(1-e^{2x})\right), \quad (61)$$

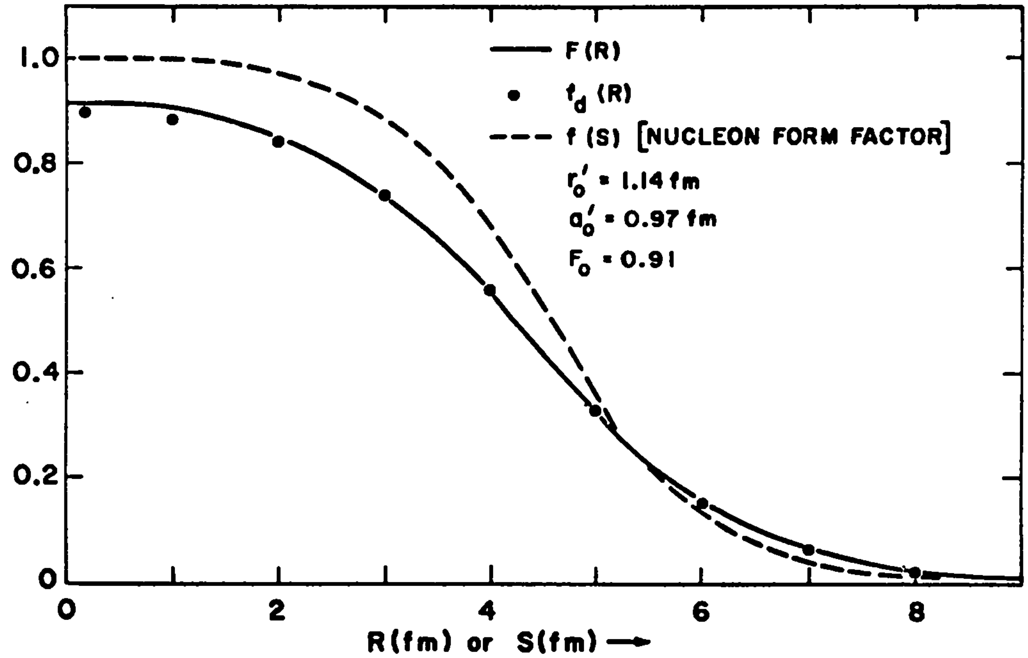
where $x = \frac{R-R_o'}{a_o'}$ for the real potential terms (f_d, h_d, and m_d) and $x = \frac{R-R_i'}{a_i'}$ for the imaginary potential terms (g_d and n_d). Often one can find a single set of R_o', a_i', R_i', and a_i' that will fit all five form factors of Eq. (61).

Figure 4 presents the results of a calculation of the form factors for deuterons elastically scattered from ^{60}Ni, with nucleon parameters from Ref. 20. It should be noticed that this model predicts a real and imaginary tensor term of about equal size. It would seem unlikely that either can be ignored.

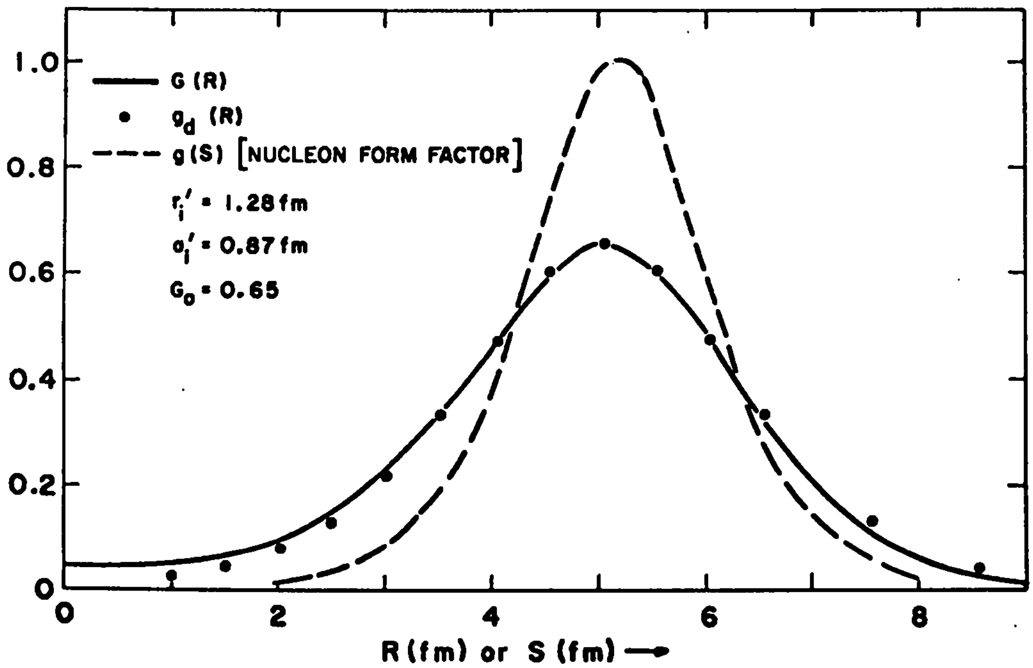
A rigorous test of this model for deuterons will be a systematic study of vector and tensor polarized deuterons elastically scattered from intermediate-weight nuclei at about 15-MeV bombarding energy. A high-intensity polarized ion source has been developed for the Los Alamos tandem accelerator, and such a study is being planned.

VI. CONCLUSIONS

The theoretical basis for a study of composite particle optical potentials has been reviewed and extended. A consequence of summing nucleon optical

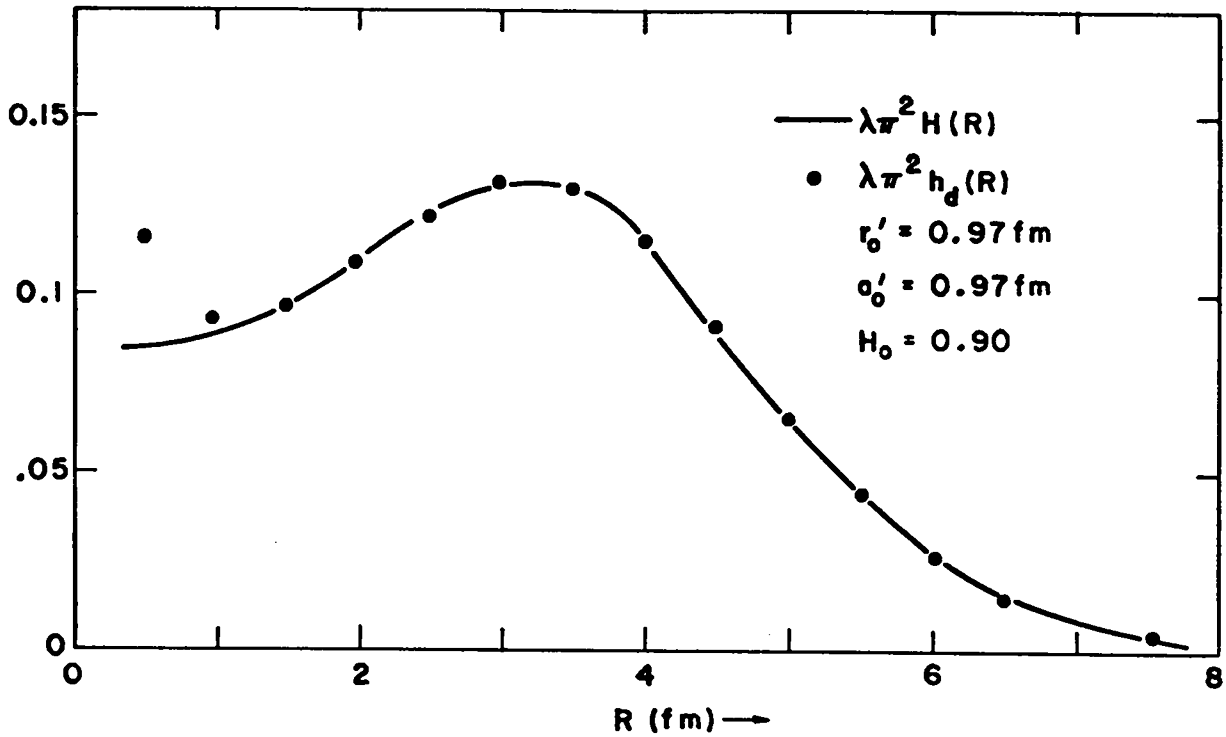


(a)



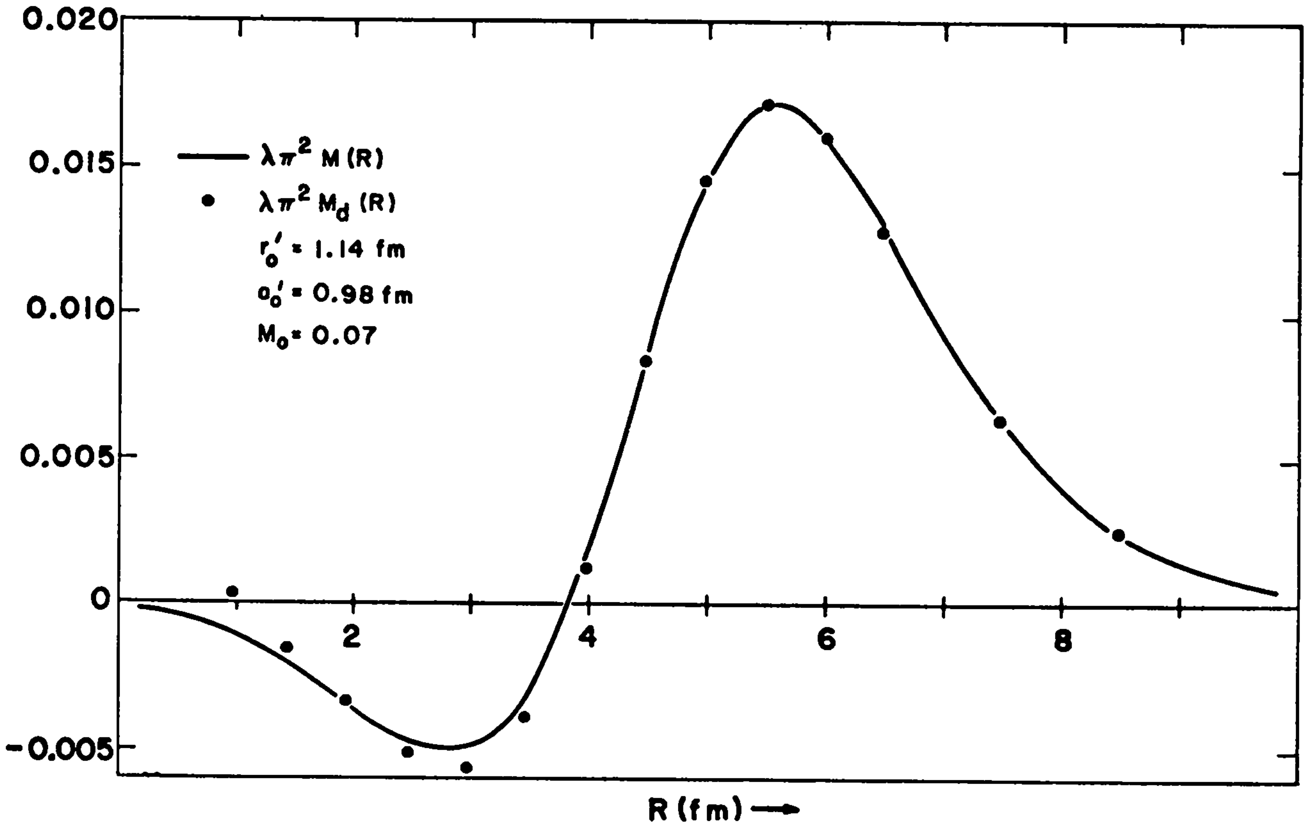
(b)

Fig. 4. Dimensionless form factors for the deuteron optical potential of ^{60}Ni. The nucleon parameters used in calculating (a) and (d) are r_o = 1.17 fm and a_o = 0.75 fm. The nucleon parameters used in calculating (c) are r_o = 1.01 fm and a_o = 0.75 fm. The nucleon parameters used in calculating (b) and (e) are r_i = 1.32 fm and a_i = 0.56 fm. It has been assumed that λ_π^2 = 2.00 fm^2.



0.15
0.1
.05
0
0
2
4
6
8
R (fm) ⟶
$\lambda\pi^2 H(R)$
$\lambda\pi^2 h_d(R)$
$r_0' = 0.97$ fm
$a_0' = 0.97$ fm
$H_0 = 0.90$

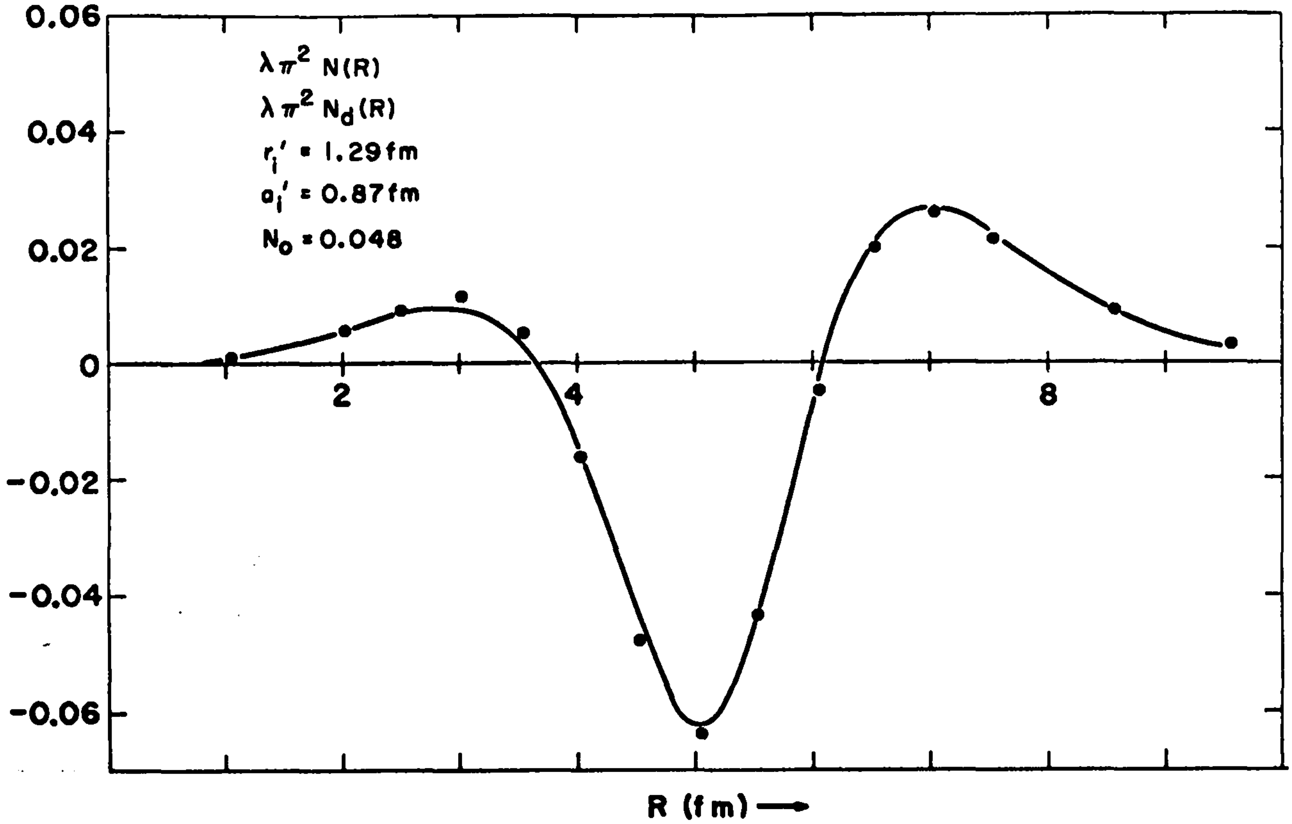
(c)



0.020
0.015
0.010
0.005
0
-0.005
2
4
6
8
R (fm) ⟶
$\lambda\pi^2 M(R)$
$\lambda\pi^2 M_d(R)$
$r_0' = 1.14$ fm
$a_0' = 0.98$ fm
$M_0 = 0.07$

(d)

Fig. 4 (cont.)



