

Here is a little write-up of the deuteron problem – one of the possible problems on the Quantum II final last month. We show how to calculate the magnetic dipole moment and the electric quadrupole moment of the deuteron. The write-up in Elton's text (which I handed out in class) was brief to say the least. It also used the quasi-classical "vector coupling model" which most of us learned in an undergraduate Modern Physics course, and did not do the Clebsch Gordon algebra which is (I think) important to understand what is really going on when we "couple" angular momenta. In the case of the deuteron, the Russell Saunders coupling of orbital and spin angular momenta yields a total angular momentum. Moreover, the presence of the tensor force allows the mixing of the $L=0$ and $L=2$ orbital angular momentum states. I tried to be very rigorous in the discussion and derivations, making sure to distinguish observables, eigenvalues, eigenstates, quantum numbers, etc. If you want to discuss any points I would be happy to do so.

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The Deuteron

We want to consider the ground state of the deuteron from the traditional nuclear physics viewpoint. That is, we want to use non-relativistic quantum mechanics to explore the bound state of a proton and neutron (each considered as a particular isotopic spin state of a nucleon). We shall simply elaborate on the formalism presented in the texts by Elton and Erder in chapters relating to the structure of the deuteron. Having found the ground state wave function we would then be able to calculate various properties of the deuteron, such as its electric quadrupole moment and its magnetic dipole moment. It turns out that the ground state wave function must be a "mixture" of relative angular momentum states with $l=0$ and $l=2$ in order to reproduce the experimental values for the electric quadrupole and magnetic dipole moments. In turn this mixing is the result of a non-central potential energy term, the tensor force, in the Hamiltonian. Indeed, this term for the tensor force commutes with neither the components of orbital angular momentum nor spin, but it does commute with the components of the total angular momentum, the operator which is the vector sum (component by component) of the operator for orbital angular momentum and the operator for spin. "Coupling" angular momenta to form a basis for the eigenstates of total angular momentum squared and one of its components is an exercise in the Clebsch Gordon algebra. Indeed, we did this for the atomic electron problem but the math is the same for the deuteron structure problem.

However, we want to be more rigorous than either of the texts by Elton or Erder in regard to "angular momentum". In that regard such procedures as replacing operators by eigenvalues will be anathema. We will spend the introduction looking at the "spin $\frac{1}{2}$ " problem with an eye toward including spin and isospin "coordinates" in the configuration space wavefunction.

Our point of view is that a nucleus is a bound state of a collection of identical indistinguishable fermions called "nucleons". Each nucleon has two internal degrees of freedom: "ordinary" spin and isospin. Both degrees of freedom are described by an intrinsic angular momentum operator. Thus the vector observable "spin" is

$$\vec{\hat{s}} = \hat{s}_x \mathbf{e}_x + \hat{s}_y \mathbf{e}_y + \hat{s}_z \mathbf{e}_z \quad (1)$$

where the unit cartesian basis vectors \mathbf{e} are introduced in anticipation of taking "cross products" and "scalar products" of the this vector operator

with other vector operators such as \vec{r} , \vec{p} , and $\vec{l} (\equiv \vec{r} \times \vec{p})$. These are indeed observables (*Hermitian quantum mechanical operators*). We have put a caret (^) above the operator (as we had done previously); we have not put a caret above the unit vectors \mathbf{e} which are in **boldface** type; but of course the \mathbf{e} 's are not operators. By definition of angular momentum operators, the components of \vec{s} obey the commutation relations

$$[\hat{s}_i, \hat{s}_j] = i\hbar \epsilon_{ijk} \hat{s}_k \quad (\text{summing over the repeated index "k"}) \quad (2)$$

where the indices $i \in \{x,y,z\}$, $j \in \{x,y,z\}$, $k \in \{x,y,z\}$ and $\epsilon_{ijk} = \pm 1$ for even/odd permutations of 1,2,3 (x,y,z) and 0 otherwise. The observable $\hat{s}^2 \equiv \hat{s}_x^2 + \hat{s}_y^2 + \hat{s}_z^2$ commutes with each component \hat{s}_i . Following our tradition we choose \hat{s}_z so that $\{\hat{s}^2, \hat{s}_z\}$ is a set of commuting observables. From our general considerations we can always find a set of spin vectors which are eigenvectors of both \hat{s}^2 and \hat{s}_z . Thus the *eigenvalue spectrum* of \hat{s}^2 is $s(s+1)\hbar^2$, where the *quantum number* $s = 0, \frac{1}{2}, 1, \dots$ and the *eigenvalue spectrum* of \hat{s}_z is $m_s \hbar$, where for a given s , the *quantum number* m_s ranges from $-s$ to $+s$ in unit steps. There are $(2s+1)$ values of m_s for a given s . Thus, in Dirac notation we write

$$\begin{aligned} \hat{s}^2 |s, m_s\rangle &= s(s+1)\hbar^2 |s, m_s\rangle \\ \hat{s}_z |s, m_s\rangle &= m_s \hbar |s, m_s\rangle \end{aligned} \quad (3)$$

where we have written the quantum numbers s , m_s and the corresponding eigenvalues $s(s+1)\hbar^2$, $m_s \hbar$ in *script*.

Again from our general considerations, we also introduce the raising and lowering operators

$$\hat{s}_{\pm} = \hat{s}_x \pm i\hat{s}_y \quad (4)$$

so that with the understanding that all ket vectors are normalized to 1

$$\begin{aligned} \hat{s}_+ |s, m_s\rangle &= \hbar[(s - m_s)(s + m_s + 1)]^{\frac{1}{2}} |s, (m_s + 1)\rangle \\ \hat{s}_- |s, m_s\rangle &= \hbar[(s + m_s)(s - m_s + 1)]^{\frac{1}{2}} |s, (m_s - 1)\rangle \end{aligned} \quad (5)$$

For spin $s = \frac{1}{2}$ there are two eigenstates $|\frac{1}{2}, \frac{1}{2}\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle$ and the most general single particle spin state can be written as a linear superposition of these two eigenstates. Thus the most general state is

$$|\chi\rangle = a|\frac{1}{2}, \frac{1}{2}\rangle + b|\frac{1}{2}, -\frac{1}{2}\rangle \quad (6)$$

where by virtue of the completeness and orthonormality of the basis vectors the constants must be given by

$$a = \langle\frac{1}{2}, \frac{1}{2}|\chi\rangle \text{ and } b = \langle\frac{1}{2}, -\frac{1}{2}|\chi\rangle. \quad (7)$$

That is, the formal statement of (6) after inserting (7)

$$\begin{aligned} |\chi\rangle &= |\frac{1}{2}, \frac{1}{2}\rangle \langle\frac{1}{2}, \frac{1}{2}|\chi\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle \langle\frac{1}{2}, -\frac{1}{2}|\chi\rangle \\ &= \left\{ |\frac{1}{2}, \frac{1}{2}\rangle \langle\frac{1}{2}, \frac{1}{2}| + |\frac{1}{2}, -\frac{1}{2}\rangle \langle\frac{1}{2}, -\frac{1}{2}| \right\} |\chi\rangle \end{aligned} \quad (8)$$

implies the Dirac "outer product" form is the identity operator:

$$\left\{ |\frac{1}{2}, \frac{1}{2}\rangle \langle\frac{1}{2}, \frac{1}{2}| + |\frac{1}{2}, -\frac{1}{2}\rangle \langle\frac{1}{2}, -\frac{1}{2}| \right\} = \hat{1}. \quad (9)$$

In general, a linear operator $\hat{G} \equiv G(\hat{s}_x, \hat{s}_y, \hat{s}_z)$ on the spin space yields

$$\hat{G}|\chi\rangle = |\Gamma\rangle = \{ (a) \hat{G}|\frac{1}{2}, \frac{1}{2}\rangle + (b) \hat{G}|\frac{1}{2}, -\frac{1}{2}\rangle \}. \quad (10)$$

As we did in Quantum Mechanics II, we wish to represent this relation in some convenient basis. That is, the states $|\chi\rangle$ and $|\Gamma\rangle$ will each be represented as a 2×1 column matrix of complex numbers and the general operator \hat{G} will be represented by a 2×2 square matrix. Since \hat{G} itself is some function of the observables $\hat{s}_x, \hat{s}_y, \hat{s}_z$, all we need do is find the matrix representatives of these operators in the chosen basis for then the matrix G representing \hat{G} is the same function of the matrices s_x, s_y, s_z as is the operator relation itself:

$$G = G(s_x, s_y, s_z). \quad (11)$$

We choose the basis of eigenstates of s^2 and s_z , that is $\{ |\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle \}$. Thus we need to represent the equation

$$|\Upsilon\rangle = \hat{s}_i |\chi\rangle = \hat{s}_i |\frac{1}{2}, \frac{1}{2}\rangle \langle\frac{1}{2}, \frac{1}{2}|\chi\rangle + \hat{s}_i |\frac{1}{2}, -\frac{1}{2}\rangle \langle\frac{1}{2}, -\frac{1}{2}|\chi\rangle \quad (12)$$

and so in turn need to find $\hat{s}_i |\frac{1}{2}, \frac{1}{2}\rangle$ and $\hat{s}_i |\frac{1}{2}, -\frac{1}{2}\rangle$, for $i = x, y, z$. But each

of these can presumably be expanded as

$$\begin{aligned}\hat{S}_i |\frac{1}{2}, \frac{1}{2}\rangle &= |\frac{1}{2}, \frac{1}{2}\rangle \langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle \\ \hat{S}_i |\frac{1}{2}, -\frac{1}{2}\rangle &= |\frac{1}{2}, \frac{1}{2}\rangle \langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle\end{aligned}\quad (13)$$

whence (12) becomes

$$\begin{aligned}|\Upsilon\rangle &= \{ |\frac{1}{2}, \frac{1}{2}\rangle \langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle \} \langle \frac{1}{2}, \frac{1}{2} | \chi\rangle \\ &\quad + \{ |\frac{1}{2}, \frac{1}{2}\rangle \langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle \} \langle \frac{1}{2}, -\frac{1}{2} | \chi\rangle \\ &= |\frac{1}{2}, \frac{1}{2}\rangle \langle \frac{1}{2}, \frac{1}{2} | \Upsilon\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle \langle \frac{1}{2}, -\frac{1}{2} | \Upsilon\rangle\end{aligned}\quad (14)$$

where the last step simply recognizes that $|\Upsilon\rangle$ can be expanded in the $\{ |\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle \}$ basis. But the basis vectors are linearly independent and thus we can equate the coefficients of each basis vector on the left and right to find the two equations:

$$\begin{aligned}\langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle \langle \frac{1}{2}, \frac{1}{2} | \chi\rangle + \langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle \langle \frac{1}{2}, -\frac{1}{2} | \chi\rangle &= \langle \frac{1}{2}, \frac{1}{2} | \Upsilon\rangle \\ \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle \langle \frac{1}{2}, \frac{1}{2} | \chi\rangle + \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle \langle \frac{1}{2}, -\frac{1}{2} | \chi\rangle &= \langle \frac{1}{2}, -\frac{1}{2} | \Upsilon\rangle\end{aligned}\quad (15)$$

which rewritten in matrix form is

$$\begin{bmatrix} \langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle & \langle \frac{1}{2}, \frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle \\ \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, \frac{1}{2}\rangle & \langle \frac{1}{2}, -\frac{1}{2} | \hat{S}_i | \frac{1}{2}, -\frac{1}{2}\rangle \end{bmatrix} \begin{bmatrix} \langle \frac{1}{2}, \frac{1}{2} | \chi\rangle \\ \langle \frac{1}{2}, -\frac{1}{2} | \chi\rangle \end{bmatrix} = \begin{bmatrix} \langle \frac{1}{2}, \frac{1}{2} | \Upsilon\rangle \\ \langle \frac{1}{2}, -\frac{1}{2} | \Upsilon\rangle \end{bmatrix}. \quad (16)$$

Specifically, this is a matrix representation in the $\{ |\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle \}$ basis of the vector relationship (12). The elements of the matrices are complex numbers. The square matrix must be Hermitian.