(e)

potentials is that the spin-orbit well depth is decreased by the number of nucleons in the composite particle. The model therefore predicts small polarization values for elastically scattered mass-3 nuclei. The validity of this model has not been confirmed or denied by existing experiments.

And, finally, we have suggested specific form factors for the tensor portion of the deuteron optical potential.

ACKNOWLEDGMENTS

The authors thank D. D. Armstrong, J. G. Beery, D. D. Dodder, L. Heller, and L. Rodberg for helpful discussions on various aspects of this work. One of us (PK) is particularly thankful for the encouragement and suggestions of J. L. Gammel concerning the deuteron optical model calculations of Appendix C.

APPENDIX A: IRVING-GUNN WAVE FUNCTION

I. COORDINATE SYSTEM

The coordinate system is defined in Fig. 1. We define in addition,

$$\vec{r}_{12} = \vec{r}_1 - \vec{r}_2 = \vec{r}$$

$$\vec{r}_{32} = \vec{r}_3 - \vec{r}_2 = \vec{\rho} + \frac{\vec{r}}{2}$$

$$\vec{r}_{31} = \vec{r}_3 - \vec{r}_1 = \vec{\rho} - \frac{\vec{r}}{2} .$$

It follows that $\xi^2 \equiv |\vec{r}_{12}|^2 + |\vec{r}_{32}|^2 + |\vec{r}_{31}|^2 = 2\rho^2 + \frac{3}{2} r^2$. It will be necessary to discuss the center-of-mass coordinates to some degree.

$$\vec{r}^{(1)}_{cm} = -\frac{1}{3}\vec{\rho} + \frac{1}{2}\vec{r}$$

$$\vec{r}^{(2)}_{cm} = -\frac{1}{3}\vec{\rho} - \frac{1}{2}\vec{r}$$

$$\vec{r}^{(3)}_{cm} = \frac{2}{3}\vec{\rho} .$$

The expectation value of the momentum squared (or kinetic energy) of any one of the nucleons must be the same as any other. Therefore, for our purposes we need calculate only $(\vec{\nabla}^{(3)}_{cm})^2$.

$$\frac{\partial}{\partial x^{(3)}_{cm}} = \frac{\partial x_\rho}{\partial x^{(3)}_{cm}} \cdot \frac{\partial}{\partial x_\rho} = \frac{3}{2}\frac{\partial}{\partial x_\rho}$$

$$\left(\frac{\partial}{\partial x^{(3)}_{cm}}\right)^2 = \frac{3}{2} \cdot \frac{\partial x_\rho}{\partial x^{(3)}_{cm}} \cdot \frac{\partial^2}{\partial x^2} = \frac{9}{4}\frac{\partial^2}{\partial x^2} \text{, etc.}$$

Therefore,

$$(\vec{\nabla}^{(3)}_{cm})^2 = \frac{9}{4}\nabla^2_\rho = \frac{9}{4}\frac{1}{\rho^2}\frac{\partial}{\partial\rho}\rho^2\frac{\partial}{\partial\rho} , \qquad \text{(A-1)}$$

where the last equation holds for the function which depends on only the magnitude of $\vec{\rho}$.

II. NORMALIZATION

The Irving-Gunn wave function for mass-3 nuclei may be written

$$\chi = \frac{A\, e^{-\frac{\alpha}{2}(r_{12}^2+r_{31}^2+r_{32}^2)^{1/2}}}{(r_{12}^2+r_{31}^2+r_{32}^2)^{1/2}} = \frac{A\, e^{-\frac{\alpha}{2}\xi}}{\xi}\,, \tag{A-2}$$

where $\xi = (2\rho^2 + \frac{3}{2} r^2)^{1/2}$. We require that the integral $\mathcal{J} = 1$, where

$$\mathcal{J} = (4\pi)^2 \int_0^\infty \int_0^\infty \chi^2\, \rho^2\, r^2\, d\rho\, dr\,.$$

Let $x = \sqrt{2}\,\alpha\rho$ and $y = \sqrt{3/2}\,\alpha r$, then

$$\mathcal{J} = \frac{(4\pi A)^2}{3^{3/2}\cdot\alpha^4} \int_0^\infty x^2\, dx \int_0^\infty y^2\, dy\, \frac{e^{-\sqrt{x^2+y^2}}}{(x^2+y^2)}\,.$$

Let $x = R\cos\theta$ and $y = R\sin\theta$, and integrate over the first quadrant of the element $RdRd\theta = dxdy$. The integral is separable and we find

$$\mathcal{J} = \frac{(4\pi A)^2}{3^{3/2}\alpha^4} \left\{\int_0^{\pi/2} \sin^2\theta\cos^2\theta\, d\theta\right\}\left\{\int_0^\infty R^3\, e^{-R}\, dR\right\}.$$

The first integral has the value $\pi/16$ and the second integral is one of the integrals

$$\int_0^\infty R^N\, e^{-R}\, dR = N!\,.$$

Setting $\mathcal{J} = 1$ we find

$$A = \frac{3^{1/4}\alpha^2}{\pi^{3/2}\sqrt{2}}\,. \tag{A-3}$$

III. MEAN SQUARE RADIUS

The mean square radius of a nucleon (measured, of course, from the center of mass of the triton) can be obtained by choosing particle 3. In that case,

$$<R^2_{rms}< = <|r^{(3)}_{cm}|^2> = \frac{4}{9} <\xi^2>$$

$$<R^2_{rms}> = \frac{4}{9} \cdot \frac{1}{2\alpha^2} <R^2 \cos^2\theta> .$$

The integral obviously separates again, and since

$$\int_0^{\pi/2} \cos^4\theta \sin^2\theta d\theta = \frac{1}{2} \int_0^{\pi/2} \cos^2\theta \sin^2\theta d\theta ,$$

$$<R^2_{rms}> = \frac{4}{9} \cdot \frac{1}{4\alpha^2} <R^2> = \frac{4}{9} \cdot \frac{1}{4\alpha^2} \cdot \frac{5!}{3!} .$$

Therefore,

$$<R^2_{rms}> = \frac{20}{9} \cdot \frac{1}{\alpha^2} .$$

In particular,

$$<R^2_{rms}> = 3.77 \text{ fm}^2 \qquad \text{for} \qquad \alpha = 0.768 \text{ fm}^{-1} .$$

IV. THE AVERAGE KINETIC ENERGY

The average kinetic energy of a nucleon within the triton can be calculated by choosing particle 3 again, and finding

$$T_3 = \left\langle \frac{p_3^2}{2M_3} \right\rangle = -\frac{\hbar^2}{2M} <(\vec{\nabla}^{(3)}_{cm.})^2> ,$$

from Eq. (A-1),

$$T_3 = (-\frac{\hbar^2}{2M}) \cdot \frac{9}{4} <\nabla^2_\rho> . \qquad \text{(A-4)}$$

Using Eq. (A-2)

$$\frac{\partial}{\partial\rho} \chi(\rho,r) = \frac{\partial}{\partial\rho} (A \frac{e^{-\frac{\alpha}{2}\xi}}{\xi}) = A \frac{\partial\xi}{\partial\rho} \cdot \frac{\partial}{\partial\xi} (\frac{e^{-\frac{\alpha}{2}\xi}}{\xi})$$

$$\frac{\partial\chi}{\partial\rho} = -\rho \left(\frac{\alpha}{\xi} + \frac{2}{\xi^2}\right) \chi(\rho,r) .$$

Next,

$$\frac{1}{\rho^2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial\chi}{\partial\rho}\right) = \frac{2}{\rho}\frac{\partial\chi}{\partial\rho} + \frac{\partial^2\chi}{\partial\rho^2}$$

$$= -3\left(\frac{\alpha}{\xi}+\frac{2}{\xi^2}\right)\chi(\rho,r) + 2\rho^2\left(\frac{\alpha}{\xi^3}+\frac{4}{\xi^4}\right)\chi(\rho,r) + \rho^2\left(\frac{\alpha}{\xi}+\frac{2}{\xi^2}\right)^2\chi(\rho,r) .$$

Therefore,

$$\nabla^2_\rho\,\chi(\rho,r) = \left[-3\left(\frac{\alpha}{\xi}+\frac{2}{\xi^2}\right) + \rho^2\left(\frac{\alpha^2}{\xi^2}+\frac{6\alpha}{\xi^3}+\frac{12}{\xi^4}\right)\right]\chi(\rho,r) , \qquad \text{(A-5)}$$

with the substitutions $\xi = R/\alpha$ and $\rho = \dfrac{R\cos\theta}{\alpha\sqrt{2}}$, Eq. (A-5) becomes

$$\alpha^2\left[-3\left(\frac{1}{R}+\frac{2}{R^2}\right) + \frac{\cos^2\theta}{2}\left(1+\frac{6}{R}+\frac{12}{R^2}\right)\right]\chi(\rho,r) . \qquad \text{(A-6)}$$

The integrals again separate, and performing the integration over θ, Eq. (A-6) gives

$$<\nabla^2_\rho> = \alpha^2 <\frac{1}{4} - \frac{3}{2R} - eR^2>$$

$$= \alpha^2\left[\frac{1}{4} - \frac{3}{2}\frac{2!}{3!} - 3\frac{1}{3!}\right]$$

$$= -\frac{3}{4}\alpha^2$$

$$<\nabla^2_\rho> = -\frac{3}{4}\alpha^2 . \qquad \text{(A-7)}$$

Substituting Eq. (A-7) into Eq. (A-4), we find

$$T_3 = \left(\frac{\hbar^2}{2M}\right)\cdot\frac{27}{16}\alpha^2 .$$

If T_3 is expressed in MeV and α is expressed in $fm^{-2} = (10^{-15}\text{ meter})^{-2}$, then

$$T_3 = \left(\frac{\hbar^2}{2Me}\right)\cdot\frac{27}{16}\alpha^2 ,$$

where T_3 is expressed in electron volts and e is the electron charge in coulombs.

$$\frac{\hbar^2}{2Me} = 20.7 \text{ MeV - fm}^2 \ .$$

Therefore,

$$T_3 = (20.7) \cdot \frac{27}{16} \alpha^2 \text{ MeV} \ .$$

For $\alpha = 0.768 \text{ fm}^{-2}$,

$$\boxed{T_3 = 20.6 \text{ MeV}} \qquad \text{(average kinetic energy per nucleon).} \qquad (A-8)$$

APPENDIX B: POLARIZATION FROM ELASTIC SCATTERING IN THE BORN APPROXIMATION

For reference, we calculate here the polarization which one obtains from first using Born approximations with optical potentials. Consider the total Hamiltonian as $H = H_o + H_1$ where

$$H_1 = V(r) + iW(r) + V_{so}(r)\,\vec{\sigma}\cdot\vec{L}$$

$$V(r) = -V_o\, f(r)$$

$$W(r) = -W_o\, g(r)$$

$$V_{so}(r) = \lambda_\pi^2\, V_{so} \cdot \frac{1}{r}\frac{df(r)}{dr}$$

$$\lambda_\pi^2 = 2\ \text{fm}^{-2}\ . \qquad \text{(B-1)}$$

In the first Born approximation, the scattering amplitude $F(\theta)$ can be written

$$F(\theta) = \frac{1}{4\pi}\iiint d\vec{r}\, e^{-i\vec{K}\cdot\vec{r}}\, U(r)\ , \qquad \text{(B-2)}$$

where $U(r) = \frac{2\mu}{h^2} H_1(r)$, μ is reduced mass. The initial momentum is $\vec{k}_i$ and the final momentum is $\vec{k}_f$ and $\vec{K} \equiv \vec{k}_i - \vec{k}_f$. The angle between $\vec{k}_i$ and $\vec{k}_f$ is θ, the center-of-mass scattering angle. Define the Fourier transforms

$$\mathcal{F}(K) = \frac{\mu}{2\pi\hbar^2}\iiint e^{-i\vec{K}\cdot\vec{r}}\, f(r)\, d\vec{r}$$

$$\mathcal{G}(K) = \frac{\mu}{2\pi\hbar^2}\iiint e^{-i\vec{K}\cdot\vec{r}}\, g(r)\, d\vec{r}\ . \qquad \text{(B-3)}$$

Substituting Eq. (B-3) into Eq. (B-2)

$$F(\theta) = -V_o\,\mathcal{F}(K) - iW_o\,\mathcal{G}(K) + \frac{\mu\lambda_\pi^2 V_{so}}{2\pi\hbar^2}\iiint e^{-i\vec{k}_f\cdot\vec{r}}\left(\frac{1}{r}\frac{df}{dr}\right)\vec{\sigma}\cdot\vec{L}\; e^{i\vec{k}_i\cdot\vec{r}}\, d\vec{r}\ . \qquad \text{(B-4)}$$

The integral in Eq. (B-4) can be rewritten

$$\iiint e^{-i\vec{k}_f\cdot\vec{r}} \left(\frac{1}{r}\frac{df}{dr}\right) \vec{\sigma}\cdot\vec{r} \times \frac{\vec{\nabla}}{i} e^{i\vec{k}_i\cdot\vec{r}} \, d\vec{r}$$

$$= \vec{\sigma} \cdot \iiint e^{-i\vec{K}\cdot\vec{r}} \vec{\nabla}f(r) \times \vec{k}_i \, d\vec{r}$$

$$= - \vec{\sigma} \cdot \vec{k}_i \times \iiint (\vec{\nabla} e^{-i\vec{K}\cdot\vec{r}}) f(r) \, d\vec{r} ,$$

where the last step included an integration by parts. Therefore, the integral in Eq. (B-4) becomes

$$-i \vec{\sigma} \cdot \vec{k} \times \vec{K} \mathcal{J}(K) \cdot \frac{2\pi h^2}{\mu} , \tag{B-5}$$

and for elastic scattering,

$$\vec{k}_i \cdot \vec{K} = \vec{k}_i \cdot \vec{k}_f = k_i^2 \sin\theta \, \hat{n} ,$$

where $\hat{n}$ is a unit vector perpendicular to the reaction plane. Equation (B-4) can now be written

$$F(\theta) = -V_o \mathcal{J}(K) - iW_o \mathcal{A}(K) - i \, [\lambda_\pi^2 V_{so} k_i^2 \sin\theta \, \mathcal{J}(K)] \, \vec{\sigma} \cdot \vec{n}$$

$$= a(\theta) + b(\theta) \, \vec{\sigma} \cdot \vec{n} ,$$

where

$$a(\theta) = -V_o \mathcal{J}(K) - iW_o \mathcal{A}(K)$$

$$b(\theta) = -iV_{so} \, [\lambda_\pi^2 k_i^2 \sin\theta \, \mathcal{J}(K)] . \tag{B-6}$$

In terms of a and b, $FF^\dagger$ can be written

$$FF^\dagger = [\,|a|^2 + |b|^2] \, 1 + [ab^* + a^*b] \, \sigma_y$$

$$= [\,|a|^2 + |b|^2] \, 1 + 2[\mathrm{Re}(a^*b)] \, \sigma_y .$$

The cross section is (cf. Ref. 21)

$$I_o = \frac{1}{2} \mathrm{Tr} \, (FF^\dagger) = [\,|a|^2 + |b|^2] ,$$

and the polarization, P_y, is

$$I_o P_y = \frac{1}{2} \mathrm{Tr}\,(FF^\dagger \sigma_y) = 2\mathrm{Re}(a^*b) \ . \qquad \text{(B-7)}$$

Since b is pure imaginary, it may be noted in passing that the first Born approximation predicts a zero polarization for a real potential. Substituting Eq. (B-6) into Eq. (B-7), we find

$$P_y = \frac{2[iW_o \mathcal{G}(K)\ (-i)\lambda_\pi^2 V_{so} k_i^2 \sin\theta\, \mathcal{F}(K)]}{[V_o^2 \mathcal{F}^2 + W_o^2 \mathcal{G}^2] + V_{so}^2 [\lambda_\pi^2 k_i^2 \sin\theta\, \mathcal{F}]^2}$$

or

$$P_y = \frac{2W_o V_{so} \mathcal{G}(K) \mathcal{F}(K)(\lambda_\pi^2 k_i^2)\sin\theta}{[V_o^2 \mathcal{F}^2 + W_o^2 \mathcal{G}^2] + V_{so}^2 [\lambda_\pi^2 k_i^2 \sin\theta\, \mathcal{F}]^2}$$

For the usual optical potentials, $V_o >> W_o > V_{so}$. Therefore, we may write

$$P_y \propto \frac{W_o V_{so}}{V_o^2} \ .$$

Of special interest in this report is the fact that, for composite particles, the ratio (W_o/V_o) is independent of the number of nucleons in the composite particle, and therefore

$$P_y \propto \frac{V_{so}}{V_o} \ .$$

APPENDIX C: THE DEUTERON OPTICAL POTENTIAL

I. Consider the deuteron as a proton and a neutron bombarding a core, and assume that the total potential can be written as the sum of individual (two-body) potentials (see Sec. III of the report).

A.

$$H_d = T_{pn} + V_{pn}$$

$$H_{dc} = T_{dc} + U$$

$$= T_{dc} + V_{pc} + V_{nc}$$

$$H = H_{dc} + H_d$$

$$H\Psi = E\Psi$$

$$H_d\chi_d = \varepsilon_d\chi_d$$

$$H_{dc}\Phi_{dc} = E_{dc}\Phi_{dc}$$

$$E = E_{dc} + \varepsilon_d \ .$$

B. The coordinate system is shown in Fig. 2 where

$$\vec{R} = \frac{\vec{r}_p + \vec{r}_n}{2} - \vec{r}_c \qquad \vec{s}_p = \vec{R} + \frac{\vec{r}}{2}$$

$$\vec{r} = \vec{r}_p - \vec{r}_n \qquad \vec{s}_n = \vec{R} - \frac{\vec{r}}{2}$$

$$\vec{s}_p = \vec{r}_p - \vec{r}_c$$

$$\vec{s}_n = \vec{r}_n - \vec{r}_p \ .$$

C. Neglecting the distortion term,

$$\Psi(\vec{R},\vec{r}) = \Phi(\vec{R})\ \chi(\vec{r})$$

(subscripts are dropped). Then,

$$(H_d + T_{dc} + V_{pc} + V_{nc})\Psi = (\varepsilon_d + E_{dc})\Psi \ .$$

Multiplying this equation from the left by $\chi^\dagger$ and integrating over $\vec{r}$,

$$[(\chi,H_d\chi) + T_{dc}(\chi,\chi) + (\chi,[V_{pc}+V_{nc}]\chi)]\ \Phi(\vec{R}) = (\varepsilon_d+E_{dc})(\varepsilon,\varepsilon)\ \Phi(\vec{R}) \ .$$

$$\underset{\varepsilon_d}{\shortparallel} \qquad \underset{1}{\shortparallel} \qquad \underset{1}{\shortparallel}$$

Therefore,

$$(T_{dc} + U(\vec{R}))\ \Phi(\vec{R}) = E_{dc}\ \Phi(\vec{R}) \ ,$$

where we have identified

$$U(\vec{R}) = \int [\chi(\vec{r}),[V_{pc}(\vec{s}_p) + V_{nc}(\vec{s}_n)]\ \chi(\vec{r})]\ d\vec{r} \ ,$$

as the deuteron potential in $H_{dc}\Phi(\vec{R}) = E_{dc}\Phi(\vec{R})$.

D. The problem is to calculate $U(\vec{R})$. To do do, we assume an optical potential for the nucleons, which does not distinguish between protons and neutrons (this is simpler, but not necessary).

$$V_{pc}(\vec{s}) = V_{nc}(\vec{s}) = V_c(s) + V^N_{so}(s)\ \vec{\sigma}\cdot\vec{L} \ .$$

Notice that if we reverse the directions of $\vec{r}$, $\vec{s}_p \to \vec{s}_n$, etc., we need only calculate the effect of χ one one of the nucleons. We will need

$$\vec{s} = \vec{R} + \frac{\vec{r}}{2} \qquad ; \qquad \vec{\nabla}_s = \frac{1}{2}\vec{\nabla}_R + \vec{\nabla}_r$$

$$\vec{L}_j = \frac{1}{i}\vec{s}_j \times \vec{\nabla}_j \qquad ; \qquad \vec{S}_K = \frac{1}{2}\vec{\sigma}_K \ .$$

For convenience, we take $\hbar = 1$. We must evaluate

$$U_1(\vec{R}) = \int d\vec{r}\ [\chi, 2V_c(s)\ \chi(\vec{r})]$$

and

$$U_2(\vec{R}) = \frac{1}{i}\int d\vec{r}\ [\chi, V_{so}(s)(\vec{\sigma}_1 + \vec{\sigma}_2)\cdot\vec{s}\times\vec{\nabla}_s\ \chi] \ .$$

II. HULTHEN WAVE FUNCTION

A. The Hulthen wave function is of the form

$$\chi(\vec{r}) = \frac{1}{\sqrt{4\pi}} \left[\frac{u(r)}{r} + \frac{w(r)}{r\sqrt{8}} S_{12}(\theta,\phi) \right] ,$$

where

$$S_{12} = 3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - \vec{\sigma}_1 \quad \vec{\sigma}_2 .$$

Since the deuteron is always in a triplet configuration, we replace $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ by 1.

B. Find $(S_{12})^2$

$$S_{12} \cdot S_{12} = \left[3 \frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - 1 \right] \left[3 \frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - 1 \right]$$

$$= 9 \underbrace{\left[\frac{(\vec{\sigma}_1 \cdot \vec{r})}{r} \right]^2}_{1} \underbrace{\left[\frac{(\vec{\sigma}_2 \cdot \vec{r})}{r} \right]^2}_{1} - 6 \frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} + 1$$

$$= 10 - 6 \frac{(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2}$$

$$S_{12} \cdot S_{12} = 8 - 2 \left[3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - 1 \right] = 8 - 2S_{12}$$

$$(S_{12})^2 = 8 - 2S_{12} .$$

C. Expand $S_{12}(\hat{r})$ for triplet states:

$$S_{12}(\hat{r}) = 3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - 1$$

$$= 3[(\sigma_1^x \sin\theta\cos\phi + \sigma_1^y \sin\theta\sin\phi + \sigma_1^z \cos\theta)(\sigma_2^x \sin\theta\cos\phi + \sigma_2^y \sin\theta\sin\phi + \sigma_2^z \cos\theta)] - 1$$

$$S_{12} = 3[(\sigma_1^x \sigma_2^x \sin^2\theta\cos^2\phi + \sigma_1^y \sigma_2^y \sin^2\theta\sin^2\phi + \sigma_1^z \sigma_2^z \cos^2\theta)$$

$$+ (\sigma_1^x \sigma_2^y + \sigma_1^y \sigma_2^x) \sin^2\theta\cos\phi\sin\phi$$

$$+ (\sigma_1^x \sigma_2^z + \sigma_1^z \sigma_2^x) \sin\theta\cos\theta\cos\phi$$

$$+ (\sigma_1^y \sigma_2^z + \sigma_1^z \sigma_2^y) \sin\theta\cos\theta\sin\phi] - 1 \ .$$

D. Important special case: $\int_0^{2\pi} S_{12}\, d\phi \qquad (S_{12}^2 = 8 - 2S_{12})$.

For this case, all ϕ terms will integrate to zero except

$$\int_0^{2\pi} \cos^2\phi d\phi = \int_0^{2\pi} \sin^2\phi d\phi = \tfrac{1}{2}(2\pi) \quad \text{and} \quad \int_0^{2\pi} d\phi = 2\pi \ .$$

The only surviving terms are

$$\int_0^{2\pi} \frac{S_{12}(\hat{r})}{2\pi}\, d\phi = 3[\tfrac{1}{2}(\sigma_1^x \sigma_2^x \sin^2\theta + \sigma_1^y \sigma_2^y \sin^2\theta) + \sigma_1^z \sigma_2^z \cos^2\theta] - 1$$

but

$$\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y = \vec{\sigma}_1 \cdot \vec{\sigma}_2 - \sigma_1^z \sigma_2^z = 1 - \sigma_1^z \sigma_2^z \ .$$

Therefore,

$$\int \frac{S_{12}(\hat{r})}{2\pi}\, d\phi = 3[\tfrac{1}{2}(1 - \sigma_1^z \sigma_2^z) \sin^2\theta + \sigma_1^z \sigma_2^z \cos^2\theta] - 1$$

$$= \frac{3}{2} \sin^2\theta + \sigma_1^z \sigma_2^z (3\cos^2\theta - \frac{3}{2} \sin^2\theta) - 1$$

$$= 3\, \sigma_1^z \sigma_2^z (\frac{3}{2} \cos^2\theta - \frac{1}{2}) - (\frac{3}{2} \cos^2\theta - \frac{1}{2}) \ .$$

If the z axis is oriented along $\vec{R}$, $\sigma^z = \frac{\vec{\sigma}\cdot\vec{R}}{R}$ and since

$$(\frac{3}{2} \cos^2\theta - \frac{1}{2}) = P_2(\theta) \ ,$$

the Legendre polynomial $P_\ell(\theta)$ for $\ell = 2$, we find

$$\frac{1}{2\pi} \int S_{12}(\hat{r})\ d\phi = [3(\vec{\sigma}_1 \cdot \hat{R})(\vec{\sigma}_2 \cdot \hat{R}) - 1]\ P_2(\theta)$$

or

$$\frac{1}{2\pi} \int_0^{2\pi} S_{12}(\hat{r})\ d\phi = S_{12}(\hat{R})\ P_2(\theta)\ .$$

III. EVALUATION OF $U_1(\vec{R})$

A. Since U_1 contains only $V_c(s)$, the potential is

$$U_1(\vec{R}) = \frac{2}{(4\pi)} \int d\vec{r}\ u(r)\ V_c(s)\ u(r)\ \frac{1}{r^2}$$

$$+ \frac{4}{(4\pi)} \int d\vec{r}\ u(r)\ V_c(s)\ \frac{w(r)}{\sqrt{8}}\ S_{12}(\hat{r})\ \frac{1}{r^2}$$

$$+ \frac{2}{(4\pi)} \int d\vec{r}\ \frac{w(r)}{\sqrt{8}}\ V_c(s)\ \frac{w(r)}{\sqrt{8}}\ S_{12}^2(\hat{r})\ \frac{1}{r^2}\ .$$

B. The first ingegral stands. The second becomes

$$\frac{4}{(4\pi)\sqrt{8}} \left\{ \int d\vec{r}\ \frac{u(r)}{r}\ V_c(s)\ \frac{w(r)}{r}\ P_2(\theta) \right\} S_{12}(\hat{R})\ .$$

The third term becomes

$$\frac{2}{(4\pi)} \int d\vec{r}\ \frac{w(r)}{r}\ V_c(s)\ \frac{w(r)}{r}\ [1 - \tfrac{1}{4}\ S_{12}(\hat{r})]\ ,$$

which clearly gives a central term and a tensor term.