The matrix elements follow from the general abstract commutation relations of the operators themselves. Indeed, writing \hat{S}_x and \hat{S}_y in terms of \hat{S}_+ and \hat{S}_- and then using the properties (5) of the raising and lowering we find

$$\begin{aligned}\langle \frac{1}{2}, m_S^- | \hat{S}_x | \frac{1}{2}, m_S \rangle &= \frac{1}{2} [\langle \frac{1}{2}, m_S^- | \hat{S}_+ + \hat{S}_- | \frac{1}{2}, m_S \rangle] \\ &= \frac{1}{2} \hbar [\delta_{m_S^-, (m_S+1)} + \delta_{m_S^-, (m_S-1)}]\end{aligned}\quad (17a)$$

$$\begin{aligned} \langle \frac{1}{2}, m_s^- | \hat{s}_y | \frac{1}{2}, m_s \rangle &= (-i) \frac{1}{2} [\langle \frac{1}{2}, m_s^- | \hat{s}_+ - \hat{s}_- | \frac{1}{2}, m_s \rangle] \\ &= (-i) \frac{1}{2} \hbar [\delta_{m_s^-, (m_s+1)} - \delta_{m_s^-, (m_s-1)}] \end{aligned} \quad (17b)$$

$$\langle \frac{1}{2}, m_s^- | \hat{s}_z | \frac{1}{2}, m_s \rangle = m_s \hbar \delta_{m_s^-, m_s} \quad (17c)$$

and thus the 2x2 matrices representing the operators in basis $\{|\frac{1}{2}, m_s\rangle\}$ are:

$$\begin{aligned} \tilde{s}_x &= \begin{pmatrix} 0 & \frac{1}{2}\hbar \\ \frac{1}{2}\hbar & 0 \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}\hbar \sigma_x \\ \tilde{s}_y &= \begin{pmatrix} 0 & -\frac{1}{2}i\hbar \\ \frac{1}{2}i\hbar & 0 \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{2}\hbar \sigma_y \\ \tilde{s}_z &= \begin{pmatrix} \frac{1}{2}\hbar & 0 \\ 0 & -\frac{1}{2}\hbar \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2}\hbar \sigma_z \\ \tilde{s}^2 &= \tilde{s}_x^2 + \tilde{s}_y^2 + \tilde{s}_z^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

★ The set of σ matrices are called the Pauli matrices.
 ★ $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
 ★ The matrix commutators $[\tilde{s}_i, \tilde{s}_j] = i\hbar \epsilon_{ijk} \tilde{s}_k$
 ★ and so $[\sigma_i, \sigma_j] = 2i \epsilon_{ijk} \sigma_k$

Instead of choosing \hat{s}_z along with \hat{s}^2 as members of the commuting set we could choose \hat{s}_x or \hat{s}_y . But even more generally, with \mathbf{n} a unit vector defining some arbitrary direction in space, we could take \hat{s}^2 and $\vec{s} \cdot \mathbf{n}$ as the set of commuting observables. With the unit vector

$$\mathbf{n} = (\sin\theta \cos\phi) \mathbf{e}_x + (\sin\theta \sin\phi) \mathbf{e}_y + \cos\theta \mathbf{e}_z \quad (19)$$

the (abstract) operator is

$$\hat{s}_{\mathbf{n}} = \vec{s} \cdot \mathbf{n} = (\sin\theta \cos\phi) \hat{s}_x + (\sin\theta \sin\phi) \hat{s}_y + \cos\theta \hat{s}_z. \quad (20)$$

If we use the Pauli 2x2 matrices to represent the operators we write

$$\begin{aligned} \vec{s} \cdot \mathbf{n} &= (\sin\theta \cos\phi) \left[\frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] + (\sin\theta \sin\phi) \left[\frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right] + \cos\theta \left[\frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \\ \tilde{s}_{\mathbf{n}} \equiv \vec{s} \cdot \mathbf{n} &= \frac{1}{2}\hbar \begin{pmatrix} \cos\theta & \sin\theta(\cos\phi - i \sin\phi) \\ \sin\theta(\cos\phi + i \sin\phi) & -\cos\theta \end{pmatrix} \end{aligned} \quad (21)$$

(continued)

$$\underline{s}_n = \frac{1}{2}\hbar \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \quad (21)$$

We should understand that this \underline{s}_n is a matrix representation of the operator \hat{s}_n in the basis $\{ |\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle \}$. We can find the eigenvalues of \hat{s}^2 and \hat{s}_n most simply by diagonalizing their 2x2 matrix representations. The eigenvalues of the above 2x2 matrix follow from the characteristic equation. Letting the eigenvalue $\Lambda = \frac{1}{2}\hbar\lambda$ we have

$$\det \left[\left(\frac{1}{2}\hbar \right) \begin{pmatrix} \cos\theta - \lambda & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta - \lambda \end{pmatrix} \right] = 0 \quad (22)$$

or

$$\left(\frac{1}{2}\hbar \right)^2 [-\cos^2\theta + \lambda^2 - \sin^2\theta] = 0$$

so that $\lambda = \pm 1$ and the eigenvalues are $\Lambda = \pm \frac{1}{2}\hbar$. Of course $\underline{s}^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and so the eigenvalues of \hat{s}^2 and \hat{s}_n are also $\frac{3}{4}\hbar^2$ and $\pm \frac{1}{2}\hbar$. The new eigenvectors are, of course, not $\{ |s, m_s\rangle \} \equiv \{ |\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle \}$, the eigenvectors of \hat{s}^2 and \hat{s}_z . Rather, we designate the new eigenvectors as $\{ |\frac{1}{2}, \uparrow\rangle, |\frac{1}{2}, \downarrow\rangle \}$ and accordingly

$$\hat{s}^2 |\frac{1}{2}, \uparrow\rangle = \frac{3}{4}\hbar^2 |\frac{1}{2}, \uparrow\rangle \quad \hat{s}_n |\frac{1}{2}, \uparrow\rangle = +\frac{1}{2}\hbar |\frac{1}{2}, \uparrow\rangle \quad (23)$$

$$\hat{s}^2 |\frac{1}{2}, \downarrow\rangle = \frac{3}{4}\hbar^2 |\frac{1}{2}, \downarrow\rangle \quad \hat{s}_n |\frac{1}{2}, \downarrow\rangle = -\frac{1}{2}\hbar |\frac{1}{2}, \downarrow\rangle$$

The coefficients for expanding the new vectors in terms of the old basis can be found in the usual way. We are guaranteed (by the fundamental theorem of linear algebra) that the pair of equations written in matrix form

$$\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} u_{\frac{1}{2}\lambda} \\ u_{-\frac{1}{2}\lambda} \end{pmatrix} = \lambda \begin{pmatrix} u_{\frac{1}{2}\lambda} \\ u_{-\frac{1}{2}\lambda} \end{pmatrix} \quad (24)$$

has a *nontrivial* solution (i.e. are "consistent") if and only if (in this case) $\lambda = \pm 1$. The non-trivial solutions are given only up to a normali-

zation factor times an arbitrary phase factor. We abbreviate the basis vectors $\{|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle\}$ by $\{|\frac{1}{2}\rangle, |-\frac{1}{2}\rangle\}$ and $\{|\frac{1}{2}, \uparrow\rangle, |\frac{1}{2}, \downarrow\rangle\}$ by $\{|\uparrow\rangle, |\downarrow\rangle\}$. Thus

$$\cos\theta u_{\frac{1}{2}\lambda} + \sin\theta e^{-i\phi} u_{-\frac{1}{2}\lambda} = \lambda u_{\frac{1}{2}\lambda}$$

$$\sin\theta e^{i\phi} u_{\frac{1}{2}\lambda} - \cos\theta u_{-\frac{1}{2}\lambda} = \lambda u_{-\frac{1}{2}\lambda}$$

and so

$$u_{\frac{1}{2}\lambda} = \frac{\sin\theta e^{-i\phi}}{\lambda - \cos\theta} u_{-\frac{1}{2}\lambda} \quad (25a)$$

$$u_{\frac{1}{2}\lambda} = \frac{(\lambda + \cos\theta)e^{-i\phi}}{\sin\theta} u_{-\frac{1}{2}\lambda} \quad (25b)$$

which are consistent (as they must be) for $\lambda = 1$ and $\lambda = -1$. The normalization condition requires that

$$|u_{\frac{1}{2}\lambda}|^2 + |u_{-\frac{1}{2}\lambda}|^2 = 1. \quad (26)$$

Doing the algebra we obtain

$$\left\{ \frac{\sin^2\theta}{1 - 2\lambda\cos\theta + \cos^2\theta} + 1 \right\} |u_{-\frac{1}{2}\lambda}|^2 = 1$$

$$\left\{ \frac{2(1 - \lambda\cos\theta)}{(\lambda - \cos\theta)^2} \right\} |u_{-\frac{1}{2}\lambda}|^2 = 1 \quad (27)$$

Specifically for $\lambda = 1$ we get

$$u_{-\frac{1}{2}\lambda=1} = \left\{ \frac{1}{2}(1 - \cos\theta) \right\}^{\frac{1}{2}} e^{i\gamma} = \sin(\frac{1}{2}\theta) e^{i\gamma} \quad (28a)$$

where $e^{i\gamma}$ (γ real) is an arbitrary phase factor and from (28a) and (25b)

$$u_{\frac{1}{2}\lambda=1} = \frac{(1 + \cos\theta)e^{-i\phi}}{\sin\theta} \cdot \left\{ \frac{1}{2}(1 - \cos\theta) \right\}^{\frac{1}{2}} e^{i\gamma} = \cos(\frac{1}{2}\theta) e^{-i(\phi-\gamma)} \quad (28b)$$

Then continuing for $\lambda = -1$ we find

$$u_{-\frac{1}{2}\lambda=-1} = \left\{ \frac{1}{2}(1 + \cos\theta) \right\}^{\frac{1}{2}} e^{i\delta} = \cos(\frac{1}{2}\theta) e^{i\delta} \quad (29a)$$

and

$$u_{\frac{1}{2}\lambda=-1} = \frac{(-1 + \cos\theta)e^{-i\phi}}{\sin\theta} \cdot \left\{ \frac{1}{2}(1 + \cos\theta) \right\}^{\frac{1}{2}} e^{i\delta} = -\sin(\frac{1}{2}\theta) e^{-i(\phi-\delta)} \quad (29b)$$

δ is a second arbitrary phase factor. We take $\gamma = \delta = 0$. Therefore the unitary transformation matrix is

$$\tilde{U} = \begin{pmatrix} u_{\frac{1}{2}\uparrow} & u_{\frac{1}{2}\downarrow} \\ u_{-\frac{1}{2}\uparrow} & u_{-\frac{1}{2}\downarrow} \end{pmatrix} = \begin{pmatrix} \cos(\frac{1}{2}\theta) e^{-i\phi} & -\sin(\frac{1}{2}\theta) e^{-i\phi} \\ \sin(\frac{1}{2}\theta) & \cos(\frac{1}{2}\theta) \end{pmatrix} \quad (30)$$

and so the basis $\{|\frac{1}{2}, \uparrow\rangle, |\frac{1}{2}, \downarrow\rangle\}$ expanded in the basis $\{|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle\}$ is

$$\begin{aligned} |\frac{1}{2}, \uparrow\rangle &= [\cos(\frac{1}{2}\theta) e^{-i\phi}] |\frac{1}{2}, \frac{1}{2}\rangle + [\sin(\frac{1}{2}\theta)] |\frac{1}{2}, -\frac{1}{2}\rangle \\ |\frac{1}{2}, \downarrow\rangle &= [-\sin(\frac{1}{2}\theta) e^{-i\phi}] |\frac{1}{2}, \frac{1}{2}\rangle + [\cos(\frac{1}{2}\theta)] |\frac{1}{2}, -\frac{1}{2}\rangle \end{aligned} \quad (31)$$

The inverse transformation is

$$\tilde{U}^\dagger = \begin{pmatrix} u_{\uparrow\frac{1}{2}}^\dagger & u_{\uparrow-\frac{1}{2}}^\dagger \\ u_{\downarrow\frac{1}{2}}^\dagger & u_{\downarrow-\frac{1}{2}}^\dagger \end{pmatrix} = \begin{pmatrix} \cos(\frac{1}{2}\theta) e^{i\phi} & \sin(\frac{1}{2}\theta) \\ -\sin(\frac{1}{2}\theta) e^{i\phi} & \cos(\frac{1}{2}\theta) \end{pmatrix} \quad (32)$$

and so

$$\begin{aligned} |\frac{1}{2}, \frac{1}{2}\rangle &= [\cos(\frac{1}{2}\theta) e^{i\phi}] |\frac{1}{2}, \uparrow\rangle + [-\sin(\frac{1}{2}\theta) e^{i\phi}] |\frac{1}{2}, \downarrow\rangle \\ |\frac{1}{2}, -\frac{1}{2}\rangle &= [\sin(\frac{1}{2}\theta)] |\frac{1}{2}, \uparrow\rangle + [\cos(\frac{1}{2}\theta)] |\frac{1}{2}, \downarrow\rangle \end{aligned} \quad (33)$$