C. We conclude that U_1 contains a central part, $U_{1C}(\vec{R})$ and a tensor part, $U_{1T}(\vec{R})\ S_{12}(\hat{R})$ where:

$$U_{1C}(\vec{R}) = \frac{1}{(4\pi)} \int d\vec{r}\ \frac{u(r)}{r}\ V_c(s)\ \frac{u(r)}{r} + \frac{2}{(4\pi)} \int d\vec{r}\ \frac{w(r)}{r}\ V_c(s)\ \frac{w(r)}{r}$$

$$U_{1T}(\vec{R}) = \frac{2}{(4\pi)} \int d\vec{r}\ \frac{u(r)}{r}\ V_c(s)\ \frac{w(r)}{r}\ P_2(\theta) - \frac{1}{2(4\pi)} \int d\vec{r}\ \frac{w(r)}{r}\ V_c(s)\ \frac{w(r)}{r}\ P_2(\theta)\ .$$

IV. THE APPROACH TO $U_2(\vec{R})$

A. Since $\frac{1}{i}(\vec{s} \times \vec{\nabla}_s) = \frac{1}{i}(\vec{R} + \frac{\vec{r}}{2}) \times (\frac{1}{2}\vec{\nabla}_R + \vec{\nabla}_r)$, we must evaluate:

$$U_2(\vec{R}) = \frac{1}{(i)(4\pi)} \int d\vec{r} \left[\frac{u(r)}{r} + \frac{w(r)}{r\sqrt{8}} S_{12}\right] V_{so}(s)(\vec{\sigma}_1+\vec{\sigma}_2)\cdot(\vec{R}+\frac{\vec{r}}{2})\times(\frac{1}{2}\vec{\nabla}_R+\vec{\nabla}_r)\left[\frac{u(r)}{r} + \frac{w(r)}{r\sqrt{8}} S_{12}\right].$$

B. The plan:

1. Show that any contribution from $\vec{r} \times \vec{\nabla}_R$ comes from a component of $\vec{r}$ along $\vec{R}$. Thus we will have

$$\frac{1}{i}(\vec{R} + \frac{\vec{r}}{2}) \times \vec{\nabla}_R = \frac{1}{i}(1 + \frac{\vec{r}\cdot\vec{R}}{2R^2})\, \vec{R} \times \vec{\nabla}_R = (1 + \frac{\vec{r}\cdot\vec{R}}{2R^2})\, \vec{L}\ .$$

2. Calculate the contributions from $\vec{R} \times \vec{\nabla}_r$ which will consist of central terms and tensor terms.

3. Write $\frac{1}{i}\vec{r} \times \vec{\nabla}_r = \vec{\ell}$, an operator on S_{12} which can be written as

$$\vec{j} = \vec{\ell} + \vec{S}\ ,$$

and $\vec{\ell}$ is an Hermitian operator for χ (or S_{12}). We will find

$$\vec{S}\cdot\vec{\ell} = \frac{j(j+1) - \ell(\ell+1) - S(S+1)}{2}\ .$$

V. CONSIDER THE $\vec{\nabla}_R$ TERM

$$\int V_{so}(s) \left\{\chi(\vec{r})\ [\vec{\sigma}_1 + \vec{\sigma}_2]\ \chi(\vec{r})\right\} \cdot (\vec{R} + \frac{\vec{r}}{2}) \times \vec{\nabla}_R \cdot d\vec{r}\ .$$

A. Calculate $\chi(\vec{\sigma}_1 + \vec{\sigma}_2)\chi$

$$\frac{1}{4\pi r^2}\left[u(r) + \frac{w(r)}{\sqrt{8}} S_{12}\right] \vec{\sigma}_1 \left[u(r) + \frac{w(r)}{\sqrt{8}} S_{12}\right]$$

$$= \frac{1}{4\pi r^2}\left[u^2\vec{\sigma}_1 + \frac{u(r)w(r)}{\sqrt{8}}(\vec{\sigma}_1 S_{12} + S_{12}\vec{\sigma}_1) + \frac{w^2}{8} S_{12}\vec{\sigma}_1 S_{12}\right].$$

Note that

$$S_{12}(\vec{r}) = \frac{3}{r^2}\Big\{(\sigma_1^x\,\sigma_2^x\,x^2 + \sigma_1^y\,\sigma_2^y\,y^2 + \sigma_1^z\,\sigma_2^z\,z^2)$$

$$+ (\sigma_1^x\,\sigma_2^y + \sigma_1^y\,\sigma_2^x)\ xy$$

$$+ (\sigma_1^x\,\sigma_2^z + \sigma_1^z\,\sigma_2^x)\ xz$$

$$+ (\sigma_1^y\,\sigma_2^z + \sigma_1^z\,\sigma_2^y)\ yz\Big\} - 1\ .$$

B. Then, since $\sigma_1^j\,\sigma_1^K + \sigma_1^K\,\sigma_1^j = 0$,

$$\sigma_1^x\,S_{12} + S_{12}\,\sigma_1^x = \frac{2\cdot 3}{r^2}\Big\{\sigma_2^x\,x^2 + \sigma_2^y\,xy + \sigma_2^z\,xz\Big\} - 2\sigma_1^x\ ,$$

or

$$(\sigma_1^x\,S_{12} + S_{12}\,\sigma_1^x)\hat{i} = \frac{6x\hat{i}}{r^2}\,(\vec{\sigma}_2\cdot\vec{r}) - 2\sigma_1^x\,\hat{i}\ .$$

Adding the three components,

$$\vec{\sigma}_1\,S_{12} + S_{12}\,\vec{\sigma}_1 = 6\hat{r}(\vec{\sigma}_2\cdot\hat{r}) - 2\vec{\sigma}_1\ .$$

Likewise,

$$\vec{\sigma}_2\,S_{12} + S_{12}\,\vec{\sigma}_2 = 6\hat{r}(\vec{\sigma}_1\cdot\hat{r}) - 2\vec{\sigma}_2\ .$$

Then

$$[(\vec{\sigma}_1 + \vec{\sigma}_2)\,S_{12} + S_{12}(\vec{\sigma}_1 + \vec{\sigma}_2)] = 6\hat{r}[(\vec{\sigma}_1 + \vec{\sigma}_2)\cdot\hat{r}] - 2(\vec{\sigma}_1 + \vec{\sigma}_2)\ .$$

C. $S_{12}(\vec{\sigma}_1 + \vec{\sigma}_2)S_{12}$

Since $(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} + S_{12}(\vec{\sigma}_1+\vec{\sigma}_2) = 6\hat{r}[(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r}] - 2(\vec{\sigma}_1+\vec{\sigma}_2)$,

multiply from the left by S_{12},

$$S_{12}(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} = 6\,S_{12}\,\hat{r}[(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r}] - 2S_{12}(\vec{\sigma}_1+\vec{\sigma}_2) - S_{12}^2(\vec{\sigma}_1+\vec{\sigma}_2)\ ,$$

since

$$S_{12}^2 = 8 - 2S_{12}\ ,$$

$$S_{12}(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} = 6[3(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) - 1][(\vec{\sigma}_1\cdot\hat{r}) + (\vec{\sigma}_2\cdot\hat{r})]\hat{r} - 8(\vec{\sigma}_1+\vec{\sigma}_2)\ .$$

NOTE: $(\vec{\sigma}_1 \cdot \hat{r})^2 \equiv 1$. Then

$$S_{12}(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} = 6[3(\vec{\sigma}_2\cdot\hat{r}) + 3(\vec{\sigma}_1\cdot\hat{r}) - (\vec{\sigma}_1\cdot\hat{r}) - (\vec{\sigma}_2\cdot\hat{r})] - 8(\vec{\sigma}_1+\vec{\sigma}_2) ,$$

or

$$S_{12}(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} = 12[(\vec{\sigma}_1\cdot\hat{r}) + (\vec{\sigma}_2\cdot\hat{r})]r - 8(\vec{\sigma}_1+\vec{\sigma}_2) .$$

It may be helpful to note that

$$S_{12}\, \vec{\sigma}_1\, S_{12} = 6[3(\vec{\sigma}_1\cdot\hat{r}) - (\vec{\sigma}_2\cdot\hat{r})] - 8\vec{\sigma}_1 .$$

D. Again, $\chi(\vec{\sigma}_1 + \vec{\sigma}_2)\chi$

$$\chi(\vec{r})(\vec{\sigma}_1+\vec{\sigma}_2)\chi(\vec{r}) = \frac{1}{4\pi r^2}\left\{u^2(\vec{\sigma}_1+\vec{\sigma}_2) + \frac{u(r)w(r)}{\sqrt{8}}[(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} + S_{12}(\vec{\sigma}_1+\vec{\sigma}_2)] + \frac{w^2}{8} S_{12}(\vec{\sigma}_1+\vec{\sigma}_2)S_{12}\right\}$$

$$= \frac{1}{4\pi r^2}\left\{u^2(\vec{\sigma}_1+\vec{\sigma}_2) + \frac{u(r)w(r)}{\sqrt{8}}[6((\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r})\hat{r} - 2(\vec{\sigma}_1+\vec{\sigma}_2)] + \frac{w^2}{8}[12(\vec{\sigma}_1\cdot\hat{r} + \vec{\sigma}_2\cdot\hat{r})\hat{r} - 8(\vec{\sigma}_1+\vec{\sigma}_2)]\right\}.$$

Then

$$\chi(\vec{r})(\vec{\sigma}_1+\vec{\sigma}_2)\chi(\vec{r}) = \frac{1}{4\pi r^2}\left\{\left[u^2 - \frac{uw}{\sqrt{2}} - w^2\right](\vec{\sigma}_1+\vec{\sigma}_2) + 3\left[\frac{u(r)w(r)}{\sqrt{2}} + \frac{w^2}{2}\right][(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r}]\hat{r}\right\}.$$

Also note that

$$\chi(r)\vec{\sigma}_1\chi(r) = \frac{1}{4\pi r^2}\left\{\left[u^2 - \frac{uw}{\sqrt{2}} - w^2\right]\vec{\sigma}_1 + \left[\frac{3}{\sqrt{2}}w(u-\frac{w}{8})\vec{\sigma}_2\cdot\hat{r} + \frac{9}{4}w^2(\vec{\sigma}_1\cdot\hat{r})\right]\hat{r}\right\}.$$

E. We have now

$$\left\{\frac{1}{i}\int d\vec{r}\; V_{so}(s)\;[\chi(\vec{r})(\vec{\sigma}_1+\vec{\sigma}_2)\chi(\vec{r})]\cdot(\vec{R}+\frac{\vec{r}}{2})\right\}\times\vec{\nabla}_R\;.$$

1. Using the expansion of $\chi(\vec{\sigma}_1 + \vec{\sigma}_2)\chi$ from D, we first consider the coefficient of $(\vec{\sigma}_1 + \vec{\sigma}_2)$:

$$\frac{1}{i}\int d\vec{r}\; V_{so}(s)\left\{\left[u^2-\frac{uw}{\sqrt{2}}-w^2\right](\vec{\sigma}_1+\vec{\sigma}_2)\cdot(\vec{R}+\frac{\vec{r}}{2})\right\}\times\vec{\nabla}_R\;.$$

The only ϕ terms come in through $\vec{r}$ and they integrate to zero. This gives a $\cos\theta\,\hat{k}$ term:

$$r\cos\theta\;\hat{k}=\frac{\vec{r}\cdot\vec{R}}{R^2}\vec{R}$$

and

$$\frac{1}{i}\int d\vec{r}\; V_{so}(s)\left\{\left[u^2-\frac{uw}{\sqrt{8}}-w^2\right](\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{R}(1+\frac{\vec{r}\cdot\vec{R}}{2R^2})\right\}\times\vec{\nabla}_R$$

$$=\left\{\int d\vec{r}\; V_{so}(s)\left[u^2-\frac{uw}{\sqrt{2}}-w^2\right](1+\frac{\vec{r}\cdot\vec{R}}{2R^2})\right\}(\vec{\sigma}_1+\vec{\sigma}_2)\cdot(\frac{1}{i}R\times\vec{\nabla}_R)\;.$$

2. Next we notice that the $\hat{r}\cdot\hat{r}\times\vec{\nabla}_R$ term vanishes.

3. We have left

$$\left\{\frac{1}{4\pi}\int\frac{1}{r}\,d\vec{r}\; V_{so}(s)\;3\left[\frac{uw}{\sqrt{2}}+\frac{w^2}{2}\right][(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r}]\hat{r}\right\}\cdot\vec{R}\times\vec{\nabla}_R$$

$$(\vec{\sigma}_j\cdot\hat{r})\hat{r}=(\sigma_j^x\sin\theta\cos\phi+\sigma_j^y\sin\theta\sin\phi+\sigma_j^z\cos\theta)(\sin\theta\cos\phi\,\hat{i}+\sin\theta\sin\phi\,\hat{j}+\cos\theta\,\hat{k})\;.$$

Integrating over ϕ,

$$\frac{1}{2\pi}\int_0^{2\pi}(\vec{\sigma}_j\cdot\hat{r})\;\hat{r}\,d\phi=\frac{1}{2}(\sigma_j^x\;\hat{i}+\sigma_j^y\;\hat{j})\sin^2\theta+\hat{k}\;\sigma_j^z\cos^2\theta$$

$$=\frac{1}{2}\vec{\sigma}_j\;\sin^2\theta+\sigma_2^z\;(\cos^2\theta-\frac{1}{2}\sin^2\theta)\;\hat{k}\;.$$

The last is zero because $\hat{k}\cdot\hat{R}\times\vec{\nabla}_R = 0$. Thus, the relevant term becomes

$$\frac{1}{2\pi}\int_0^{2\pi} (\vec{\sigma}_j\cdot\hat{r})\ \hat{r}d\phi = (\frac{1}{2}\sin^2\theta)\ \vec{\sigma}_j\ ,$$

and the desired integral is

$$\left[\frac{1}{4\pi}\int d\vec{r}\ V_{so}(s)\ \cdot \frac{3w}{r^2}\frac{u}{\sqrt{2}} + \frac{w}{2}\cdot\frac{1}{2}\sin^2\theta\right]\cdot(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{L}\ .$$

F. Does the spin-orbit term of deuteron have the Thomas form? Consider only the u^2 term for the spin-orbit term.

$$\frac{\partial S}{\partial R} = \frac{R + \frac{\vec{r}\cdot\vec{R}}{2R}}{S}$$

$$f_d^0(R) = \int u^2\ f(s)\ d\vec{r}$$

$$\frac{1}{R}\frac{\partial f_d^0}{\partial R} = \frac{1}{R}\int u^2\ \frac{\partial f(s)}{\partial R}\ d\vec{r} = \frac{1}{R}\int u^2\ (\frac{\partial f}{\partial s})\ \frac{\partial s}{\partial R}\ d\vec{r}$$

$$= \frac{1}{R}\int u^2\ \cdot\ (\frac{1}{s}\frac{\partial f}{\partial s})\ \cdot\ s\left[\frac{R + \frac{\vec{r}\cdot\vec{R}}{2R}}{S}\right] d\vec{r}$$

$$= \int u^2\ d\vec{r}\ h(s)\ (1 + \frac{\vec{r}\cdot\vec{R}}{2R^2})$$

$$\frac{1}{R}\frac{\partial f_d^0}{\partial R} = h_d^0\ ,$$

so that the largest contribution (from u^2) is of the Thomas form. However, in general it is not.