We take the basis $\{|\frac{1}{2}, \uparrow\rangle, |\frac{1}{2}, \downarrow\rangle\}$ as defining part of the "configuration space" representation, where the "coordinate" label $\xi = \uparrow$ or \downarrow . Thus, if we abbreviate the notation so that the basis $|\alpha\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$, $|\beta\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$, and the basis $|\uparrow\rangle = |\frac{1}{2}, \uparrow\rangle$, $|\downarrow\rangle = |\frac{1}{2}, \downarrow\rangle$ we have

$$\chi_{\frac{1}{2}}^{\frac{1}{2}}(\xi) = \langle \xi | \alpha \rangle = \begin{cases} \langle \uparrow | \alpha \rangle = \cos(\frac{1}{2}\theta) e^{i\phi}, & \text{for } \xi = \uparrow \\ \langle \downarrow | \alpha \rangle = -\sin(\frac{1}{2}\theta) e^{i\phi}, & \text{for } \xi = \downarrow \end{cases} \quad (34)$$

$$\chi_{\frac{1}{2}}^{-\frac{1}{2}}(\xi) = \langle \xi | \beta \rangle = \begin{cases} \langle \uparrow | \beta \rangle = \sin(\frac{1}{2}\theta), & \text{for } \xi = \uparrow \\ \langle \downarrow | \beta \rangle = \cos(\frac{1}{2}\theta), & \text{for } \xi = \downarrow \end{cases}$$

$$\tilde{\alpha} = \chi_{\frac{1}{2}}^{\frac{1}{2}} \equiv \begin{pmatrix} \cos(\frac{1}{2}\theta) e^{i\phi} \\ -\sin(\frac{1}{2}\theta) e^{i\phi} \end{pmatrix}; \quad \tilde{\beta} = \chi_{\frac{1}{2}}^{-\frac{1}{2}} \equiv \begin{pmatrix} \sin(\frac{1}{2}\theta) \\ \cos(\frac{1}{2}\theta) \end{pmatrix} \quad (35)$$

The labels \uparrow and \downarrow suggest the spin is aligned parallel or antiparallel to \mathbf{n} and often are referred to as "spin up" and "spin down". More often than not, we choose $\mathbf{n} = \mathbf{e}_z$ whence $\theta = 0$ whence

$$\langle \uparrow | \alpha \rangle = 1, \langle \downarrow | \alpha \rangle = 0; \langle \uparrow | \beta \rangle = 0, \langle \downarrow | \beta \rangle = 1. \quad (36)$$

For a single particle with three spatial degrees of freedom and spin $\frac{1}{2}$ the configuration space representation is based upon appending the eigenstates of \hat{x} , \hat{y} , \hat{z} , to the eigenstates of \hat{s}^2 and $\hat{s}_n \equiv \hat{s} \cdot \mathbf{n}$. Thus we have the basis

$$\{ |\vec{r}, \xi\rangle \equiv |x, y, z, \xi\rangle \equiv |x, y, z\rangle \otimes |\frac{1}{2}, \xi\rangle; \begin{array}{l} -\infty \leq x \leq \infty \\ -\infty \leq y \leq \infty \\ -\infty \leq z \leq \infty \end{array} \xi = \uparrow, \downarrow \} \quad (37)$$

The state vector $|\Psi(t)\rangle$ is represented in configuration space by a wave function defined over the range of eigenvalues of the four observables \hat{x} , \hat{y} , \hat{z} , \hat{s}_n (given that always $s = \frac{1}{2}$ and thus need not be specified):

$$\langle \vec{r}, \xi | \Psi(t) \rangle = \Psi(\vec{r}, \xi; t) = \Psi(x, y, z, \xi; t). \quad (38)$$

The wavefunction thus is a set of scalar products (complex numbers) defined over the "space and spin coordinates" of the particle.

This would be a sufficient (i.e. a complete) description of a single particle state where, as in the case of an electron, "ordinary spin" is the only internal degree of freedom. For a nucleon, however, there is a second internal degree of freedom called isospin. This degree of freedom is also represented in terms of angular momentum algebra of spin $\frac{1}{2}$, for empirically, there are two states of the nucleon; with $i = \frac{1}{2}$ always, the $m_i = +\frac{1}{2}$ is the nucleon state called a proton and $m_i = -\frac{1}{2}$ is the nucleon state called a neutron. Thus we introduce $\hat{i} = \hat{i}_x \mathbf{e}_x + \hat{i}_y \mathbf{e}_y + \hat{i}_z \mathbf{e}_z$ and $\hat{i}^2 = \hat{i}_x^2 + \hat{i}_y^2 + \hat{i}_z^2$. Analogously to "ordinary spin" the two eigenstates of \hat{i}^2 and \hat{i}_z satisfy

$$\begin{aligned} \hat{i}^2 |i, m_i\rangle &= i(i+1) |i, m_i\rangle = \frac{3}{4} |i, m_i\rangle, \quad (\text{as } i = \frac{1}{2}) \\ \hat{i}_z |i, m_i\rangle &= m_i |i, m_i\rangle, \quad (\text{for } m_i = \pm \frac{1}{2}). \end{aligned} \quad (39)$$

Note that we have not included factors of \hbar since the algebra does not require a mechanical angular momentum. We introduce a set of 2×2

matrices $\tau_{\tilde{x}}, \tau_{\tilde{y}}, \tau_{\tilde{z}}$ analogous to the σ 's. Thus,

$$i_{\tilde{x}} = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{1}{2} \tau_{\tilde{x}}; \quad i_{\tilde{y}} = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{1}{2} \tau_{\tilde{y}}; \quad i_{\tilde{z}} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{1}{2} \tau_{\tilde{z}} \quad (40)$$

But once again we could choose to diagonalize \hat{i}^2 and $\hat{i}_{\tilde{n}} \equiv \hat{i} \cdot \tilde{n}$. Analogous to the ordinary spin, we define the eigenbasis of $\{\hat{i}^2, \hat{i}_{\tilde{z}}\}$ such that $|\frac{1}{2}, \frac{1}{2}\rangle \equiv |p\rangle$ (proton) and $|\frac{1}{2}, -\frac{1}{2}\rangle \equiv |n\rangle$ (neutron) and the eigenbasis of $\{\hat{i}^2, \hat{i}_{\tilde{n}}\}$ as $|\frac{1}{2}, \frac{1}{2}\rangle \equiv |\frac{1}{2}, \eta=/\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle = |\eta=\backslash\rangle$.

We define η the isospin coordinate $\eta = /, \backslash$ and in a similar fashion

$$\begin{aligned} \Upsilon_{\frac{1}{2}}^{\frac{1}{2}}(\eta) &= \langle \eta | i = \frac{1}{2}, m_i = \frac{1}{2} \rangle = \begin{cases} \cos(\frac{1}{2}\theta) e^{i\phi} = \langle / | p \rangle \\ -\sin(\frac{1}{2}\theta) e^{i\phi} = \langle \backslash | p \rangle \end{cases} \\ \Upsilon_{\frac{1}{2}}^{-\frac{1}{2}}(\eta) &= \langle \eta | \frac{1}{2} = \frac{1}{2}, m_i = -\frac{1}{2} \rangle = \begin{cases} \sin(\frac{1}{2}\theta) = \langle / | n \rangle \\ \cos(\frac{1}{2}\theta) = \langle \backslash | n \rangle \end{cases} \end{aligned} \quad (41)$$

$$\tilde{p} = \Upsilon_{\frac{1}{2}}^{\frac{1}{2}} \equiv \begin{pmatrix} \cos(\frac{1}{2}\theta) e^{i\phi} \\ -\sin(\frac{1}{2}\theta) e^{i\phi} \end{pmatrix}; \quad \tilde{n} = \Upsilon_{\frac{1}{2}}^{-\frac{1}{2}} \equiv \begin{pmatrix} \sin(\frac{1}{2}\theta) \\ \cos(\frac{1}{2}\theta) \end{pmatrix} \quad (42)$$

and again for $\theta = 0$ $\langle / | p \rangle = 1$; $\langle \backslash | p \rangle = 0$; $\langle / | n \rangle = 0$; $\langle \backslash | n \rangle = 1$.

Thus the configuration space for a nucleon is expanded to include isospin and the basis vectors for the configuration space representation are

$$\left\{ |\vec{r}, \xi, \eta\rangle = |x, y, z\rangle \otimes |s=\frac{1}{2}, \xi\rangle \otimes |i=\frac{1}{2}, \eta\rangle \begin{array}{l} -\infty \leq x \leq \infty \\ -\infty \leq y \leq \infty \\ -\infty \leq z \leq \infty \end{array} \left. \begin{array}{l} \xi = \uparrow, \downarrow \\ \eta = /, \backslash \end{array} \right\} \quad (43)$$

and the wavefunction for a single nucleon is

$$\langle x, y, z, \xi, \eta | \Psi(t) \rangle = \Psi(x, y, z, \xi, \eta; t) \quad (45)$$

which depends on five coordinates. As usual \otimes denotes the "direct product" so that the complete set of basis vectors is formed by taking every vector in each of the three sets to form the triplet.

So far this entire discussion has focused on a single nucleon. We can construct two particle (and many particle) states in the usual fashion by "vector coupling" direct products. Thus we shall let " α " indicate the pair of quantum numbers " $\frac{1}{2}, \frac{1}{2}$ " and " β " indicate " $\frac{1}{2}, -\frac{1}{2}$ " for ordinary spin. Then for the two particle spin observables

$$\hat{S}^2 = (\vec{s}_1 + \vec{s}_2) \cdot (\vec{s}_1 + \vec{s}_2) \quad \text{and} \quad \hat{S}_Z = (\hat{s}_{1Z} + \hat{s}_{2Z}) . \quad (46)$$

The two-particle eigenstates which satisfy

$$\begin{aligned} \hat{S}^2 |S, M_S\rangle &= S(S+1)\hbar^2 |S, M_S\rangle \\ \hat{S}_Z |S, M_S\rangle &= M_S \hbar |S, M_S\rangle \end{aligned} \quad (47)$$

are explicitly

$$\begin{aligned} |S=1, M_S=1\rangle &= |\alpha\rangle_1 |\alpha\rangle_2 \\ |S=1, M_S=0\rangle &= \frac{1}{\sqrt{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} \\ |S=1, M_S=-1\rangle &= |\beta\rangle_1 |\beta\rangle_2 \end{aligned} \quad \left. \vphantom{\begin{aligned} |S=1, M_S=1\rangle \\ |S=1, M_S=0\rangle \\ |S=1, M_S=-1\rangle \end{aligned}} \right\} \begin{array}{l} \text{Three triplets} \\ S=1, \text{ with the} \\ \text{three choices} \\ M_S = 1, 0, -1. \end{array} \quad (48)$$

and

$$|S=0, M_S=0\rangle = \frac{1}{\sqrt{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 - |\alpha\rangle_2 |\beta\rangle_1 \} \quad \left. \vphantom{|S=0, M_S=0\rangle} \right\} \begin{array}{l} \text{one singlet} \\ \text{spin function} \end{array}$$

These two particle states are arrived at using the Russel Saunders vector coupling scheme where the coefficients 1, or $\pm\frac{1}{\sqrt{2}}$ are simply the Clebsch Gordon coefficients for coupling two $s = \frac{1}{2}$ spin states. Indeed the spin states of two nucleons (each with $s = \frac{1}{2}$) can only be $S = 1$, with $M_S = 1, 0, -1$ and $S=0$ with $M_S = 0$. The configuration space representations of the two nucleon spin states ($\chi_{S, M_S}(\xi_1, \xi_2) = \langle \xi_1, \xi_2 | S, M_S \rangle$) are

$$\begin{aligned} \chi_{1,1}(\xi_1, \xi_2) &= \alpha(\xi_1) \alpha(\xi_2) \\ \chi_{1,0}(\xi_1, \xi_2) &= \frac{1}{\sqrt{2}} \{ \alpha(\xi_1) \beta(\xi_2) + \alpha(\xi_2) \beta(\xi_1) \} \\ \chi_{1,-1}(\xi_1, \xi_2) &= \beta(\xi_1) \beta(\xi_2) \end{aligned} \quad \left. \vphantom{\begin{aligned} \chi_{1,1}(\xi_1, \xi_2) \\ \chi_{1,0}(\xi_1, \xi_2) \\ \chi_{1,-1}(\xi_1, \xi_2) \end{aligned}} \right\} \begin{array}{l} \text{Three triplet} \\ \text{two particle} \\ \text{spin functions} \end{array} \quad (49)$$

and

$$\chi_{0,0}(\xi_1, \xi_2) = \frac{1}{\sqrt{2}} \{ \alpha(\xi_1) \beta(\xi_2) - \alpha(\xi_2) \beta(\xi_1) \} \quad \left. \vphantom{\chi_{0,0}(\xi_1, \xi_2)} \right\} \begin{array}{l} \text{One singlet} \\ \text{two particle} \\ \text{spin function} \end{array}$$

Similarly, for the isotopic spin, the eigenstates of

$$\begin{aligned}\hat{I}^2 |I, M_I\rangle &= I(I+1) |I, M_I\rangle \\ \hat{I}_Z |I, M_I\rangle &= M_I |I, M_I\rangle\end{aligned}\tag{50}$$

$$\begin{aligned}|I=1, M_I=1\rangle &= |p\rangle_1 |p\rangle_2 \\ |I=1, M_I=0\rangle &= \frac{\sqrt{2}}{2} \{ |p\rangle_1 |n\rangle_2 + |p\rangle_2 |n\rangle_1 \} \\ |I=1, M_I=-1\rangle &= |n\rangle_1 |n\rangle_2\end{aligned}\left. \begin{array}{l} \\ \\ \end{array} \right\} \begin{array}{l} \text{Three triplets} \\ I=1, \text{ for the} \\ \text{three choices} \\ M_I = 1, 0, -1. \end{array}\tag{51}$$

and

$$|I=0, M_I=0\rangle = \frac{\sqrt{2}}{2} \{ |p\rangle_1 |n\rangle_2 - |p\rangle_2 |n\rangle_1 \} \left. \begin{array}{l} \\ \end{array} \right\} \begin{array}{l} \text{one singlet} \\ I=0, M_I=0 \end{array}$$

for which the configuration space representations are:

$$\begin{aligned}\Upsilon_{1,1}(\eta_1, \eta_2) &= p(\eta_1) p(\eta_2) \\ \Upsilon_{1,0}(\eta_1, \eta_2) &= \frac{\sqrt{2}}{2} \{ p(\eta_1) n(\eta_2) + p(\eta_2) n(\eta_1) \} \\ \Upsilon_{1,-1}(\eta_1, \eta_2) &= n(\eta_1) n(\eta_2)\end{aligned}\left. \begin{array}{l} \\ \\ \end{array} \right\} \begin{array}{l} \text{Three triplet} \\ \text{two particle} \\ \text{isospin functions} \end{array}\tag{52}$$

$$\Upsilon_{0,0}(\eta_1, \eta_2) = \frac{\sqrt{2}}{2} \{ p(\eta_1) n(\eta_2) - p(\eta_2) n(\eta_1) \} \left. \begin{array}{l} \\ \end{array} \right\} \begin{array}{l} \text{one singlet} \\ \text{two particle} \\ \text{isospin function} \end{array}$$

where $\Upsilon_{I, M_I}(\eta_1, \eta_2) \equiv \langle \eta_1, \eta_2 | I, M_I \rangle$. Again we have simply vector coupled the nucleon states using Clebsch Gordon algebra to get the two nucleon isospin states. There are no factors of \hbar in the isospin algebra.

We have spent the introduction discussing the spin and isospin states of two nucleons. We now turn to the real problem at hand, determining the ground state wavefunction of the deuteron with which we will be able to calculate the properties of the deuteron such as its electric quadrupole and magnetic dipole moments. The deuteron is a two body problem and so the first item of business is to separate the center of mass and internal (relative) spatial coordinates. We do this is the usual way; however, we do want to do it explicitly since there is a specific problem for the deuteron which we must address.

We consider the spatial observables for the two nucleon problem.

The nucleons are identical fermions and so $m_1 \equiv m_2$. "1" and "2" are the particle labels and lower case and upper case quantities are the relative and center of mass observables respectively. Note the caret and the arrow; we express one set of vector operators (observables) in terms of the other set. With μ the reduced mass, the "new" coordinates are

$$\left. \begin{aligned} \vec{r} &= \vec{r}_2 - \vec{r}_1 \\ \vec{R} &= \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2} = \frac{1}{2} [\vec{r}_1 + \vec{r}_2] \end{aligned} \right\} \left\{ \begin{aligned} \vec{r}_1 &= \vec{R} - \vec{r} (\mu/m_1) = \vec{R} - \frac{1}{2} \vec{r} \\ \vec{r}_2 &= \vec{R} + \vec{r} (\mu/m_2) = \vec{R} + \frac{1}{2} \vec{r} \end{aligned} \right. \quad (53)$$

and the "new" momenta are

$$\left. \begin{aligned} \vec{p} &= \left(\frac{\mu}{m_2}\right) \vec{p}_2 - \left(\frac{\mu}{m_1}\right) \vec{p}_1 = \frac{1}{2} [\vec{p}_2 - \vec{p}_1] \\ \vec{P} &= [\vec{p}_1 + \vec{p}_2] \end{aligned} \right\} \left\{ \begin{aligned} \vec{p}_1 &= (\mu/m_2) \vec{P} - \vec{p} = \frac{1}{2} \vec{P} - \vec{p} \\ \vec{p}_2 &= (\mu/m_1) \vec{P} + \vec{p} = \frac{1}{2} \vec{P} + \vec{p} \end{aligned} \right. \quad (54)$$

The orbital angular momentum observables are therefore

$$\vec{l}_1 = \vec{r}_1 \times \vec{p}_1 = (\vec{R} - \frac{1}{2} \vec{r}) \times (\frac{1}{2} \vec{P} - \vec{p}) = \frac{1}{2} [(\vec{R} \times \vec{P}) + (\vec{r} \times \vec{p})] - \frac{1}{4} \vec{r} \times \vec{P} - \vec{R} \times \vec{p} \quad (55)$$

and

$$\vec{l}_2 = \vec{r}_2 \times \vec{p}_2 = (\vec{R} + \frac{1}{2} \vec{r}) \times (\frac{1}{2} \vec{P} + \vec{p}) = \frac{1}{2} [(\vec{R} \times \vec{P}) + (\vec{r} \times \vec{p})] + \frac{1}{4} \vec{r} \times \vec{P} + \vec{R} \times \vec{p}$$

so that

$$\vec{l}_1 + \vec{l}_2 = \vec{R} \times \vec{P} + \vec{r} \times \vec{p} = \vec{L} + \vec{l}$$

Here,

$$\vec{L} = \vec{R} \times \vec{P} \quad \text{and} \quad \vec{l} = \vec{r} \times \vec{p} \quad (56)$$

are the observables for the angular momentum of the center of mass and the relative angular momentum of the pair about the center of mass respectively. The kinetic energy operator is

$$\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} = \frac{[(\mu/m_2) \vec{P} - \vec{p}]^2}{2m_1} + \frac{[(\mu/m_1) \vec{P} + \vec{p}]^2}{2m_2} = \frac{\hat{P}^2}{2M} + \frac{p^2}{2\mu} \quad (57)$$

where $M = m_1 + m_2 = 2m$ and $\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{1}{2}m$, with $m_1 = m_2 = m$.
 m is the mass of a "nucleon".

The Hamiltonian is

$$\begin{aligned}\hat{H} &= \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + V(\vec{r}_1, \vec{r}_2, \vec{l}_1, \vec{l}_2, \vec{s}_1, \vec{s}_2, \vec{i}_1, \vec{i}_2) \\ &= \frac{P^2}{2M} + \frac{p^2}{2\mu} + V(\vec{r}, \vec{l}, \vec{s}_1, \vec{s}_2, \vec{i}_1, \vec{i}_2)\end{aligned}\quad (58)$$

where the second line is a consequence of the two nucleons being identical particles and the assumption (which is not rigorously true) that the interaction energy operator does not depend on the center of mass coordinates. In effect, we claim to carry out the calculation of the internal energy in the center of mass frame and thus take not only $\langle \vec{L} \rangle = \vec{0}$, but also individually $\langle \vec{R} \rangle \equiv \vec{0}$ and $\langle \vec{P} \rangle \equiv \vec{0}$. I presume you see the contradiction in this last ansatz! Nevertheless, we essentially dropped all reference to the center of mass effects from this point. In particular in considering the spin orbit interaction, we take

$$\vec{l}_1 = \frac{1}{2} \vec{l} \quad \text{and} \quad \vec{l}_2 = \frac{1}{2} \vec{l} \quad (59)$$

so that

$$\vec{l}_1 \cdot \vec{s}_1 + \vec{l}_2 \cdot \vec{s}_2 = \frac{1}{2} \vec{l} \cdot [\vec{s}_1 + \vec{s}_2] \quad (60)$$

Dropping the center of mass operators, we take the "internal" (relative) Hamiltonian for the deuteron to be

$$\hat{H} = \frac{p^2}{2\mu} + V_C(r) + V_{SO}(r) [\kappa] \frac{1}{2} \vec{l} \cdot (\vec{s}_1 + \vec{s}_2) + V_T(r) [\lambda] \hat{T}_{12}(\vec{r}, \vec{s}_1, \vec{s}_2) \quad (61)$$

where the tensor operator

$$\hat{T}_{12} = 3 (\vec{s}_1 \cdot \vec{r})(\vec{s}_2 \cdot \vec{r})/r^2 - \vec{s}_1 \cdot \vec{s}_2 \quad (62)$$

We have included factors $[\kappa]$ and $[\lambda]$ (not found in the texts) since the operators to the right in each term have dimensions of angular momentum squared. We anticipate the $[\kappa]$ and $[\lambda] \sim \text{a constant}/\hbar^2$ in order that "V" has dimensions of energy. There are indeed additional terms in the general form of the nucleon nucleon interaction, but we settle on just these three. (For example, the Coulomb interaction between two nucleons both with $m_i = +\frac{1}{2}$ (i.e two protons) is not operative in the deuteron. This would emerge from the formalism since, as we shall see, the deuteron must be an isospin singlet.)

The tensor operator is such that its "angular average" vanishes:

$$\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \hat{T}_{12}(r, \theta, \phi, \hat{s}_1, \hat{s}_2) = \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \left\{ \frac{3}{r^2} (\hat{s}_{1x} \hat{s}_{2x} r^2 \sin^2\theta \cos^2\phi + \hat{s}_{1y} \hat{s}_{2y} r^2 \sin^2\theta \sin^2\phi + \hat{s}_{1z} \hat{s}_{2z} r^2 \cos^2\theta + \text{"cross terms which vanish"} - \hat{s}_1 \cdot \hat{s}_2 \right\} = 0. \quad (63)$$

The potential energy factors have the Yukawa form

$$V_\nu(r) = \begin{cases} \infty, & r \leq r_c \\ V_{0\nu} \frac{e^{-\mu_\nu r}}{\mu_\nu r}, & r > r_c \end{cases} \quad (64)$$

for $\nu = "c"$ (central), "so" (spin orbit), or "T" (tensor) potential. In each term r_c is the (same) "hard core radius."

The problem is to find the ground state energy and wave function, i.e. the lowest energy solution to

$$\hat{H}\Psi(\vec{r}, \xi_1, \xi_2, \eta_1, \eta_2) = E\Psi(\vec{r}, \xi_1, \xi_2, \eta_1, \eta_2) \quad (65)$$

so that knowing Ψ we may evaluate the ground state properties of the deuteron (e.g. its magnetic moment and electric quadrupole moment). We have chosen the configuration space representation for the Hamiltonian whence we can find a set of partial differential equations for the ground state. However, we first need to get a handle on the form of Ψ . The tensor interaction contains the factor

$$\begin{aligned} \hat{T}_{12} &= 3 (\hat{s}_1 \cdot \hat{r}) (\hat{s}_2 \cdot \hat{r}) / r^2 - \hat{s}_1 \cdot \hat{s}_2 \\ &= 3 (\hat{s}_{1j} \hat{x}_j) (\hat{s}_{2k} \hat{x}_k) / r^2 - \hat{s}_{1j} \hat{s}_{2j} \\ &= \{3 \hat{x}_j \hat{x}_k / r^2 - \delta_{jk}\} \hat{s}_{1j} \hat{s}_{2k} \end{aligned} \quad (66)$$

where we sum over the repeated indices. This factor commutes with the components of total angular momentum

$$\hat{J}_i = \hat{l}_i + \hat{s}_{1i} + \hat{s}_{2i} \quad (67)$$

but not with the observables \hat{l}_i and $(\hat{s}_{1i} + \hat{s}_{2i})$ separately. To see this we write the orbital angular momentum components as

$$\hat{l}_i = \epsilon_{imn} \hat{x}_m \hat{p}_n \quad (68)$$

(summing over the repeated indices m, n) and consider the commutator

$$\begin{aligned} [\hat{T}_{12}, \hat{l}_i] &= [\{3\hat{x}_j \hat{x}_k / r^2 - \delta_{jk}\}, \epsilon_{imn} \hat{x}_m \hat{p}_n] \hat{s}_{1j} \hat{s}_{2k} \\ &= (3\epsilon_{imn} / r^2) [\hat{x}_j \hat{x}_k, \hat{x}_m \hat{p}_n] \hat{s}_{1j} \hat{s}_{2k} \end{aligned} \quad (69)$$

Consider the factor

$$\begin{aligned} [\hat{x}_j \hat{x}_k, \hat{x}_m \hat{p}_n] &= [\hat{x}_j \hat{x}_k, \hat{x}_m] \hat{p}_n - \hat{x}_m [\hat{p}_n, \hat{x}_j \hat{x}_k] \\ &= \hat{x}_j \hat{x}_k \hat{x}_m \hat{p}_n - \hat{x}_m \hat{x}_j \hat{x}_k \hat{p}_n - \hat{x}_m \hat{p}_n \hat{x}_j \hat{x}_k + \hat{x}_m \hat{x}_j \hat{x}_k \hat{p}_n \\ &= 0 - \hat{x}_m \{ [\hat{p}_n, \hat{x}_j] \hat{x}_k - \hat{x}_j [\hat{x}_k, \hat{p}_n] \} \\ &= 0 - \hat{x}_m \{ -i\hbar \delta_{jn} \hat{x}_k - \hat{x}_j (i\hbar \delta_{kn}) \} \end{aligned} \quad (70)$$