G. Conclusion for the $\frac{1}{i}\ (\vec{R} + \frac{\vec{r}}{2}) \times \frac{1}{2}\ \vec{\nabla}_R$ term:

$$\frac{1}{2i}\int V_{so}(s)\ [\chi(r)[\vec{\sigma}_1+\vec{\sigma}_2]\chi(\vec{r})]\ \cdot\ (\vec{R} + \frac{\vec{r}}{2})\times\vec{\nabla}_R\ d\vec{r}$$

$$= \frac{1}{4\pi}\cdot\left\{\frac{1}{2}\int d\vec{r}\ \frac{V_{so}(s)}{r^2}\left\{\left[u^2 - \frac{uw}{\sqrt{2}} - w^2\right]\left(1 + \frac{\vec{r}\cdot\vec{R}}{2R^2}\right) + \frac{3w}{\sqrt{8}}\ [u + \frac{w}{\sqrt{2}}]\sin^2\theta\right\}\right\}(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{L}\ .$$

Or, if we write $\vec{S} = \frac{1}{2}\ (\vec{\sigma}_1+\vec{\sigma}_2)$, this is the "$\vec{S}\cdot\vec{L}$" term in the potential.

VI. THE $\vec{R} \times \vec{\nabla}_r$ TERM

Next we consider

$$\frac{1}{i} \int d\vec{r}\; V_{so}(s) \left\{ \chi(\vec{r})(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \vec{R} \times \vec{\nabla}_r\, \chi(\vec{r}) \right\} .$$

A. Calculate $\vec{\nabla}_r\, \chi(\vec{r})$:

1. In spherical coordinates,

$$\vec{\nabla}_r = \frac{\vec{r}}{r}\frac{\partial}{\partial r} + \frac{\hat{\varepsilon}_\theta}{r}\frac{\partial}{\partial \theta} + \frac{\hat{\varepsilon}_\phi}{r\sin\theta}\frac{\partial}{\partial \phi} ,$$

where

$$\hat{r} = \sin\theta\cos\phi\,\hat{i} + \sin\theta\sin\phi\,\hat{j} + \cos\theta\,\hat{k}$$

$$\hat{\varepsilon}_\theta = \cos\theta\cos\phi\,\hat{i} + \cos\theta\sin\phi\,\hat{j} - \sin\theta\,\hat{k}$$

$$\hat{\varepsilon}_\phi = -\sin\phi\,\hat{i} + \cos\phi\,\hat{j}$$

2. $\vec{\nabla}_r\, S_{12}\,(\theta,\phi)$

Note that $\vec{\nabla}_r(\hat{r}) = \frac{\hat{\varepsilon}_\theta}{r}(\hat{\varepsilon}_\theta) + \frac{\hat{\varepsilon}_\phi}{r}(\hat{\varepsilon}_\phi)$. Then

$$\begin{aligned}
\vec{\nabla}_r S_{12} &= 3(\vec{\sigma}_1 \cdot \vec{\nabla}_r\,\hat{r})(\vec{\sigma}_2\cdot\hat{r}) + 3(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2 \cdot \vec{\nabla}_r\,\hat{r}) \\
&= \frac{3}{r}[(\vec{\sigma}_1\cdot\hat{\varepsilon}_\theta)(\vec{\sigma}_2\cdot\hat{r})\hat{\varepsilon}_\theta+(\vec{\sigma}_1\cdot\hat{\varepsilon}_\phi)(\vec{\sigma}_2\cdot\hat{r})\hat{\varepsilon}_\phi+(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{\varepsilon}_\theta)\hat{\varepsilon}_\theta+(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{\varepsilon}_\phi)\hat{\varepsilon}_\phi] \\
&= \frac{3}{r}\left\{(\vec{\sigma}_2\cdot\hat{r})[(\vec{\sigma}_1\cdot\hat{\varepsilon}_\theta)\hat{\varepsilon}_\theta+(\vec{\sigma}_1\cdot\hat{\varepsilon}_\phi)\hat{\varepsilon}_\phi]+(\vec{\sigma}_1\cdot\hat{r})[(\vec{\sigma}_2\cdot\hat{\varepsilon}_\theta)\hat{\varepsilon}_\theta+(\vec{\sigma}_2\cdot\hat{\varepsilon}_\phi)\hat{\varepsilon}_\phi]\right\} \\
&= \frac{3}{r}\left\{(\vec{\sigma}_2\cdot\hat{r})[\vec{\sigma}_1-(\vec{\sigma}_1\cdot\hat{r})\hat{r}]+(\vec{\sigma}_1\cdot\hat{r})[\vec{\sigma}_2-(\vec{\sigma}_2\cdot\hat{r})\hat{r}]\right\} \\
\vec{\nabla}_r S_{12} &= \frac{3}{r}\left\{(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2+(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1-2(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r})\hat{r}\right\} .
\end{aligned}$$

3. $\vec{\nabla}_r\, \chi(\vec{r})$:

$$\vec{\nabla}_r\, \chi(\vec{r}) = \vec{\nabla}_r \left\{ \frac{1}{(4\pi)^{\frac{1}{2}} r} \left[u(r) + \frac{w(r)}{\sqrt{8}} S_{12} \right] \right\}$$

$$\vec{\nabla}_r\, \chi(\vec{r}) = \frac{r}{(4\pi)^{\frac{1}{2}}} \left[\frac{d}{dr}\left(\frac{u(r)}{r}\right) + \frac{S_{12}}{\sqrt{8}} \frac{d}{dr}\left(\frac{w(r)}{r}\right) \right]$$

$$+ \frac{w(r)}{(4\pi)^{\frac{1}{2}} r\sqrt{8}} \vec{\nabla}_r\, S_{12}$$

$$\vec{\nabla}_r \chi(\vec{r}) = \frac{1}{(4\pi)^{\frac{1}{2}}} \left\{ \left[\frac{d}{dr}\left(\frac{u(r)}{r}\right) + \frac{S_{12}}{\sqrt{8}} \frac{d}{dr}\left(\frac{w(r)}{r}\right)\right]\hat{r} \right.$$

$$\left. + \frac{3w(r)}{r^2\sqrt{8}} \left[(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1 - 2(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r})\hat{r}\right]\right\}.$$

Or, since $(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) = \dfrac{S_{12} + 1}{3}$,

$$\vec{\nabla}_r \chi(\vec{r}) = \frac{1}{(4\pi)^{\frac{1}{2}}} \left\{ \left[\frac{d}{dr}\left(\frac{u}{r}\right) - \frac{w(r)}{r^2\sqrt{2}} + \frac{1}{\sqrt{8}}\left[\frac{d}{dr}\left(\frac{w(r)}{r}\right) - \frac{2w(r)}{r^2}\right] S_{12}\right]\hat{r} \right.$$

$$\left. + \frac{3w(r)}{r^2\sqrt{8}} \left[(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1\right]\right\}.$$

B. Often used relations:

1. $\sigma_j \sigma_k = \delta_{jk} + i\, e^{ik\ell} \sigma_\ell$

$e^{jk\ell} = 1$, ijk + permutation of 1, 2, 3

$= 0$, not permutation

$= -1$, $jk\ell$ odd permutation

i.e,, if $j = k$,

$\sigma_j\sigma_j = 1$

if $j = 1,\ k = 2,$

$\sigma_x\sigma_y = i\,\sigma_z$

if $j = 2,\ k = 1,$

$\sigma_y\sigma_x = -i\,\sigma_z$.

Therefore,

$$\sigma_x\sigma_y + \sigma_y\sigma_x = 0$$

$$\sigma_x\sigma_y - \sigma_y\sigma_x = i\,2\sigma_z \text{ , etc.}$$

2. $(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = (\vec{A}\cdot\vec{B}) + i\ \vec{\sigma}\cdot(\vec{A}\times\vec{B})$, where $\vec{A}$ and $\vec{B}$ are two vectors which commute with $\vec{\sigma}$. Example: Let $\vec{\sigma} = \vec{\sigma}_1$, $\vec{A} = \hat{k}$, $\vec{B} = \vec{\sigma}_2$,

$$(\vec{\sigma}_1\cdot\hat{k})(\vec{\sigma}_1\cdot\vec{\sigma}_2) = (\hat{k}\cdot\vec{\sigma}_2) + i\ \vec{\sigma}_1\cdot(\hat{k}\cdot\vec{\sigma}_2)\ .$$

Since $(\vec{\sigma}_1\cdot\vec{\sigma}_2) = 1$ for triplet states,

$$\vec{\sigma}_1\cdot\hat{k}\times\vec{\sigma}_2 = i(\sigma_2^z - \sigma_1^z)$$

$$\vec{\sigma}_2\cdot\hat{k}\times\vec{\sigma}_1 = -i(\sigma_2^z - \sigma_1^z)\ .$$

3. In a triple scalar product, the dot and cross can be interchanged.

$$\vec{\sigma}\cdot\hat{k}\times\vec{\sigma} = \begin{vmatrix} \sigma_x & \sigma_y & \sigma_z \\ 0 & 0 & 1 \\ \sigma_x & \sigma_y & \sigma_z \end{vmatrix} = -\sigma_x\sigma_y + \sigma_y\sigma_x = -2i\ \sigma_z$$

$$-\vec{\sigma}\times\vec{\sigma}\cdot\hat{k} = -\begin{vmatrix} \sigma_x & \sigma_y & \sigma_z \\ \sigma_x & \sigma_y & \sigma_z \\ 0 & 0 & 1 \end{vmatrix} = -\sigma_x\sigma_y + \sigma_y\sigma_x = -2i\ \sigma_z$$

or

$$-\vec{\sigma}\times\vec{\sigma}\cdot\hat{k} = -2i\ \vec{\sigma}\cdot\hat{k} = -2i\ \sigma_z\ .$$

4. $$\vec{\sigma}_1(\vec{\sigma}_1\cdot\hat{r}) + (\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_1 = {}_1(\sigma_1^x \frac{x}{r} + \sigma_1^y \frac{y}{r} + \sigma_1^z \frac{z}{r}) + (\sigma_1^x \frac{x}{r} + \sigma_1^y \frac{y}{r} + \sigma_1^z \frac{z}{r})\vec{\sigma}_1 + 2\frac{x}{r}\hat{i} + 2\frac{y}{r}\hat{j} + 2\frac{z}{r}\hat{k}\ ,$$

or

$$\vec{\sigma}_1(\vec{\sigma}_1\cdot\hat{r}) + (\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_1 = 2\ \hat{r}\ .$$

C. "Standard Forms"

1. $$(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times \frac{1}{2\pi} \int_0^{2\pi} [(\vec{\sigma}_1 \cdot \hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2 \cdot \hat{r})\vec{\sigma}_1] d\phi$$

$$= (\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times [\sigma_1^z\vec{\sigma}_2+\sigma_2^z\vec{\sigma}_1] = -\hat{k} \cdot (\vec{\sigma}_1+\vec{\sigma}_2) \times [\sigma_1^z\vec{\sigma}_2+\sigma_2^z\vec{\sigma}_1]$$

$$= -\hat{k} \cdot [(\vec{\sigma}_1 \times \vec{\sigma}_2)(\sigma_1^z-\sigma_2^z)] - [4i\ \sigma_1^z\sigma_2^z]$$

$$= -4i\ \sigma_1^z\sigma_2^z + 2i\ (\vec{\sigma}_1 \cdot \vec{\sigma}_2 - \sigma_1^z\sigma_2^z)$$

$$= -2i\ [3\sigma_1^z\sigma_2^z - 1]$$

$$= -2i\ S_{12}\ (\hat{R})\ .$$

2. $$(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times \frac{1}{2\pi} \int_0^{2\pi} S_{12}\ \hat{r}\ d\phi$$

$$\frac{1}{2\pi} \int_0^{2\pi} S_{12}\ \hat{r}\ d\phi = \frac{3}{2} \sin^2\theta\cos\theta \left[(\sigma_1^x\sigma_2^z+\sigma_1^z\sigma_2^x)\hat{i} + (\sigma_1^y\sigma_2^z+\sigma_1^z\sigma_2^y)\hat{j} + ()\hat{k}\right]$$

$$= \frac{3}{2} \sin^2\theta\cos\theta\ \ [\sigma_1\sigma_2^z+\sigma_2\sigma_1^z+()\hat{k}]$$

$$\downarrow$$

$$\hat{k} \times \hat{k} = 0$$

$$= -(3i)\ \sin^2\theta\cos\theta\ S_{12}\ (\hat{R})\ .$$

3. $$(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times \frac{1}{2\pi} \int_0^{2\pi} [(\vec{\sigma}_1 \cdot \hat{r})\vec{\sigma}_1 + (\vec{\sigma}_2 \cdot \hat{r})\vec{\sigma}_2] d\phi$$

$$= -(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times [\vec{\sigma}_1\sigma_1^z+\vec{\sigma}_2\sigma_2^z]$$

$$= (\vec{\sigma}_1 \times \vec{\sigma}_1) \cdot \hat{k}\ \sigma_1^z - \vec{\sigma}_1 \times \vec{\sigma}_2 \cdot \hat{k}\ [\sigma_1^z-\sigma_2^z] + \vec{\sigma}_2 \times \vec{\sigma}_2 \cdot \hat{k}\ \sigma_2^z$$

$$= 2i[(\sigma_1^z)^2 + (\sigma_2^z)^2] - [(\sigma_1^x\sigma_2^y - \sigma_1^y\sigma_2^x)(\sigma_1^z-\sigma_2^z)]$$

$$= 4i + 2i(\vec{\sigma}_1 \cdot \vec{\sigma}_2 - \sigma_1^z\sigma_2^z) = 6i - 2i\ \sigma_1^z\sigma_2^z\ .$$

SUMMARY:

STANDARD FORM I

$$(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times \frac{1}{2\pi} \int_0^{2\pi} [(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]d\phi = -2i\ S_{12}\ (\hat{R})$$