Using the result (70) in (69) we have

$$\begin{aligned} [\hat{T}_{12}, \hat{l}_i] &= \{3i\hbar \epsilon_{imn} / r^2\} \{ \hat{x}_m \hat{x}_k \delta_{jn} + \hat{x}_m \hat{x}_j \delta_{kn} \} \hat{s}_{1j} \hat{s}_{2k} \\ &= (3i\hbar \epsilon_{imn} / r^2) \{ \hat{x}_m \hat{x}_k \hat{s}_{1n} \hat{s}_{2k} + \hat{x}_m \hat{x}_j \hat{s}_{1j} \hat{s}_{2n} \} \\ &= (3i\hbar / r^2) \{ (\vec{r} \times \vec{s}_1)_i (\vec{r} \cdot \vec{s}_2) + (\vec{r} \cdot \vec{s}_1) (\vec{r} \times \vec{s}_2)_i \} \end{aligned} \quad (71)$$

which clearly is not the null operator. Similarly, the commutator

$$\begin{aligned} [\hat{T}_{12}, \hat{s}_{1i}] &= [\{3\hat{x}_j \hat{x}_k / r^2 - \delta_{jk}\} \hat{s}_{1j} \hat{s}_{2k}, \hat{s}_{1i}] \\ &= \{3\hat{x}_j \hat{x}_k / r^2 - \delta_{jk}\} [\hat{s}_{1j}, \hat{s}_{1i}] \hat{s}_{2k} \\ &= \{3\hat{x}_j \hat{x}_k / r^2 - \delta_{jk}\} \{i\hbar \epsilon_{jim} \hat{s}_{1m}\} \hat{s}_{2k} \\ &= -3i\hbar / r^2 \{ \epsilon_{ijm} \hat{x}_j \hat{s}_{1m} \} (\hat{x}_k \hat{s}_{2k}) + i\hbar \epsilon_{ikm} \hat{s}_{1m} \hat{s}_{2k} \\ &= -3i\hbar / r^2 \{ (\vec{r} \times \vec{s}_1)_i (\vec{r} \cdot \vec{s}_2) - i\hbar (\vec{s}_1 \times \vec{s}_2)_i \} \end{aligned} \quad (72)$$

With the symmetry of \vec{s}_1 and \vec{s}_2 in \hat{T}_{12} it is clear that

$$[\hat{T}_{12}, \hat{s}_{2i}] = -3i\hbar/r^2 \{ (\vec{r} \times \vec{s}_2)_i (\vec{r} \cdot \vec{s}_1) - i\hbar (\vec{s}_2 \times \vec{s}_1)_i \} \quad (73)$$

It follows from (71), (72), (73) and the fact $\vec{s}_1 \times \vec{s}_2 = -\vec{s}_2 \times \vec{s}_1$ that

$$[\hat{T}_{12}, \hat{J}_i] = [\hat{T}_{12}, \{ \hat{l}_i + \hat{s}_{1i} + \hat{s}_{2i} \}] = \hat{0}. \quad (74)$$

Thus the components of the total angular momentum commute with \hat{T}_{12} although the components of the relative orbital angular momentum and the components of the spin do not separately commute with \hat{T}_{12} . Thus \hat{J}^2 and one of its components, say \hat{J}_z , can be included along with the Hamiltonian in a complete set of commuting observables. Equivalently stated l is not a good quantum number, but J and M_J are good quantum numbers. A priori, S is also not a good quantum number (since the components \hat{S}_i do not commute with \hat{H}). However, other constraints (see the following arguments) make S a good quantum number for the ground state.

We write out the configuration space form for \hat{T}_{12} . We note that

$$\vec{r} \cdot \vec{s} = \frac{1}{2} (\hat{r}_+ \hat{s}_- + \hat{r}_- \hat{s}_+) + \hat{r}_0 \hat{s}_0 \quad \text{and} \quad \vec{s}_1 \cdot \vec{s}_2 = \frac{1}{2} [\hat{s}_{1+} \hat{s}_{2-} + \hat{s}_{1-} \hat{s}_{2+}] + \hat{s}_{10} \hat{s}_{20}$$

Defining $\hat{r}_+ = (x + iy)/r = \sin\theta e^{i\phi}$, $\hat{r}_- = (x - iy)/r = \sin\theta e^{-i\phi}$, $\hat{r}_0 = \cos\theta$ we find that the tensor operator can be written

$$\begin{aligned} \hat{T}_{12} &= 3(\vec{r} \cdot \vec{s}_1)(\vec{r} \cdot \vec{s}_2) - \vec{s}_1 \cdot \vec{s}_2 = \\ &= 3 \left\{ \frac{1}{4} [r_+^2 s_{1-} s_{2-} + r_+ r_- (s_{1-} s_{2+} + s_{1+} s_{2-}) + r_-^2 s_{1+} s_{2+}] + r_0^2 s_{10} s_{20} \right. \\ &\quad \left. + \frac{1}{2} [r_+ r_0 (\hat{s}_{1-} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2-}) + r_- r_0 (\hat{s}_{1+} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2+})] \right\} \\ &\quad - \left\{ \frac{1}{2} [\hat{s}_{1+} \hat{s}_{2-} + \hat{s}_{1-} \hat{s}_{2+}] + \hat{s}_{10} \hat{s}_{20} \right\} \\ &= \frac{3}{4} [r_+^2 \hat{s}_{1-} \hat{s}_{2-} + r_-^2 \hat{s}_{1+} \hat{s}_{2+}] + \left[\left(\frac{3}{4} r_+ r_- - \frac{1}{2} \right) (\hat{s}_{1-} \hat{s}_{2+} + \hat{s}_{1+} \hat{s}_{2-}) \right] + [3r_0^2 - 1] \hat{s}_{10} \hat{s}_{20} \\ &\quad + \frac{3}{2} [r_+ r_0 (\hat{s}_{1-} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2-}) + r_- r_0 (\hat{s}_{1+} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2+})] \quad (75) \end{aligned}$$

Now the six angular factors can be expressed in terms of the five spheri-

cal harmonics for $l=2$. Check to see that in fact

$$\begin{aligned}
 r_+^2 &= \sin^2\theta e^{2i\phi} = [32\pi/15]^{\frac{1}{2}} Y_2^2(\theta, \phi) \\
 r_-^2 &= \sin^2\theta e^{-2i\phi} = [32\pi/15]^{\frac{1}{2}} Y_2^{-2}(\theta, \phi) \\
 \frac{3}{4}r_+r_- - \frac{1}{2} &= \frac{3}{4}\sin^2\theta - \frac{1}{2} = \frac{1}{4} - \frac{3}{4}\cos^2\theta = -\frac{1}{4}(3\cos^2\theta - 1) = -[\pi/5]^{\frac{1}{2}} Y_2^0(\theta, \phi) \\
 r_+r_0 &= \sin\theta\cos\theta e^{i\phi} = -[8\pi/15]^{\frac{1}{2}} Y_2^1(\theta, \phi) \\
 r_-r_0 &= \sin\theta\cos\theta e^{-i\phi} = +[8\pi/15]^{\frac{1}{2}} Y_2^{-1}(\theta, \phi) \\
 3r_0^2 - 1 &= (3\cos^2\theta - 1) = [16\pi/5]^{\frac{1}{2}} Y_2^0(\theta, \phi)
 \end{aligned} \tag{76}$$

We obtained these results using Shankar's text. Thus we have for the tensor operator factor

$$\begin{aligned}
 \hat{T}_{12} &= 3(\hat{r} \cdot \hat{s}_1)(\hat{r} \cdot \hat{s}_2) - \hat{s}_1 \cdot \hat{s}_2 = \\
 &= \frac{3}{4} [r_+^2 \hat{s}_{1-} \hat{s}_{2-} + r_-^2 \hat{s}_{1+} \hat{s}_{2+}] + [(\frac{3}{4}r_+r_- - \frac{1}{2})(\hat{s}_{1-} \hat{s}_{2+} + \hat{s}_{1+} \hat{s}_{2-})] + [3r_0^2 - 1] \hat{s}_{10} \hat{s}_{20} \\
 &\quad + \frac{3}{2} [r_+r_0(\hat{s}_{1-} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2-}) + r_-r_0(\hat{s}_{1+} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2+})] \} \\
 &= \frac{3}{4} [32\pi/15]^{\frac{1}{2}} \{ Y_2^2(\theta, \phi) \hat{s}_{1-} \hat{s}_{2-} + Y_2^{-2}(\theta, \phi) \hat{s}_{1+} \hat{s}_{2+} \} \\
 &\quad - [\pi/5]^{\frac{1}{2}} Y_2^0(\theta, \phi) [\hat{s}_{1-} \hat{s}_{2+} + \hat{s}_{1+} \hat{s}_{2-}] + [16\pi/5]^{\frac{1}{2}} Y_2^0(\theta, \phi) \hat{s}_{10} \hat{s}_{20} \\
 &\quad + \frac{3}{2} [8\pi/15]^{\frac{1}{2}} \{ -Y_2^1(\theta, \phi) [\hat{s}_{1-} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2-}] + Y_2^{-1}(\theta, \phi) [\hat{s}_{1+} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2+}] \} \\
 &= [6\pi/5]^{\frac{1}{2}} \{ Y_2^2(\theta, \phi) \hat{s}_{1-} \hat{s}_{2-} + Y_2^{-2}(\theta, \phi) \hat{s}_{1+} \hat{s}_{2+} \\
 &\quad - Y_2^1(\theta, \phi) [\hat{s}_{1-} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2-}] + Y_2^{-1}(\theta, \phi) [\hat{s}_{1+} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2+}] \} \\
 &\quad [16\pi/5]^{\frac{1}{2}} Y_2^0(\theta, \phi) \{ \hat{s}_{10} \hat{s}_{20} - \frac{1}{4} [\hat{s}_{1-} \hat{s}_{2+} + \hat{s}_{1+} \hat{s}_{2-}] \} \tag{77}
 \end{aligned}$$

\hat{T}_{12} is an operator on the space and "ordinary" spin factors in the wave function. We will examine in detail the results of applying the operator to the wavefunction (or equivalently the state vector). In anticipation of doing so we have on the following page all the results of the six operators $\hat{s}_{1-} \hat{s}_{2-}$; $\hat{s}_{1+} \hat{s}_{2+}$; $[\hat{s}_{1-} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2-}]$; $[\hat{s}_{1+} \hat{s}_{20} + \hat{s}_{10} \hat{s}_{2+}]$; $\hat{s}_{10} \hat{s}_{20}$; $[\hat{s}_{1-} \hat{s}_{2+} + \hat{s}_{1+} \hat{s}_{2-}]$ on the three triplet spin functions, $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$.

The six operations on the three triplet states are:

$$[\hat{S}_1 - \hat{S}_{2+} + \hat{S}_{1+} \hat{S}_{2-}] \begin{cases} |\alpha\rangle_1 |\alpha\rangle_2 & = |\emptyset\rangle \\ \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} & = \hbar^2 \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} \\ |\beta\rangle_1 |\beta\rangle_2 & = |\emptyset\rangle \end{cases} \quad (78a)$$

$$[\hat{S}_{10} \hat{S}_{2+} + \hat{S}_{1+} \hat{S}_{20}] \begin{cases} |\alpha\rangle_1 |\alpha\rangle_2 & = |\emptyset\rangle \\ \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} & = \sqrt{\frac{1}{2}} \hbar^2 |\alpha\rangle_1 |\alpha\rangle_2 \\ |\beta\rangle_1 |\beta\rangle_2 & = -\sqrt{\frac{1}{2}} \hbar^2 \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} \end{cases} \quad (78b)$$

$$[\hat{S}_1 - \hat{S}_{20} + \hat{S}_{10} \hat{S}_{2-}] \begin{cases} |\alpha\rangle_1 |\alpha\rangle_2 & = \sqrt{\frac{1}{2}} \hbar^2 \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} \\ \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} & = -\sqrt{\frac{1}{2}} \hbar^2 |\beta\rangle_1 |\beta\rangle_2 \\ |\beta\rangle_1 |\beta\rangle_2 & = |\emptyset\rangle \end{cases} \quad (78c)$$

$$[\hat{S}_{10} \hat{S}_{20}] \begin{cases} |\alpha\rangle_1 |\alpha\rangle_2 & = \frac{1}{4} \hbar^2 |\alpha\rangle_1 |\alpha\rangle_2 \\ \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} & = -\frac{1}{4} \hbar^2 \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} \\ |\beta\rangle_1 |\beta\rangle_2 & = \frac{1}{4} \hbar^2 |\beta\rangle_1 |\beta\rangle_2 \end{cases} \quad (78d)$$

$$[\hat{S}_{1+} \hat{S}_{2+}] \begin{cases} |\alpha\rangle_1 |\alpha\rangle_2 & = |\emptyset\rangle \\ \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} & = |\emptyset\rangle \\ |\beta\rangle_1 |\beta\rangle_2 & = \hbar^2 |\alpha\rangle_1 |\alpha\rangle_2 \end{cases} \quad (78e)$$

$$[\hat{S}_1 - \hat{S}_{2-}] \begin{cases} |\alpha\rangle_1 |\alpha\rangle_2 & = \hbar^2 |\beta\rangle_1 |\beta\rangle_2 \\ \sqrt{\frac{1}{2}} \{ |\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1 \} & = |\emptyset\rangle \\ |\beta\rangle_1 |\beta\rangle_2 & = |\emptyset\rangle \end{cases} \quad (78f)$$

The fact that the nucleons are fermions implies the entire wave function must be antisymmetric under the exchange of all the coordinates. As

$1 \leftrightarrow 2$ we have $\vec{r} \rightarrow -\vec{r}$ ($r=r, \theta \rightarrow \pi - \theta, \phi \rightarrow \phi + \pi$), $\xi_1 \leftrightarrow \xi_2$ and $\eta_1 \leftrightarrow \eta_2$.