STANDARD FORM II

$$(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times \frac{1}{2\pi} \int_0^{2\pi} S_{12}\ (\hat{r})\hat{r}\ d\phi = -3i\ \sin^2\theta\cos\theta\ S_{12}\ (\hat{R})$$

STANDARD FORM III

$$(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times \frac{1}{2\pi} \int_0^{2\pi} [(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_1 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_2]d\phi = 6i - 2i\ \sigma_1^z\sigma_2^z\ .$$

D. Definition of Terms

1. $$\chi(\vec{r})(\vec{\sigma}_1+\vec{\sigma}_2) = \frac{1}{(4\pi)^{\frac{1}{2}}r}\left\{u(\vec{\sigma}_1+\vec{\sigma}_2) + \frac{w}{\sqrt{8}}\ S_{12}\ (\vec{\sigma}_1+\vec{\sigma}_2)\right\}$$

$$= \frac{1}{(4\pi)^{\frac{1}{2}}r}\left\{u(\vec{\sigma}_1+\vec{\sigma}_2) + \frac{w}{\sqrt{8}}\left[6\hat{r}[(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r}] - 2(\vec{\sigma}_1+\vec{\sigma}_2) - (\vec{\sigma}_1+\vec{\sigma}_2)S_{12}\right]\right\}$$

$$\chi(\vec{r})(\vec{\sigma}_1+\vec{\sigma}_2) = \frac{1}{(4\pi)^{\frac{1}{2}}r}\left\{[u- \frac{w}{\sqrt{2}}](\vec{\sigma}_1+\vec{\sigma}_2)- \frac{w}{\sqrt{8}}(\vec{\sigma}_1+\vec{\sigma}_2)S_{12}+ \frac{6w}{\sqrt{8}}\hat{r}[(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r}]\right\} .$$

Also

$$\vec{\nabla}_r\ \chi(\vec{r}) = \frac{1}{(4\Pi)}\left\{\left[[\frac{d}{dr}\ (\frac{u}{r}) - \frac{w(r)}{r^2\sqrt{2}}]\ \hat{r} + \frac{1}{\sqrt{8}}\ [\frac{d}{dr}\ (\frac{w}{r}) - \frac{2w}{r^2}]\ S_{12}\ \hat{r}\right] + \frac{3w}{r^2\sqrt{8}}\ [(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]\right\} .$$

We wish to evaluate:

$$\frac{1}{i}\int d\vec{r}\ \chi(\vec{r})\ V_{so}(s)\ (\vec{\sigma}_1+\vec{\sigma}_2)\ \cdot\ \hat{R} \times \vec{\nabla}_r\ \chi(\vec{r})$$

$$= \frac{R}{4\pi i}\int d\vec{r}\ V_{so}(s)\left\{\left[d(r)(\vec{\sigma}_1+\vec{\sigma}_2)+e(r)(\vec{\sigma}_1+\vec{\sigma}_2)S_{12}+f(r)[(\vec{\sigma}_1\cdot\hat{r})+(\vec{\sigma}_2\cdot\hat{r})]\hat{r}\right] \cdot \hat{k} \times \left[a(r)\hat{r}+b(r)S_{12}\hat{r}+c(r)[(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]\right]\right\} ,$$

where

$$\chi(\vec{r})(\vec{\sigma}_1+\vec{\sigma}_2) = d(\vec{\sigma}_1+\vec{\sigma}_2) + e(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} + f[(\vec{\sigma}_1\cdot\hat{r}) + (\vec{\sigma}_2\cdot\hat{r})]\hat{r}$$

$$d(r) = \frac{1}{r}\left[u - \frac{w}{\sqrt{2}}\right]$$

$$e(r) = -\frac{w}{r\sqrt{8}}$$

$$f(r) = \frac{6w}{r\sqrt{8}}$$

and

$$\vec{\nabla}_r\, \chi(\vec{r}) = a(r)\hat{r} + b(r)S_{12}\,\hat{r} + c(r)[(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1] ,$$

where

$$a(r) = \left[\frac{d}{dr}\left(\frac{u}{r}\right) - \frac{w}{r^2\sqrt{2}}\right] \quad ; \quad b(r) = \frac{1}{\sqrt{8}}\left[\frac{d}{dr}\left(\frac{w}{r}\right) - \frac{2w}{r^2}\right]$$

$$c(r) = \frac{3w}{r^2\sqrt{8}} .$$

E. Evaluations of the $\vec{R} \times \vec{\nabla}_r$ terms:

1. The d-a term = 0, ($\hat{k} \times \hat{k} = 0$).

2. The d-b term $= \frac{R}{4\pi i}\int d\vec{r}\; V_{so}(s)\; d(r)\; b(r)\; (\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times S_{12}\,\hat{r}$.

Using Standard Form II this gives

$$-\frac{3R}{4\pi}\left\{\int d\vec{r}\; V_{so}(s) \cdot (d\cdot b)\, \sin^2\theta\cos\theta\right\} S_{12}(\hat{R}) .$$

3. The d-c term $= \frac{R}{4\pi i}\int d\vec{r}\; V_{so}(s)(d\cdot c)\left[(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times [(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]\right]$

Using Standard Form I this gives

$$-\frac{2R}{4\pi}\left\{\int d\vec{r}\; V_{so}(s) \cdot (dc)\right\} S_{12}(\hat{R}) .$$

4. The e-a term $= \frac{R}{4\pi i}\int d\vec{r}\; V_{so}(s)(ea)\left[(\vec{\sigma}_1+\vec{\sigma}_2) \cdot \hat{k} \times S_{12}\,\hat{r}\right]$.

Again, Standard Form II gives

$$-\frac{3R}{4\pi}\left\{\int d\vec{r}\ V_{so}(s)\cdot(ea)\ \sin^2\theta\cos\theta\right\} S_{12}(\hat{R}) \ .$$

5. The e-b term $= \frac{R}{4\pi i}\int d\vec{r}\ V_{so}(s)(eb)\ \left[(\vec{\sigma}_k+\vec{\sigma}_2)\cdot\hat{k}\times S_{12}^2\ \hat{r}\right]$, but $S_{12}^2 = 8 - 2S_{12}$, the term with 8 vanishes, leaving

$$\frac{6R}{4\pi}\left\{\int d\vec{r}\ V_{so}(s)\cdot(e\cdot b)\ \sin^2\theta\cos\theta\right\} S_{12}(\hat{R}) \ .$$

6. The e-c term $= \frac{R}{4\pi i}\int d\vec{r}\ V_{so}(s)\cdot(ec)\ \left[(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{k}\times S_{12}[(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2+(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]\right]$

but

$$[3(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) - 1][(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 + (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]$$

$$= 3(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_2 + 3(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_1 - (\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2 - (\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1 \ .$$

Then the integral becomes

$$\frac{R}{4\pi i}\int d\vec{r}\ V_{so}(s)(e\cdot c)\left\{(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{k}\times\left[3[(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_2+(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_1] - [(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2+(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]\right]\right\} \ .$$

Using Standard Forms I and III, the brackets give

$$18i - 6i\ \sigma_1^z\sigma_2^z + 6i\ \sigma_1^z\sigma_2^z - 2i = 16i \ .$$

Or this term becomes

$$\frac{16R}{4\pi}\int d\vec{r}\ V_{so}(s)\cdot(e\cdot c) \qquad \text{(a central term)} \ .$$

7. The f-a term = 0 because $\hat{r}\times\hat{r} = 0$.

8. The f-b term = 0 because $\hat{r}\times\hat{r} = 0$.

9. The f-c term

$$= \frac{R}{4\pi i}\int d\vec{r}\ V_{so}(s)(f\cdot c)\left[\hat{r}\cdot\hat{k}\times[(\vec{\sigma}_k\cdot\hat{r})+(\vec{\sigma}_2\cdot\hat{r})][(\vec{\sigma}_1\cdot\hat{r})\vec{\sigma}_2+(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1]\right] \ .$$

The brackets give

$$\vec{\sigma}_2 + (\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_1 + (\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r})\vec{\sigma}_2+\vec{\sigma}_1$$

$$= [(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) + 1]\ (\vec{\sigma}_1+\vec{\sigma}_2)\ .$$

The "1" in the brackets contributes zero, so we can subtract $-\frac{4}{3}(\vec{\sigma}_1+\vec{\sigma}_2)$. Thus, the term becomes

$$S_{12}(\vec{\sigma}_1+\vec{\sigma}_2) \Rightarrow -(\vec{\sigma}_1+\vec{\sigma}_2)S_{12} \qquad \text{(because other terms are zero).}$$

Then we have left

$$\frac{S_{12}}{3}(\vec{\sigma}_1+\vec{\sigma}_2)\ .$$

Therefore, the f-c term becomes

$$-\frac{R}{4\pi i}\int d\vec{r}\ V_{so}(s)(f\cdot c)\left[\hat{r}\cdot\hat{k}\times(\vec{\sigma}_1+\vec{\sigma}_2)\frac{S_{12}}{3}\right]$$

$$= +\frac{R}{4\pi i}\cdot\frac{1}{3}\int d\vec{r}\ V_{so}(s)(f\cdot c)\left[(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{k}\times S_{12}\,\hat{r}\right],$$

which gives

$$-\frac{1}{4\pi}\left\{\int d\vec{r}\ V_{so}(s)(f\cdot c)\ \sin^2\theta\cos\theta\right\} S_{12}(\hat{R})\ .$$

F. Summary of $\vec{R}\times\vec{\nabla}_r$ terms:

$$\frac{3R\cdot S_{12}(R)}{4\pi}\int d\vec{r}\ V_{so}(s)\sin^2\theta\cos\theta\left[-d\cdot b - e\cdot a + 2e\cdot b - \frac{f\cdot c}{3}\right]$$

$$+\frac{2R\ S_{12}(R)}{4\pi}\int d\vec{r}\ V_{so}(s)(d\cdot c) + \frac{16R}{4\pi}\int d\vec{r}\ V_{so}(s)\cdot(e\cdot c)\ .$$

But the brackets become

$$= \frac{1}{r\sqrt{8}}\left\{-[u - \frac{w}{\sqrt{2}}][\frac{d}{dr}(\frac{w}{r}) - \frac{2w}{r^2}] + w[\frac{d}{dr}(\frac{u}{r}) - \frac{w}{r^2\sqrt{2}}]\right.$$

$$\left. - \frac{2w}{\sqrt{8}}[\frac{d}{dr}(\frac{w}{r}) - \frac{2w}{r^2}] - \frac{6w}{\sqrt{8}}[\frac{w}{r^2}]\right\}$$

$$= \frac{1}{r\sqrt{8}} \Big\{ w \frac{d}{dr}\left(\frac{u}{r}\right) - u \frac{d}{dr}\left(\frac{w}{r}\right) + \frac{w}{\sqrt{2}} \frac{d}{dr}\left(\frac{w}{r}\right) - \frac{w^2}{r^2\sqrt{2}}$$

$$- \frac{2w^2}{\sqrt{2}r^2} + \frac{2uw}{r^2} + \frac{2w^2}{\sqrt{2}r^2} - \frac{w}{\sqrt{2}} \frac{d}{dr}\left(\frac{w}{r}\right) - \frac{6w^2}{\sqrt{8}r^2} \Big\}$$

$$= \frac{1}{r\sqrt{8}} \left\{ w \frac{d}{dr}\left(\frac{u}{r}\right) - u \frac{d}{dr}\left(\frac{w}{r}\right) + \frac{2uw}{r^2} - \frac{4}{\sqrt{2}} \frac{w^2}{r^2} \right\}.$$

Let $u' = \frac{du}{dr}$; $w' = \frac{dw}{dr}$. Then

$$= \frac{1}{r\sqrt{8}} \left\{ (wu' - uw') + \frac{2uw}{r^2} - \frac{4}{\sqrt{2}} \frac{w^2}{r^2} \right\} .$$

Therefore, the $\vec{R} \times \vec{\nabla}_r$ term is

$$\frac{3R}{4\pi} \int d\vec{r}\, V_{so}(s) \frac{\sin^2\theta\cos\theta}{r\sqrt{8}} \left\{ (wu' - uw') + \frac{2uw}{r^2} - \frac{4}{\sqrt{2}} \frac{w^2}{r^2} \right\} S_{12}(\hat{R})$$

$$- \frac{3R}{4\pi} \int d\vec{r}\, V_{so}(s) \frac{w}{r^3\sqrt{2}} [u - \frac{w}{\sqrt{2}}]\, S_{12}(\hat{R})$$

$$- \frac{6R}{4\pi} \int d\vec{r}\, V_{so}(s) \frac{w^2}{r^3} .$$

VII. THE $\frac{1}{i}\, \vec{r} \times \vec{\nabla}_r = \ell$ TERM

$$\frac{1}{2} \int d\vec{r}\, V_{so}(s)\, \chi(\vec{r})\, (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{\ell}\, \chi(\vec{r})$$

$$\vec{\ell}\, \chi(\vec{r}) = \vec{\ell} \cdot \frac{1}{(4\pi)^{\frac{1}{2}}} \left[\frac{u}{r} + \frac{w}{r\sqrt{8}} S_{12} \right]$$

$$= 0 + \frac{1}{(4\pi)^{\frac{1}{2}}} \frac{w}{r\sqrt{8}} S_{12} \quad ,$$

where $\vec{\ell}$ is now a vector, $(\ell = 2)$, and can be moved anywhere. Putting it back into the integral as a number, we note that

$$\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2) = \vec{S} \quad ; \quad \vec{J} = \vec{\ell} + \vec{S} .$$

Therefore,

$$\frac{j(j+1) - \ell(\ell+1) - S(S+1)}{2} = \vec{\ell} \cdot \vec{S} \ ,$$

where $j = 1$, $\ell = 2$, $S = 1$. Therefore,

$$\vec{\ell} \cdot \vec{S} = - \frac{6}{2} = - 3 \ .$$

Then the $\vec{\ell}$ term becomes

$$- \frac{3}{(4\pi)^{\frac{1}{2}}} \int d\vec{r} \ V_{so}(s) \ \chi(\vec{r}) \ \frac{w}{r\sqrt{8}} \ S_{12}$$

$$= - \frac{3}{(4\pi)} \int d\vec{r} \ V_{so}(s) \ [\frac{u}{r^2} \frac{w}{\sqrt{8}} S_{12} + \frac{w^2}{8r^2} (8 - 2S_{12})] \ ,$$

which yields a central part

$$- \frac{3}{(4\pi)} \int d\vec{r} \ V_{so}(s) \ \frac{w^2}{r^2} \ ,$$

and a tensor part

$$- \frac{3}{(4\pi)} \left\{ \int d\vec{r} \ V_{so}(s) \left[\frac{uw}{r^2\sqrt{8}} - \frac{w^2}{4r^2} \right] \right\} S_{12}(\hat{R}) \ .$$

VIII. SUMMARY

The problem is to calculate

$$U(\vec{R}) = \int d\vec{r} \ \chi(\vec{r}) [2V_C(s) + V_{so}(s)(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot (\vec{R} + \frac{\vec{r}}{2}) \ (\frac{1}{2} \vec{\nabla}_R + \vec{\nabla}_r)] \ \chi(\vec{r})$$

$$= U_1(\vec{R}) + U_2(R) \ ,$$

where U_1 contains V_C and U_2 contains V_{so}.