Experimentally, the lowest state corresponds to $l = 0$ (approximately) but the fact that it has an electric quadrupole moment means there is an admixture of higher angular momentum states. Possibilities are

$\left. \begin{array}{l} l=0, S=0 \Rightarrow J=0 \\ l=0, S=1 \Rightarrow J=1 \end{array} \right\} \text{even parity}$	$\left. \begin{array}{l} l=1, S=0 \Rightarrow J=1 \\ l=1, S=1 \Rightarrow J=0,1,2 \end{array} \right\} \text{odd parity}$	$\left. \begin{array}{l} l=2, S=0 \Rightarrow J=2 \\ l=2, S=1 \Rightarrow J=1,2,3 \end{array} \right\} \text{even parity}$	<ul style="list-style-type: none"> ★ The parity operator acts on the ★ wavefunction such that ★ $P \Psi(\vec{r}, \xi_1 \xi_2 \eta_1 \eta_2) = \Psi(-\vec{r}, \xi_1 \xi_2 \eta_1 \eta_2)$ ★ For a particular term with a ★ given value l, the result is ★ $\Psi(-\vec{r}, \xi_1 \xi_2 \eta_1 \eta_2) = (-1)^l \Psi(\vec{r}, \xi_1 \xi_2 \eta_1 \eta_2)$
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$l=1$ is ruled out because the wave function should also be an eigenfunction of parity and since $l=0$ is present only even l 's (even parity) contributions can mix with the $l=0$. Moreover, with $l=2$, if $S=0$ only $J=2$ would be possible but there is no $J=2$ for $l=0$. Indeed, for both $l=0$ and $l=2$ the coupling of l and $S=1$ can yield $J=1$, with our choice of $M_J = 1$.

The $l=0$ term coupled with $S=1$ via the Clebsch Gordon algebra to give $J=1, M_J=1$ has only one term, since m_l is necessarily 0, $M_S=1$ in order that $M_J = m_l + M_S = 1$.) Therefore we have

$$|l=0, S=1; J=1, M_J=1\rangle = |l=0; m_l=0\rangle \otimes |S=1, M_S=1\rangle = |0,0\rangle |\alpha\rangle_1 |\alpha\rangle_2 \quad (79)$$

which in configuration space is the function we define as

$$\begin{aligned} F_{01,11}(\theta, \phi; \xi_1, \xi_2) &= \langle \theta, \phi, \xi_1, \xi_2 | l=0, S=1; J=1, M_J=1 \rangle \\ &= Y_0^0(\theta, \phi) \alpha(\xi_1) \alpha(\xi_2) = \frac{1}{\sqrt{4\pi}} \alpha(\xi_1) \alpha(\xi_2) \quad . \end{aligned} \quad (80)$$

Similarly, coupling $l=2$ with $S=1$ to yield $J=1, M_J=1$, we have

$$\begin{aligned} |l=2, S=1; J=1, M_J=1\rangle &= \sqrt{0.1} \{ |l=2, m_l=0\rangle \otimes [|\alpha\rangle_1 |\alpha\rangle_2] \} \\ &\quad - \sqrt{0.3} \{ |l=2, m_l=1\rangle \otimes [\sqrt{\frac{1}{2}} (|\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1)] \} \\ &\quad + \sqrt{0.6} \{ |l=2, m_l=2\rangle \otimes [|\beta\rangle_1 |\beta\rangle_2] \} \end{aligned} \quad (81)$$

with the configuration space representation

$$\begin{aligned}
F_{21,11}(\theta, \phi; \xi_1 \xi_2) &= \langle \theta, \phi, \xi_1 \xi_2 | l=2, S=1; J=1, M_J=1 \rangle \\
&= \sqrt{0.1} \{ Y_2^0(\theta, \phi) [\alpha(\xi_1) \alpha(\xi_2)] \} \\
&\quad - \sqrt{0.3} \{ Y_2^1(\theta, \phi) [\sqrt{\frac{1}{2}}(\alpha(\xi_1) \beta(\xi_2) + \alpha(\xi_2) \beta(\xi_1))] \} \\
&\quad + \sqrt{0.6} \{ Y_2^2(\theta, \phi) [\beta(\xi_1) \beta(\xi_2)] \} .
\end{aligned} \tag{82}$$

The Clebsch Gordon coefficients for coupling $l=2, S=1 \rightarrow J=1, M_J=1$ are

$$\begin{aligned}
(l=2, S=1, m_l=0, M_S=1 | l=2, S=1, J=1, M_J=1) &= \sqrt{0.1} \\
(l=2, S=1, m_l=1, M_S=0 | l=2, S=1, J=1, M_J=1) &= -\sqrt{0.3} \\
(l=2, S=1, m_l=2, M_S=-1 | l=2, S=1, J=1, M_J=1) &= \sqrt{0.6} .
\end{aligned} \tag{83}$$

The pair of functions defined over angles θ, ϕ and spins ξ_1, ξ_2 form an orthonormal set in the sense that

$$\sum_{\xi_1=\uparrow, \downarrow} \sum_{\xi_2=\uparrow, \downarrow} \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi F_{l-1,11}^*(\theta, \phi, \xi_1, \xi_2) F_{l,11}(\theta, \phi, \xi_1, \xi_2) = \delta_{l-1} \tag{84}$$

Moreover, since all the components \hat{J}_1 commute with \hat{T}_{12} and the parity operator also commutes with \hat{T}_{12} , we argue that \hat{T}_{12} operating on either function $F_{01,11}$ or $F_{21,11}$ must simply be a linear combination of both.

There are no other functions of $J=1, M_J=1$ and even parity which can arise from coupling an even l with a triplet ($S=1$) spin state. Thus

$$\begin{aligned}
\hat{T}_{12} F_{01,11} &= a F_{01,11} + b F_{21,11} \\
\hat{T}_{12} F_{21,11} &= c F_{01,11} + d F_{21,11} .
\end{aligned} \tag{85}$$

These operations will occur as we evaluate the expectation value of the tensor potential energy term using a trial wave function which contains the factors $F_{01,11}(\theta, \phi, \xi_1, \xi_2)$ and $F_{21,11}(\theta, \phi, \xi_1, \xi_2)$ in a linear superposition of the $l=0$ and $l=2$ states coupled to give $J=1, M_J=1$. We thus digress to examine the implications of (85) explicitly.

Using (77) on the abstract spin vectors we find by way of the results in (78a) through (78f) that

$$\begin{aligned}
\hat{T}_{12} F_{01,11} &= \hat{T}_{12} Y_0^0(\theta, \phi) |\alpha\rangle_1 |\alpha\rangle_2 = \hat{T}_{12} \frac{1}{\sqrt{4\pi}} |\alpha\rangle_1 |\alpha\rangle_2 \\
&= \frac{1}{\sqrt{4\pi}} \hbar^2 \{ [6\pi/5]^{\frac{1}{2}} [Y_2^2(\theta, \phi) |\beta\rangle_1 |\beta\rangle_2 \\
&\quad - Y_2^1(\theta, \phi) (\sqrt{2}) [\sqrt{2} (|\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1)] \\
&\quad + [16\pi/5]^{\frac{1}{2}} Y_2^0(\theta, \phi) \cdot \frac{1}{4} |\alpha\rangle_1 |\alpha\rangle_2 \} \\
&= \frac{1}{\sqrt{4\pi}} \hbar^2 \times \\
&\{ [\pi/5]^{\frac{1}{2}} Y_2^0(\theta, \phi) |\alpha\rangle_1 |\alpha\rangle_2 - [3\pi/5]^{\frac{1}{2}} Y_2^1(\theta, \phi) [\sqrt{2} (|\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1)] \\
&\quad + [6\pi/5]^{\frac{1}{2}} Y_2^2(\theta, \phi) |\beta\rangle_1 |\beta\rangle_2 \} \\
&= \frac{1}{\sqrt{4\pi}} \hbar^2 \times \{ \sqrt{2\pi} \times \\
&\{ \sqrt{0.1} Y_2^0(\theta, \phi) |\alpha\rangle_1 |\alpha\rangle_2 - \sqrt{0.3} Y_2^1(\theta, \phi) [\sqrt{2} (|\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1)] \\
&\quad + \sqrt{0.6} Y_2^2(\theta, \phi) |\beta\rangle_1 |\beta\rangle_2 \} \} \quad (86)
\end{aligned}$$

But we recognize the curly bracket as $F_{21,11}$. Thus in configuration space we have

$$\begin{aligned}
\hat{T}_{12} F_{01,11}(\theta, \phi, \xi_1, \xi_2) &= \sqrt{\frac{1}{2}} \hbar^2 F_{21,11}(\theta, \phi, \xi_1, \xi_2) \\
&= \frac{1}{4} \hbar^2 \sqrt{8} F_{21,11}(\theta, \phi, \xi_1, \xi_2). \quad (87)
\end{aligned}$$

The additional factor " $\frac{1}{4}\hbar^2$ " (not found in Elton) arises as $\vec{s} = \frac{1}{2}\hbar \vec{\sigma}$; we need be careful to include or exclude " $\frac{1}{4}\hbar^2$ " depending on whether \vec{s} or $\vec{\sigma}$ is used in the definition of \hat{T}_{12} . But, of course, this is precisely why we introduced the factor $[\lambda]$ in the definition of the operator in (61). We conclude that in (85) $a = \frac{1}{4}\hbar^2 \sqrt{8}$ and $b = 0$; accordingly Elton says that $a = \sqrt{8}$, $b = 0$ and so our factor must be $[\lambda] = 4/\hbar^2$.

We borrow the technique introduced by Elton to find the operation of $\hat{T}_{12}F_{21,11}(\theta, \phi, \xi_1, \xi_2)$ by looking at the choice for $\theta = \frac{1}{2}\pi$, $\phi = 0$. We have

$$\begin{aligned} & \hat{T}_{12}F_{21,11} \Big|_{\theta=\frac{1}{2}\pi, \phi=0} = \\ & = \underbrace{[3\hat{s}_{1x}\hat{s}_{2x} - \hat{s}_{1x}\hat{s}_{2y} - \hat{s}_{1y}\hat{s}_{2y} - \hat{s}_{1z}\hat{s}_{2z}]}_{\hat{T}_{12}(\theta=\frac{1}{2}\pi; \phi=0)} \underbrace{\left\{ \frac{1}{\sqrt{32\pi}} [-1|\alpha\rangle_1|\alpha\rangle_2 + 3|\beta\rangle_1|\beta\rangle_2] \right\}}_{|l=2, S=1; J=1, M_J=1\rangle \Big|_{\theta=\frac{1}{2}\pi; \phi=0}} \end{aligned}$$

The operator can be written as

$$[2[\frac{1}{4}(\hat{s}_{1+} + \hat{s}_{1-})(\hat{s}_{2+} + \hat{s}_{2-})] + \frac{1}{4}(\hat{s}_{1+} - \hat{s}_{1-})(\hat{s}_{2+} - \hat{s}_{2-}) - \hat{s}_{10}\hat{s}_{20}]$$

so that

$$\begin{aligned} & [\frac{3}{4}\hat{s}_{1+}\hat{s}_{2+} + \frac{3}{4}\hat{s}_{1-}\hat{s}_{2-} + \frac{1}{4}\hat{s}_{1+}\hat{s}_{2-} + \frac{1}{4}\hat{s}_{1-}\hat{s}_{2+} - \hat{s}_{10}\hat{s}_{20}] \left\{ \frac{-|\alpha\rangle_1|\alpha\rangle_2 + 3|\beta\rangle_1|\beta\rangle_2}{\sqrt{32\pi}} \right\} \\ & = (\hbar^2) \frac{-\frac{3}{4}|\beta\rangle_1|\beta\rangle_2 + \frac{1}{4}|\alpha\rangle_1|\alpha\rangle_2 + \frac{3}{4} \cdot 3|\alpha\rangle_1|\alpha\rangle_2 - 3 \cdot \frac{1}{4}|\beta\rangle_1|\beta\rangle_2}{\sqrt{32\pi}} \\ & = (\frac{1}{4}\hbar^2) \frac{10|\alpha\rangle_1|\alpha\rangle_2 - 6|\beta\rangle_1|\beta\rangle_2}{\sqrt{32\pi}} \\ & = (\frac{1}{4}\hbar^2) \frac{8|\alpha\rangle_1|\alpha\rangle_2 - 2(-|\alpha\rangle_1|\alpha\rangle_2 + 3|\beta\rangle_1|\beta\rangle_2)}{\sqrt{32\pi}} \\ & = (\frac{1}{4}\hbar^2) \left\{ \sqrt{8} \frac{1}{\sqrt{4\pi}} |\alpha\rangle_1|\alpha\rangle_2 - 2 \frac{(-|\alpha\rangle_1|\alpha\rangle_2 + 3|\beta\rangle_1|\beta\rangle_2)}{\sqrt{32\pi}} \right\} \\ & = (\frac{1}{4}\hbar^2) \{ \sqrt{8} F_{01,11} - 2F_{21,11} \} \Big|_{\theta=\frac{1}{2}\pi, \phi=0} \quad (88) \end{aligned}$$

Now we invoke the argument that $\hat{T}_{12}F_{21,11}$ must in general be some linear combination of (only) $F_{01,11}$ and $F_{21,11}$ so we conclude for all θ and ϕ

$$\hat{T}_{12}F_{21,11} = (\frac{1}{4}\hbar^2) \{ \sqrt{8} F_{01,11} - 2F_{21,11} \} \quad (89)$$

Now we are in a position to evaluate all the Hamiltonian matrix elements, reducing them to one-dimensional radial integrals. That is, all the angular integrals and spin space inner products can be done explicitly, independently of the radial wavefunction. We proceed as follows.