A. $U_1 = U_{1C} + U_{1T} \ [(\vec{S} \cdot \hat{R})^2 - \frac{2}{3}]$

$$U_{1C} = \frac{2}{(4\pi)} \int d\vec{r} \ V_C(s) \left[(\frac{u(r)}{r})^2 + (\frac{w(r)}{r})^2 \right]$$

$$U_{1T} = \frac{6\sqrt{2}}{(4\pi)} \int d\vec{r} \ V_C(s) \ \frac{w(r)}{r^2} \ P_2(\theta) \left[u(r) - \frac{w(r)}{\sqrt{8}} \right]$$

$$[(\vec{S}\cdot\vec{R})^2 - \tfrac{2}{3}] = \tfrac{1}{6}\,[(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) - 1] = \tfrac{1}{6}\,S_{12}(\hat{R})$$

$$\vec{S} = \tfrac{1}{2}\,[\vec{\sigma}_1+\vec{\sigma}_2] \ .$$

B. $U_2 = U_{2C} + U_{2so}\,\vec{S}\cdot\vec{L} + U_{2T}\,[(\vec{S}\cdot\vec{R})^2 - \tfrac{2}{3}]$

1. Central:

$$U_{2C}(R) = -\frac{3}{(4\pi)}\int d\vec{r}\; V_{so}(s)\left[\frac{w^2}{r^2} + 2\,\frac{Rw^2}{r^3}\right] \ .$$

2. Spin-Orbit:

$$U_{2so}(R) = \frac{1}{4\pi}\int d\vec{r}\,\frac{V_{so}(s)}{r^2}\left\{\left[u^2 - \frac{uw}{\sqrt{2}} - w^2\right]\left(1 + \frac{\vec{r}\cdot\vec{R}}{2R^2}\right) + \frac{3w}{\sqrt{8}}\,[u + \frac{w}{\sqrt{2}}]\sin^2\theta\right\} \ .$$

3. Tensor:

$$U_{2T}(R) = \frac{9R}{4\pi}\int d\vec{r}\; V_{so}(s)\,\frac{\sin^2\theta\cos\theta}{r\sqrt{2}}\left[\frac{(wu'-uw')}{r} + \frac{2uw}{r^2} - \frac{4w^2}{\sqrt{2}r^2}\right]$$

$$\times\,\frac{-18R}{4\pi}\int d\vec{r}\; V_{so}(s)\,\frac{w}{r^3\sqrt{2}}\,[u - \frac{w}{\sqrt{2}}] \ .$$

C. Regrouping the potential into zeroth-order and first-order terms, we write

$$U(\vec{R}) = [U_C^{(0)}(R)+U_C^{(1)}(R)]+[U_{so}^{(0)}(R)+U_{so}^{(1)}(R)]\vec{S}\cdot\vec{L}+[U_r^{(0)}+U_T^{(1)}][(\vec{S}\cdot\vec{R})^2 - \tfrac{2}{3}] \ ,$$

where

$$U_C^{(0)}(R) = \frac{2}{(4\pi)}\int d\vec{r}\; V_C(s)\;(\tfrac{u}{r})^2$$

$$U_C^{(1)}(R) = \frac{2}{(4\pi)}\int d\vec{r}\; V_C(s)\;(\tfrac{w}{r})^2 - \frac{3}{(4\pi)}\int d\vec{r}\; V_{so}(s)\left[\frac{w^2}{r^2} + \frac{2Rw^2}{r^3}\right]$$

$$U_{so}^{(0)}(R) = \frac{1}{(4\pi)}\int d\vec{r}\,\frac{V_{so}(s)}{r^2}\left\{\left[u^2 - \frac{uw}{\sqrt{2}}\right]\left(1 + \frac{\vec{r}\cdot\vec{R}}{2R^2}\right) + \frac{3uw}{\sqrt{8}}\sin^2\theta\right\}$$

$$U_{so}^{(1)}(R) = \frac{1}{(4\pi)}\int d\vec{r}\,\frac{V_{so}}{r^2}\left[(-w^2)\left(1 + \frac{\vec{r}\cdot\vec{R}}{2R^2}\right) + \frac{3w^2}{4}\sin^2\theta\right]$$

$$U_T^{(0)}(R) = \frac{6\sqrt{2}}{(4\pi)} \int d\vec{r}\; V_C(s)\, \frac{uw}{r^2}\, P_2(\theta)$$

$$U_T^{(1)}(R) = \frac{-3}{(4\pi)} \int d\vec{r}\; V_C(s)\, P_2(\theta)\, \frac{w^2}{r^2} - \frac{18R}{(4\pi)} \int d\vec{r}\; V_{so}(s)\, \frac{w}{r^3\sqrt{2}} \left[u - \frac{w}{\sqrt{2}}\right]$$

$$+ \frac{9R}{(4\pi)} \int d\vec{r}\; V_{so}(s)\, \frac{\sin^2\theta\cos\theta}{r\sqrt{2}} \left[\frac{(wu'-uw')}{r} + \frac{2uw}{r^2} - \frac{4w^2}{\sqrt{2}r^2}\right] .$$

APPENDIX D: DEUTERON WAVE FUNCTION

I. COUPLING OF ANGULAR MOMENTUM

The deuteron is a composite particle with even parity and total spin $I = 1$. It consists of two spin-1/2 constituents, $\vec{S}_1 = 1/2\, \vec{\sigma}_1$ and $\vec{S}_2 = 1/2\, \vec{\sigma}_2$. Coupling orbital angular momentum $(\vec{L}_d)$ and spin $(\vec{S}_d = \vec{S}_1 + \vec{S}_2)$, we find

$$\vec{I}_d = \vec{L}_d + \vec{S}_d \ .$$

Since $S_d = 0$ cannot couple to $\ell = 2$ to give a spin $I_d = 1$, the spins are always parallel. Writing $S_{1/2}^{1/2} = \alpha = \binom{1}{0}$ and $S_{1/2}^{-1/2} = \beta = \binom{0}{1}$, we can form the spin wave function $y_I^{m_I}$ as

$$y_I^{m_I} = \sum_{m_j = m_1 + m_2} C_{j\ 1/2\ 1/2}^{m_j m_1 m_2}\, S_{1/2}^{m_1}\, S_{1/2}^{m_2} \ .$$

Since $I = 1$, only, for deuterons,

$$y_1^1 = \alpha_1\ \alpha_1$$

$$y_1^0 = \frac{1}{\sqrt{2}} [\alpha_1 \beta_2 + \beta_1 \alpha_2] \qquad \text{(D-1)}$$

$$y_1^{-1} = \beta_1\ \beta_2 \ .$$

II. S AND D STATES

We couple the y_1^m with the two possible angular momentum states which are allowed by parity, namely $\ell = 0, 2$.

A. Coupling of y_1^m and Y_0^0

We define the angular momentum portion of the wave function as $\phi_{I,\ell}^{m_I}$. Then

$$\phi_{1,0}^{1} = Y_0^0\, y_1^1$$

$$\phi_{1,0}^{0} = Y_0^0\, y_1^0 \qquad \text{(D-2)}$$

$$\phi_{1,0}^{-1} = Y_0^0\, y_1^{-1} \ ,$$

where $Y_\ell^{m_\ell}$ are the spherical harmonics.

B. Coupling of y_1^m and $Y_2^{m_\ell}$

$$ {}^{m_I}_{1,2} = \sum_{m_I = m + m_\ell} C_{121}^{m_I m_\ell m} \; Y_2^{m_\ell} \; y_1^m \; . $$

That is,

$$ \begin{aligned} \phi_{1,2}^{1} &= \sqrt{\tfrac{1}{10}}\, Y_2^0\, y_1^1 - \sqrt{\tfrac{3}{10}}\, Y_2^1\, y_1^0 + \sqrt{\tfrac{6}{10}}\, Y_2^2\, y_1^{-1} \\ \phi_{1,2}^{0} &= \sqrt{\tfrac{3}{10}}\, Y_1^{-1}\, y_1^1 - \sqrt{\tfrac{4}{10}}\, Y_2^0\, y_1^0 + \sqrt{\tfrac{3}{10}}\, Y_2^1\, y_1^{-1} \\ \phi_{1,2}^{-1} &= \sqrt{\tfrac{6}{10}}\, Y_2^{-2}\, y_1^1 - \sqrt{\tfrac{3}{10}}\, Y_2^{-1}\, y_1^0 + \sqrt{\tfrac{1}{10}}\, Y_2^0\, y_1^{-1} \; . \end{aligned} \qquad \text{(D-3)} $$

C. Vector Version of the Deuteron

Wave function $\Psi(\vec{r})$. We define the S and D wave vectors as ϕ_ℓ, where

$$ \vec{\phi}_0 = \begin{pmatrix} \phi_{1,0}^{1} \\ \phi_{1,0}^{0} \\ \phi_{1,0}^{-1} \end{pmatrix} \quad ; \quad \vec{\phi}_2 = \begin{pmatrix} \phi_{1,2}^{1} \\ \phi_{1,2}^{0} \\ \phi_{1,2}^{-1} \end{pmatrix} $$

$$ \mathbb{A} = \begin{pmatrix} Y_0^0 & 0 & 0 \\ 0 & Y_0^0 & 0 \\ 0 & 0 & Y_0^0 \end{pmatrix} \quad ; \quad \vec{y} = \begin{pmatrix} y_1^1 \\ y_1^0 \\ y_1^{-1} \end{pmatrix} $$

$$ \mathbb{B} = \begin{pmatrix} \sqrt{\tfrac{1}{10}}\, Y_2^0 & -\sqrt{\tfrac{3}{10}}\, Y_2^1 & \sqrt{\tfrac{6}{10}}\, Y_2^2 \\ \sqrt{\tfrac{3}{10}}\, Y_2^{-1} & -\sqrt{\tfrac{4}{10}}\, Y_2^0 & \sqrt{\tfrac{3}{10}}\, Y_2^1 \\ \sqrt{\tfrac{6}{10}}\, Y_2^{-2} & -\sqrt{\tfrac{3}{10}}\, Y_2^{-1} & \sqrt{\tfrac{1}{10}}\, Y_2^0 \end{pmatrix} . \qquad \text{(D-4)} $$

The radial part of $\vec{\Psi}$ is, of course, calculated from the Schrödinger equation. We write here the total deuteron wave function (the Hulthen wave function) in the standard form

$$\vec{\Psi}(\vec{r}) = \chi(\vec{r})\ \vec{y} = \frac{1}{\sqrt{4\pi}}\left[\frac{u(r)}{r} + \frac{w(r)}{r\sqrt{8}}\ \underset{\sim}{S_{12}}\right]\vec{y}\ , \tag{D-5}$$

where $\underset{\sim}{S_{12}}$ is here a matrix operator. The solution to the Schrödinger equation can be written as the sum of an $\ell = 0$ solution and $\ell = 2$ solution.

$$\vec{\Psi}(\vec{r}) = \frac{1}{\sqrt{4\pi}}\left[\frac{u(r)}{r}\cdot a\ \vec{\phi}_0 + \frac{w(r)}{r\sqrt{8}}\ b\ \vec{\phi}_2\right], \tag{D-6}$$

where a and b are to be determined. Since $\vec{\phi}_0 = \mathbb{A}\cdot\vec{y}$ and $\vec{\phi}_2 = \mathbb{B}\cdot\vec{y}$,

$$\vec{\Psi}(\vec{r}) = \frac{1}{\sqrt{4\pi}}\left[\frac{u(r)}{r}\cdot a\,\mathbb{A} + \frac{w(r)}{r\sqrt{8}}\ b\,\mathbb{B}\right]\vec{y}\ . \tag{D-7}$$

Comparing Eqs. (D-5) and (D-7) and using definition (D-4) we set a = 1 and we have to show that $b\,\mathbb{B} = \underset{\sim}{S_{12}}$.