Then variational trial wave function is taken to be

$$\Psi(r, \theta, \phi, \xi_1, \xi_2, \eta_1, \eta_2) = c_0 \psi_{01,11}(r, \theta, \phi, \xi_1, \xi_2, \eta_1, \eta_2) + c_2 \psi_{21,11}(r, \theta, \phi, \xi_1, \xi_2, \eta_1, \eta_2) \quad (93)$$

and the normalization condition on Ψ is that

$$\sum_{\xi_1=\uparrow}^{\uparrow} \sum_{\xi_2=\downarrow}^{\uparrow} \sum_{\eta_1=\setminus}^{\setminus} \sum_{\eta_2=\setminus}^{\setminus} \int_0^{2\pi} d\phi \int_0^{\pi} \sin\phi d\theta \int_0^{\infty} r^2 dr |\Psi(r, \theta, \phi, \xi_1, \xi_2, \eta_1, \eta_2)|^2 = 1 \quad (94)$$

which, because of the orthonormality of $\{\psi_{01,11}, \psi_{21,11}\}$ means that

$$|c_0|^2 + |c_2|^2 = 1. \quad (95)$$

Here we have dropped the explicit enumeration of the parameter lists a_0, b_0, \dots and a_2, b_2, \dots but they are still to be understood. The orthogonality of $\psi_{01,11}$ and $\psi_{21,11}$ is guaranteed because of the orthogonality of $F_{01,11}$ and $F_{21,11}$. Thus once (92) is satisfied the orthonormality of $\psi_{01,11}$ and $\psi_{21,11}$ is established. If we restrict the c_0 and c_2 to be real (which is an additional constraint on the variational formalism) we insure the normalization condition (95) in terms of a single parameter ω by taking

$$c_0 = \cos(\omega) \text{ and } c_2 = \sin(\omega) \quad (96)$$

and so the normalized trial function is

$$\Psi = \cos(\omega) \psi_{01,11} + \sin(\omega) \psi_{21,11} \quad (97)$$

and the expectation value

$$\begin{aligned} \langle \Psi | \hat{H} | \Psi \rangle &= \cos^2 \omega [\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle] + \sin^2 \omega [\langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle] \\ &\quad + \sin(\omega) \cos(\omega) [\langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle + \langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle] \end{aligned} \quad (98)$$

where the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V_c(r) + V_{SO}(r) [\kappa] \frac{1}{2} \hat{l} \cdot (\hat{s}_1 + \hat{s}_2) + V_T(r) [\lambda] T_{12}(\hat{r}, \hat{s}_1, \hat{s}_2) \quad (61)$$

I trust writing the Laplacian in spherical polar coordinates is a familiar exercise. Indeed, one can show that

$$\frac{\hat{p}^2}{2\mu} \rightarrow \frac{-\hbar^2}{2\mu} \left\{ \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{\hat{l}^2}{\hbar^2 r^2} \right\} \quad (99)$$

where \hat{l}^2 is the square of the relative orbital momentum operator

Therefore, the kinetic energy operator acting on the $\psi_{l1,11}$

$$\left\{ \frac{-\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} - \frac{\hat{l}^2}{\hbar^2 r^2} \right) \right\} \psi_{l1,11} = \quad (100)$$

$$\left\{ \frac{-\hbar^2}{2\mu} \left[\frac{\partial^2}{\partial r^2} R_l(r) + \frac{2}{r} \frac{\partial}{\partial r} R_l(r) \right] + \frac{l(l+1)\hbar^2}{2\mu r^2} R_l(r) \right\} \times$$

$$\times F_{l111}(\theta, \phi, \xi_1, \xi_2) T_0^0(\eta_1, \eta_2)$$

Moreover, in the spin-orbit term the $\hat{l} \cdot \hat{S}$ factor can be written

$$\hat{l} \cdot \hat{S} = \frac{1}{2} [\hat{l}_+ \hat{S}_- + \hat{l}_- \hat{S}_+] + \hat{l}_0 \hat{S}_0 \quad (101)$$

and so the operation of the angular - spin factors yield

$$\left\{ \frac{1}{2} [\hat{l}_+ \hat{S}_- + \hat{l}_- \hat{S}_+] + \hat{l}_0 \hat{S}_0 \right\} F_{01,11} =$$

$$\left\{ \frac{1}{2} [\hat{l}_+ \hat{S}_- + \hat{l}_- \hat{S}_+] + \hat{l}_0 \hat{S}_0 \right\} \frac{1}{\sqrt{4\pi}} \alpha(\xi_1) \alpha(\xi_2) = 0. \quad (102)$$

and

$$\left\{ \frac{1}{2} [\hat{l}_+ \hat{S}_- + \hat{l}_- \hat{S}_+] + \hat{l}_0 \hat{S}_0 \right\} F_{21,11}$$

$$\hbar^2 \left\{ \sqrt{0.1} \left\{ \frac{1}{2} [2\sqrt{3} Y_2^1(\theta, \phi) \sqrt{\frac{1}{2}} \{ \alpha(\xi_1) \beta(\xi_2) + \alpha(\xi_2) \beta(\xi_1) \}] + \right. \right.$$

$$\left. - \sqrt{0.3} \left\{ \frac{1}{2} [2\sqrt{2} Y_2^2(\theta, \phi) \beta(\xi_1) \beta(\xi_2) + 2\sqrt{3} \cdot Y_2^0(\theta, \phi) \alpha(\xi_1) \alpha(\xi_2)] \right. \right.$$

$$\left. + \sqrt{0.6} \left\{ \frac{1}{2} [2\sqrt{2} Y_2^1(\theta, \phi) \sqrt{\frac{1}{2}} \{ \alpha(\xi_1) \beta(\xi_2) + \alpha(\xi_2) \beta(\xi_1) \}] - 2Y_2^2(\theta, \phi) \beta(\xi_1) \beta(\xi_2) \right\} \right\}$$

$$= -3\hbar^2 \left\{ \left\{ \sqrt{0.1} Y_2^0 \alpha(\xi_1) \alpha(\xi_2) - \sqrt{0.3} Y_2^1(\theta, \phi) \left\{ \sqrt{\frac{1}{2}} (\alpha(\xi_1) \beta(\xi_2) + \alpha(\xi_2) \beta(\xi_1)) \right. \right. \right.$$

$$\left. \left. + \sqrt{0.6} Y_2^2(\theta, \phi) \beta(\xi_1) \beta(\xi_2) \right\} \right\}$$

$$= -3\hbar^2 F_{21,11}(\theta, \phi, \xi_1, \xi_2). \quad (103)$$

Finally in the tensor operator term we recall that

$$\hat{T}_{12} F_{01,11}(\theta, \phi, \xi_1, \xi_2) = \left(\frac{1}{4} \hbar^2 \right) \sqrt{8} F_{21,11}(\theta, \phi, \xi_1, \xi_2) \quad (87)$$

and

$$\hat{T}_{12} F_{21,11} = \left(\frac{1}{4} \hbar^2 \right) \left\{ \sqrt{8} F_{01,11} - 2F_{21,11} \right\} \quad (89)$$

So now we can reduce all the integrals to one dimensional quadratures as we integrate over the angles θ and ϕ and sum over $\xi_1 \xi_2 \eta_1 \eta_2$. If we ignore the tensor term for the moment we have for the "diagonal" terms

$$\begin{aligned} & \langle \psi_{01,11} | \left\{ \frac{-\hbar^2}{2\mu} \nabla^2 + V_c(r) + V_{LS}(r) [\kappa] \left\{ \frac{1}{2} \vec{l} \cdot (\vec{s}_1 + \vec{s}_2) \right\} \right\} | \psi_{01,11} \rangle \\ &= \int_0^\infty r^2 dr R_0(r) \left[\frac{-\hbar^2}{2\mu} \right] \left\{ \frac{d^2}{dr^2} R_0(r) + \frac{2}{r} \frac{d}{dr} R_0(r) \right\} \\ & \quad + \int_0^\infty r^2 dr R_0(r) \{ V_c(r) + V_{LS}(r) [0] \} R_0(r) \end{aligned} \quad (104)$$

and

$$\begin{aligned} & \langle \psi_{21,11} | \left\{ \frac{-\hbar^2}{2\mu} \nabla^2 + V_c(r) + V_{LS}(r) [\kappa] \left\{ \frac{1}{2} \vec{l} \cdot (\vec{s}_1 + \vec{s}_2) \right\} \right\} | \psi_{21,11} \rangle \\ &= \int_0^\infty r^2 dr R_2(r) \left[\frac{-\hbar^2}{2\mu} \right] \left\{ \frac{d^2}{dr^2} R_2(r) + \frac{2}{r} \frac{d}{dr} R_2(r) - \frac{2(2+1)}{r^2} R_2(r) \right\} \\ & \quad + \int_0^\infty r^2 dr R_2(r) \{ V_c(r) + V_{LS}(r) [-3] \} R_2(r) \end{aligned} \quad (105)$$

as $\kappa = 2/\hbar^2$ and for the "cross terms"

$$\langle \psi_{01,11} | \left\{ \frac{-\hbar^2}{2\mu} \nabla^2 + V_c(r) + V_{LS}(r) [\kappa] \left\{ \frac{1}{2} \vec{l} \cdot (\vec{s}_1 + \vec{s}_2) \right\} \right\} | \psi_{21,11} \rangle = 0 \quad (106)$$

$$\langle \psi_{21,11} | \left\{ \frac{-\hbar^2}{2\mu} \nabla^2 + V_c(r) + V_{LS}(r) [\kappa] \left\{ \frac{1}{2} \vec{l} \cdot (\vec{s}_1 + \vec{s}_2) \right\} \right\} | \psi_{01,11} \rangle = 0 \quad (107)$$

Since the cross terms all vanish this expectation value (*in which we have ignored the tensor term*) is simply

$$\langle \Psi | \hat{H} | \Psi \rangle = \cos^2 \omega [\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle] + \sin^2 \omega [\langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle] \quad (108)$$

and so for any choice of $a_0, b_0, \dots, a_2, b_2, \dots$ the minimum obtained setting

$$\frac{\partial}{\partial \omega} \langle \Psi | \hat{H} | \Psi \rangle = -\sin(2\omega) [\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle - \langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle] = 0$$

has the solution that $\omega = 0$ or $\omega = \frac{1}{2}\pi$ depending on which of the two factors $\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle$ or $\langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle$ is smaller. In other words, *neglecting the tensor term*, there is no mixing of $l=0$ and $l=2$.