III. EVALUATION OF $\underset{\sim}{S_{12}}$ (A SPIN MATRIX OPERATOR)

We have already stated that

$$\underset{\sim}{S_{12}} = \frac{3(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r})}{r^2} - \vec{\sigma}_1\cdot\vec{\sigma}_2\ , \tag{D-8}$$

where it is written with wavy lines to emphasize that the σ's are taken here as matrix operators. Before proceeding, the reader may easily convince himself of the statement that $\vec{\sigma}_1\cdot\vec{\sigma}_2$ may be replaced by 1 for triplet states by calculating

$$\vec{\sigma}_1\cdot\vec{\sigma}_2\ y_1^m = \left\{\begin{pmatrix}0&1\\1&0\end{pmatrix}_1\begin{pmatrix}0&1\\1&0\end{pmatrix}_2 + \begin{pmatrix}0&-i\\i&0\end{pmatrix}_1\begin{pmatrix}0&-i\\i&0\end{pmatrix}_2 + \begin{pmatrix}1&0\\0&-1\end{pmatrix}_1\begin{pmatrix}1&0\\0&-1\end{pmatrix}_2\right\}y_1^m\ .$$

Substituting y_1^m from Eq. (D-1) and recalling that $\alpha_i = \binom{1}{0}_i$ and $\beta_i = \binom{0}{1}_i$, one demonstrates that

$$\vec{\sigma}_1\cdot\vec{\sigma}_2\ y_1^m = y_1^m\ . \tag{D-9}$$

A. A Generator of S_{12}

One can easily demonstrate that

$$S_{12} = \frac{3}{r^2}(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r}) - \vec{\sigma}_1\cdot\vec{\sigma}_2 = \sum_{\alpha,\beta}\left[\frac{3x_\alpha x_\beta - r^2\delta_{\alpha\beta}}{r^2}\right]\sigma_1^\alpha\sigma_2^\beta\ , \qquad \text{(D-10)}$$

where x_α are components of the vector $\vec{r}$, and σ_j^α are components of the matrices $\vec{\sigma}_j$. This can be proved by explicitly expanding both sides of Eq. (D-10). Writing $T_{\alpha\beta}$ for the quantity enclosed in brackets in Eq. (D-10),

$$T_{\alpha\beta} = \frac{3x_\alpha x_\beta - r^2\delta_{\alpha\beta}}{r^2}\ , \qquad \text{(D-11)}$$

it follows that $T_{\alpha\beta}$ are linear combinations of the spherical harmonics $Y_2^{m_\ell}$.

$$\begin{aligned}
T_{11} &= 6\sqrt{\frac{2\pi}{15}}\,(Y_2^2 + Y_2^{-2}) - \sqrt{\frac{4\pi}{5}}\,Y_2^0 \\
T_{22} &= -6\sqrt{\frac{2\pi}{15}}\,(Y_2^2 + Y_2^{-2}) - \sqrt{\frac{4\pi}{5}}\,Y_2^0 \\
T_{33} &= 2\sqrt{\frac{4\pi}{5}}\,(Y_2^0) \\
T_{12} &= -3i\sqrt{\frac{2\pi}{15}}\,(Y_2^2 - Y_2^{-2}) \\
T_{23} &= -3i\sqrt{\frac{2\pi}{15}}\,(Y_2^1 - Y_2^{-1}) \\
T_{13} &= 3\sqrt{\frac{2\pi}{15}}\,(Y_2^1 + Y_2^{-1})\ .
\end{aligned} \qquad \text{(D-12)}$$

For reference we write here the spherical harmonics $Y_2^{m_\ell}$.

$$\begin{aligned}
Y_2^0 &= \sqrt{\frac{5}{16\pi}}\cdot\frac{3Z^2 - r^2}{r^2} \\
Y_2^{\pm1} &= \mp\sqrt{\frac{15}{8\pi}}\ \frac{x \pm iy}{r^2}\,Z \\
Y_2^{\pm2} &= \sqrt{\frac{15}{32\pi}}\cdot\frac{(x \pm iy)^2}{r^2}\ .
\end{aligned} \qquad \text{(D-13)}$$

B. Expansion of $\underset{\sim}{S}_{12}$ into $Y_2^{m_\ell}$

Expanding Eq. (D-10) directly, we have

$$\underset{\sim}{S}_{12}\, y_1^m = \sum_{\alpha,\beta} T_{\alpha\beta}\, \sigma_1^\alpha \sigma_2^\beta\, y_1^m$$

$$= \Big[T_{11}\, \sigma_1^x\sigma_2^x + T_{22}\, \sigma_1^y\sigma_2^y + T_{33}\, \sigma_1^z\sigma_2^z + T_{12}\, (\sigma_1^x\sigma_2^y + \sigma_1^y\sigma_2^x)$$

$$+ T_{23}(\sigma_1^y\sigma_2^z + \sigma_1^z\sigma_2^y) + T_{13}(\sigma_1^x\sigma_2^z + \sigma_1^z\sigma_2^x)\Big]\, y_1^m\ . \qquad \text{(D-14)}$$

Substituting Eq. (D-1) into Eq. (D-14), one can show that

$$\underset{\sim}{S}_{12}\, y_1^1 = T_{33}\, y_1^1 + \sqrt{2}\,(T_{13}+T_{23})\, y_1^0 + (T_{11}-T_{22}+2iT_{12})\, y_1^{-1}\ ,$$

or using Eq. (D-12),

$$\underset{\sim}{S}_{12}\, y_1^1 = 4\sqrt{2\pi}\left[\sqrt{\frac{1}{10}}\, Y_2^0\, y_1^1 - \sqrt{\frac{3}{10}}\, Y_2^1\, y_1^0 + \sqrt{\frac{6}{10}}\, Y_2^2\, y_1^{-1}\right]. \qquad \text{(D-15)}$$

Similarly,

$$\underset{\sim}{S}_{12}\, y_1^0 = 4\sqrt{2\pi}\left[\sqrt{\frac{3}{10}}\, Y_2^{-1}\, y_1^1 - \sqrt{\frac{4}{10}}\, Y_2^0\, y_1^0 + \sqrt{\frac{3}{10}}\, Y_2^1\, y_1^{-1}\right] \qquad \text{(D-16)}$$

$$\underset{\sim}{S}_{12}\, y_1^{-1} = 4\sqrt{2\pi}\left[\sqrt{\frac{6}{10}}\, Y_2^{-2}\, y_1^1 - \sqrt{\frac{3}{10}}\, Y_2^{-1}\, y_1^0 + \sqrt{\frac{1}{10}}\, Y_2^0\, y_1^{-1}\right]\ . \qquad \text{(D-17)}$$

Recalling that $\vec{y} = \begin{pmatrix} y_1^1 \\ y_1^0 \\ y_1^{-1} \end{pmatrix}$, Eqs. (D-15), (D-16), and (D-17) can be written in matrix form as

$$\underset{\sim}{S}_{12}\, \vec{y} = (\sqrt{8})(\sqrt{4\pi})\begin{pmatrix} \sqrt{\frac{1}{10}}\, Y_2^0 & -\sqrt{\frac{3}{10}}\, Y_2^1 & \sqrt{\frac{6}{10}}\, Y_2^2 \\ \sqrt{\frac{3}{10}}\, Y_2^{-1} & -\sqrt{\frac{4}{10}}\, Y_2^0 & \sqrt{\frac{3}{10}}\, Y_2^1 \\ \sqrt{\frac{6}{10}}\, Y_2^{-2} & -\sqrt{\frac{3}{10}}\, Y_2^{-1} & \sqrt{\frac{1}{10}}\, Y_2^0 \end{pmatrix}\begin{pmatrix} y_1^1 \\ y_1^0 \\ y_1^{-1} \end{pmatrix}\ . \qquad \text{(D-18)}$$

Comparing Eq. (D-5) and Eq. (D-7) by substituting Eq. (D-4) for $\mathbb{B}$ and Eq. (D-18) for $\underset{\sim}{S_{12}}$ we see that

$$\underset{\sim}{S_{12}} = \sqrt{8} \cdot \sqrt{4\pi} \ \mathbb{B} \ .$$

This accomplishes the goal of finding an explicit operator form for the deuteron wave function $\vec{\Psi}(\vec{r})$.

IV. EXPANSION OF $\underset{\sim}{S_{12}}(\hat{r})$

For completeness we show the relationship between $\underset{\sim}{S_{12}}(\hat{r})$ and $[(\vec{S}\cdot\hat{r})^2 - \frac{S(S+1)}{3}] = [(\vec{S}\cdot\hat{r})^2 - \frac{2}{3}]$ where $\vec{S} = \frac{1}{2}(\vec{\sigma}_1+\vec{\sigma}_2)$.

$$[(\vec{S}\cdot\hat{r})^2 - \frac{1}{3}|\vec{S}|^2] = \frac{1}{4}[(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\hat{r}]^2 - \frac{1}{12}(\vec{\sigma}_1+\vec{\sigma}_2)^2$$

$$= \frac{1}{4}(\vec{\sigma}_1\cdot\hat{r})^2 + \frac{1}{4}(\vec{\sigma}_2\cdot\hat{r}) + \frac{1}{2}(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) - \frac{1}{12}(\vec{\sigma}_1^2 + \vec{\sigma}_2^2 + 2\vec{\sigma}_1\cdot\vec{\sigma}_2) ,$$

but $(\vec{\sigma}\cdot\hat{r})^2 \equiv 1$, $\vec{\sigma}^2 \equiv 3$, therefore,

$$\frac{1}{2} + \frac{1}{2}(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) - \frac{1}{2} - \frac{1}{6}\vec{\sigma}_1\cdot\vec{\sigma}_2 = \frac{1}{6}[3(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) - 1] \ .$$

Therefore,

$$[(\vec{S}\cdot\hat{r})^2 - \frac{2}{3}] \equiv \frac{1}{6}[3(\vec{\sigma}_1\cdot\hat{r})(\vec{\sigma}_2\cdot\hat{r}) - 1] \ . \qquad \text{(D-19)}$$

V. NORMALIZATION

The wave function in Eq. (D-5) is required to be orthonormal; therefore,

$$\iiint \vec{\Psi}^\dagger(\vec{r}) \ \vec{\Psi}(\vec{r}) \ d\vec{r} = 1 \ .$$

Substituting the Hulthen wave function for $\vec{\Psi}$, we have the integral, I, where

$$I = \frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\left[\frac{u(r)}{r} + \frac{w(r)}{\sqrt{8}r}\underset{\sim}{S_{12}}\right]^2 r^2 \sin\theta dr d\theta d\phi \qquad \text{(D-20)}$$

$$I = \int_0^{\infty}[u^2 + w^2] \ dr \ , \qquad \text{(D-21)}$$

where Eq. (D-21) follows directly from Eq. (D-20) by recalling that $\underset{\sim}{S}_{12}^2 = 8 - 2\underset{\sim}{S}_{12}$,

$$\frac{1}{2\pi}\int_0^{2\pi} \underset{\sim}{S}_{12}(\hat{r})\, d\phi = \underset{\sim}{S}_{12}(\hat{R})\, P_2(\theta)$$

and

$$\int_0^{\pi} P_2(\theta)\, \sin\theta d\theta \equiv 0 ,$$

where $P_2(\theta)$ is the Legendre polynomial, P_ℓ, for $\ell = 2$.

The values of u(r) and w(r) which are to be used are[16]

$$u(r) = N \cos\delta\, [1 - e^{-\beta x}]\, e^{-x}$$

$$w(r) = N \sin\delta\, [1 - e^{-\gamma x}]\, e^{-x} \cdot \Lambda(x) ,$$

where

$$\Lambda(x) = 1 + 3\, \frac{[1-e^{-\gamma x}]}{x} + 3\, \frac{[1-e^{-\gamma x}]^2}{x^2}$$

and

$$x = \alpha r . \qquad \text{(D-22)}$$

We will calculate $\int_0^\infty u^2\, dr$ to demonstrate that this is normalized so as to make up 96% of the ground state of the deuteron.

$$\int_0^\infty u^2 dr = \frac{1}{\alpha}\int_0^\infty u^2 dx = \frac{N^2\cos^2\delta}{\alpha}\int_0^\infty [1 - e^{-\beta x}]^2\, e^{-2x}\, dx$$

$$\int_0^\infty u^2 dr = \frac{N^2\cos^2\delta}{\alpha}\, [\frac{1}{2} - \frac{2}{\beta+2} + \frac{1}{2(\beta+1)}] . \qquad \text{(D-23}$$

The values which properly normalize Eq. (D-22) are

$$N = 0.875041 \qquad \gamma = 2.0170 \qquad \cos\delta = 0.99947$$

$$\beta = 4.7533 \qquad \sin\delta = 0.03356 \qquad \alpha = 0.2318175 \text{ fm}^{-1} . \qquad \text{(D-24)}$$

Substituting the values of Eq. (D-24) into Eq. (D-23) we obtain

$$\int_0^\infty u^2 dr = 0.9594 .$$

VI. THE AVERAGE KINETIC ENERGY

The average kinetic energy of a nucleon in the deuteron can be calculated as

$$T_p = \left\langle \frac{p_p^2}{2M} \right\rangle = -\left\langle \frac{\hbar^2}{2m} \right\rangle \nabla_{cm}^2 = \left(-\frac{\hbar^2}{2M}\right) \cdot 4 \cdot \left\langle \nabla_r^2 \right\rangle , \quad \text{(D-25)}$$

where ∇_{cm}^2 is to be taken with respect to $\frac{1}{2}\vec{r}$, the distance to the center of mass. For this calculation, the D state of the deuteron will be neglected. To do so, we must renormalize the S wave. Let

$$u' = N' \left[1 - e^{-\beta x}\right] e^{-x} \quad , \qquad x = \alpha r ; \quad \text{(D-26)}$$

then from Eq. (D-23) we see that the restriction

$$\int_0^\infty (u')^2 \, dr = 1 , \quad \text{(D-27)}$$

gives $(N')^2 = \alpha\left[\frac{1}{2} - \frac{2}{\beta+2} + \frac{1}{2(\beta+1)}\right]^{-1}$, or from Eq. (D-24) we find

$$(N')^2 = 0.7973 \quad , \qquad N' = 0.8929 . \quad \text{(D-28)}$$

Next, we note that since $x = \alpha r$, $\nabla_r^2 = a^2 \, \nabla_x^2$ (keeping in mind that x in this sense is still a radial component). But one can show that

$$\nabla_x^2 \left(\frac{u'}{x}\right) = \frac{1}{x^2} \frac{d}{dx} x^2 \frac{\partial}{\partial x} \left(\frac{u'}{x}\right) = \frac{1}{x} \frac{\partial^2 u'}{\partial x^2}$$

$$= \frac{u'}{x} - N' \left[\beta^2 + 2\beta\right] \frac{e^{-(\beta+1)x}}{x} .$$

Then

$$\int_0^\infty \left(\frac{u'}{x}\right) \left[\nabla_r^2 \left(\frac{u'}{x}\right)\right] r^2 dr = \alpha \int_0^\infty \left(\frac{u'}{x}\right) \left[\nabla_x^2 \left(\frac{u'}{x}\right)\right] x^2 dx$$

$$= \alpha^2 \int_0^\infty u'^2 dr - N' \left[\beta^2 + 2\beta\right] \int_0^\infty u' \, e^{-(\beta+1)x} \, dx \; .$$

The first integral is one [Eq. (D-27)] and the second integral becomes

$$(N')^2 \alpha \left[\beta^2 + 2\beta\right] \left(\frac{1}{\beta+2} - \frac{1}{2(\beta+1)}\right) .$$

Therefore,

$$\langle \nabla_r^2 \rangle = \alpha^2 - (N')^2 \alpha\beta \left(1 - \frac{\beta+2}{2(\beta+1)}\right) ,$$

from Eqs. (D-28) and (D-24),

$$\langle \nabla_r^2 \rangle = - 0.309 \text{ fm}^{-2} .$$

Recalling Eq. (D-25),

$$T_p = \left(- \frac{\hbar^2}{2M}\right) \cdot 4 \langle \nabla_r^2 \rangle = \left(\frac{\hbar^2}{2M}\right) (1.237) .$$

But

$$\left(\frac{\hbar^2}{2M}\right) = 20.7 \text{ MeV} - \text{fm}^2 .$$

Therefore,

$$\boxed{T_p = 25.6 \text{ MeV}}$$ (average kinetic energy per nucleon).

(D-29).

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