The integrals involving the tensor operator for the diagonal terms are

$$\langle \psi_{01,11} | V_T(r) [\lambda] \hat{T}_{12} | \psi_{01,11} \rangle = 0; \quad (109)$$

$$\begin{aligned} \langle \psi_{21,11} | V_T(r) [\lambda] \hat{T}_{12} | \psi_{21,11} \rangle &= [4/\hbar^2] [4\hbar^2] [-2] \int_0^\infty r^2 dr R_2(r) V_T(r) R_2(r) \\ &= -2 \int_0^\infty r^2 dr R_2(r; a_2, b_2, \dots) V_T(r) R_2(r; a_2, b_2, \dots) \end{aligned} \quad (110)$$

as $\lambda = 4/\hbar^2$ and for the "cross terms"

$$\begin{aligned} \langle \psi_{21,11} | V_T(r) [\lambda] \hat{T}_{12} | \psi_{01,11} \rangle &= [4/\hbar^2] [\sqrt{2}\hbar^2] \int_0^\infty r^2 dr R_2(r) V_T(r) R_0(r) \\ &= \sqrt{8} \int_0^\infty r^2 dr R_2(r; a_2, b_2, \dots) V_T(r) R_0(r; a_0, b_0, \dots) \end{aligned} \quad (111)$$

$$\begin{aligned} \langle \psi_{01,11} | V_T(r) [\lambda] \hat{T}_{12} | \psi_{21,11} \rangle &= [4/\hbar^2] [4\hbar^2] [\sqrt{8}] \int_0^\infty r^2 dr R_2(r) V_T(r) R_2(r) \\ &= \sqrt{8} \int_0^\infty r^2 dr R_0(r; a_0, b_0, \dots) V_T(r) R_2(r; a_2, b_2, \dots) . \end{aligned} \quad (112)$$

Thus the matrix elements of the total Hamiltonian are:

$$\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle = \quad (113)$$

$$\int_0^\infty r^2 dr R_0(r) \left\{ \left[\frac{-\hbar^2}{2\mu} \right] \left\{ \frac{d^2}{dr^2} R_0(r) + \frac{2}{r} \frac{d}{dr} R_0(r) \right\} + V_c(r) \right\} R_0(r)$$

$$\langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle = \quad (114)$$

$$\begin{aligned} &= \int_0^\infty r^2 dr R_2(r) \left\{ \left[\frac{-\hbar^2}{2\mu} \right] \left\{ \frac{d^2}{dr^2} R_2(r) + \frac{2}{r} \frac{d}{dr} R_2(r) - \frac{2(2+1)}{r^2} R_2(r) \right\} \right. \\ &\quad \left. + \{ V_c(r) + V_{LS}(r) [-3] - 2V_T(r) \} \right\} R_2(r) \end{aligned}$$

and

$$\begin{aligned} &\left. \begin{aligned} \langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle \\ \langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle \end{aligned} \right\} = \sqrt{8} \int_0^\infty r^2 dr \begin{Bmatrix} R_0(r) \\ R_2(r) \end{Bmatrix} V_T(r) \begin{Bmatrix} R_2(r) \\ R_0(r) \end{Bmatrix} \quad (115) \end{aligned}$$

Of course the radial functions and thus the radial integrals are functions of the variational parameters. The expectation value of the Hamiltonian

$$\begin{aligned}
 \langle \Psi | \hat{H} | \Psi \rangle &= \cos^2 \omega [\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle] + \sin^2 \omega [\langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle] \\
 &\quad + \sin(\omega) \cos(\omega) [\langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle + \langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle] \\
 &= [\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle] - \sin^2 \omega [\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle - \langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle] \\
 &\quad + \sin(\omega) \cos(\omega) [\langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle + \langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle] \quad (116)
 \end{aligned}$$

is therefore a function of these variational parameters. It is also a function of the "mixing angle ω ". Thus

$$\langle \Psi | \hat{H} | \Psi \rangle = F(\omega; a_0, b_0, \dots, a_2, b_2, \dots) \quad (117)$$

Clearly, the function F depends upon the chosen parametric forms for the radial functions. Presumably the parameters can be optimized by

$$\frac{\partial}{\partial \lambda_i} F(\omega; a_0, b_0, \dots, a_2, b_2, \dots) = 0 \quad (118)$$

for $\lambda_i = \{\omega, a_0, b_0, \dots, a_2, b_2, \dots\}$.

In particular, for any choice of the remaining parameters

$$\begin{aligned}
 \frac{\partial}{\partial \omega} \langle \Psi | \hat{H} | \Psi \rangle &= - \sin(2\omega) [\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle - \langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle] \\
 &\quad + \cos(2\omega) [\langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle + \langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle] = 0
 \end{aligned}$$

so that the optimum choice of ω is:

$$\tan(2\omega) = \frac{[\langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle + \langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle]}{[\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle - \langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle]} \quad (119)$$

In principle we can solve (119) for the optimum value of $\omega(a_0, b_0, \dots, a_2, b_2, \dots)$ and substitute this particular ω back into (116) and optimize the resulting expression with respect to $a_0, b_0, \dots, a_2, b_2, \dots$. The arithmetic is rather arduous and so assuming $2\omega \ll 1$, $\tan(2\omega) \simeq 2\omega$, we have approximately

$$\omega \simeq \frac{\frac{1}{2} [\langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle + \langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle]}{[\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle - \langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle]} \quad (120)$$

whence

$$\langle \Psi | \hat{H} | \Psi \rangle = \frac{\{ \frac{1}{2} [\langle \psi_{21,11} | \hat{H} | \psi_{01,11} \rangle + \langle \psi_{01,11} | \hat{H} | \psi_{21,11} \rangle] \}^2}{[\langle \psi_{01,11} | \hat{H} | \psi_{01,11} \rangle - \langle \psi_{21,11} | \hat{H} | \psi_{21,11} \rangle]} \quad (121)$$

This approximate result is still a function of the variational parameters $a_0, b_0, \dots, a_2, b_2 \dots$ but because of the approximation (120) it cannot be guaranteed to be an upper bound to the exact ground state energy. Of course we could proceed without any approximation and solve (119) exactly for $\omega(a_0, b_0, \dots, a_2, b_2, \dots)$, substitute the result into (116) and minimize the resulting expression over the remaining parameter space $a_0, b_0, \dots, a_2, b_2 \dots$ to obtain a true upper bound to the exact ground state energy. On the other hand, notwithstanding the fact that (121) no longer can guarantee an upper bound, one still could search the remaining parameter space $a_0, b_0, \dots, a_2, b_2 \dots$ in order to minimize the right hand side of (121).

Minimizing (116) [or (121)] with respect to the functions $R_0(r; a_0, b_0, \dots)$ and $R_2(r; a_2, b_2, \dots)$ should yield a good value for the ground state energy. The form of these radial functions must be chosen so as to take into account the hard core potential. Thus, for both $l=0$ and $l=2$ the radial wave function is of the form

$$R_l(r; a, b, \dots) = \begin{cases} 0, & r \leq r_c \\ f_l(r; a_l, b_l, \dots) & r \geq r_c \end{cases} \quad (122)$$

where $f_l(r; a_l, b_l, \dots) = 0$ at $r = r_c$ and $f_l(r; a_l, b_l, \dots) \rightarrow 0$ as $r \rightarrow \infty$.

From this point on there is no end to the possible choices one could make for the variational functions. For instance

$$f_l(r; a, b, k) = N(a, b, k) (r - r_c)^k \{1 - e^{-a(r-r_c)}\} e^{-b(r-r_c)} \quad (123)$$

where N is a normalization factor and a, b, k are the variational parameters.

Assuming we have optimized the energy and found a reasonably good ground state wavefunction Ψ_0 , we then can calculate the magnetic moment and the electric quadrupole moment of the deuteron as follows.

The magnetic moment operator is an observable defined as

$$\begin{aligned} \vec{\mu} = & (\mu_N/\hbar) \{ [(\frac{1}{2}\hat{I}_1 + \hat{i}_{1z})g_p + (\frac{1}{2}\hat{I}_1 - \hat{i}_{1z})g_n] \vec{s}_1 + (\frac{1}{2}\hat{I}_1 + \hat{i}_{1z}) \hat{l}_1 \} \\ & + (\mu_N/\hbar) \{ [(\frac{1}{2}\hat{I}_2 + \hat{i}_{2z})g_p + (\frac{1}{2}\hat{I}_2 - \hat{i}_{2z})g_n] \vec{s}_2 + (\frac{1}{2}\hat{I}_2 + \hat{i}_{2z}) \hat{l}_2 \} \end{aligned} \quad (124)$$

and recognizing that $\hat{l}_1 = \hat{l}_2 = \frac{1}{2} \hat{I}$ [see (59)] we have

$$\begin{aligned} \vec{\mu} = & (\mu_N/\hbar) \{ [(\frac{1}{2}\hat{I}_1 + \hat{i}_{1z})g_p + (\frac{1}{2}\hat{I}_1 - \hat{i}_{1z})g_n] \vec{s}_1 + (\frac{1}{2}\hat{I}_1 + \hat{i}_{1z}) [\frac{1}{2} \hat{I}] \} \\ & + (\mu_N/\hbar) \{ [(\frac{1}{2}\hat{I}_2 + \hat{i}_{2z})g_p + (\frac{1}{2}\hat{I}_2 - \hat{i}_{2z})g_n] \vec{s}_2 + (\frac{1}{2}\hat{I}_2 + \hat{i}_{2z}) [\frac{1}{2} \hat{I}] \} \end{aligned} \quad (125)$$

Here g_p and g_n are the "gyromagnetic ratios. The empirical values for these ratios are $g_p = 5.58$ and $g_n = -3.83$. $\mu_N = [\frac{e\hbar}{2mc}]$ in cgs units. By definition the "intrinsic magnetic moments" (see Elton) are

$$\mu_p = \frac{1}{2} g_p \mu_N \quad \text{and} \quad \mu_n = \frac{1}{2} g_n \mu_N. \quad (126)$$

Note that the magnetic moment observable (125) depends on the isospin operators. In particular, we note that

$$[\frac{1}{2}\hat{I} + \hat{i}_z] |p\rangle = 1 |p\rangle; \quad [\frac{1}{2}\hat{I} + \hat{i}_z] |n\rangle = |\emptyset\rangle \quad (127)$$

and

$$[\frac{1}{2}\hat{I} - \hat{i}_z] |p\rangle = |\emptyset\rangle; \quad [\frac{1}{2}\hat{I} - \hat{i}_z] |n\rangle = 1 |n\rangle$$

so, for instance, the orbital angular momentum operator will only be operative only if the nucleon (i.e. a particle labeled 1 or 2) is in the proton state, i.e. $m_i = \frac{1}{2}$.

The magnetic moment of the deuteron is, by definition, the expectation value of the magnetic moment operator in the $J=1, M_J=1$ state.

$$\vec{\mu} = \langle \Psi_0 | \vec{\mu} | \Psi_0 \rangle \quad (128)$$

where Ψ_0 is the optimized trial function for the ground state. Indeed

$$\vec{\mu} = \cos^2\omega \langle \psi_{01,11} | \vec{\mu} | \psi_{01,11} \rangle + \sin^2\omega \langle \psi_{21,11} | \vec{\mu} | \psi_{21,11} \rangle \quad (129)$$

where we have used the fact that the "cross terms" between the $l=0$ and $l=2$ functions vanish.

We now carry out the algebra of the operator $\hat{\mu}$ on $\psi_{01,11}$ and $\psi_{21,11}$. We can bury the radial wavefunctions for the time being realizing that in the final expectation value they will simply contribute a factor of 1 as we integrate the normalized radial function over r . Thus we consider:

$$\hat{\mu} \{ Y_0^0(\theta, \phi) [|\alpha\rangle_1 |\alpha\rangle_2] \} \{ \frac{1}{\sqrt{2}} [|p\rangle_1 |n\rangle_2 - |p\rangle_2 |n\rangle_1] \} \quad (129)$$

There are two terms. We consider them one by one. The first is

$$\frac{1}{\sqrt{2}} \hat{\mu} \{ (Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |p\rangle_1 |n\rangle_2) =$$

$$(\mu_N/\hbar) \frac{1}{\sqrt{2}} \{ [g_p + 0] \hat{s}_1 + \frac{1}{2} \hat{l} + [0 + g_n] \hat{s}_2 + 0 \hat{l} \} (Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |p\rangle_1 |n\rangle_2)$$

and the second is

$$\frac{1}{\sqrt{2}} \hat{\mu} \{ (-Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |n\rangle_1 |p\rangle_2) =$$

$$(\mu_N/\hbar) \frac{1}{\sqrt{2}} \{ [0 + g_n] \hat{s}_1 + 0 \hat{l} + [g_p + 0] \hat{s}_2 + \frac{1}{2} \hat{l} \} (-Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |n\rangle_1 |p\rangle_2)$$

so that adding the results we find

$$\hat{\mu} \{ Y_0^0(\theta, \phi) [|\alpha\rangle_1 |\alpha\rangle_2] \} \{ \frac{1}{\sqrt{2}} [|p\rangle_1 |n\rangle_2 - |p\rangle_2 |n\rangle_1] \}$$

$$= (\mu_N/\hbar) \frac{1}{\sqrt{2}} \{ [g_p \hat{s}_1 + g_n \hat{s}_2] Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |p\rangle_1 |n\rangle_2$$

$$- [g_n \hat{s}_1 + g_p \hat{s}_2] Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |n\rangle_1 |p\rangle_2 \} \quad (130)$$

where we recognize that $\hat{l}_i Y_0^0 \equiv 0$ for all components $i=x,y,z$. Now preparing to do the inner product we have

$$\int_0^{2\pi} d\phi \int_0^{2\pi} \sin\theta d\theta Y_0^{0*} \langle \alpha | \langle \alpha | \{ \frac{1}{\sqrt{2}} [\langle p | \langle n | - \langle n | \langle p |] \}$$

$$(\mu_N/\hbar) \frac{1}{\sqrt{2}} \{ [g_p \hat{s}_1 + g_n \hat{s}_2] Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |p\rangle_1 |n\rangle_2$$

$$- [g_n \hat{s}_1 + g_p \hat{s}_2] Y_0^0 |\alpha\rangle_1 |\alpha\rangle_2 |n\rangle_1 |p\rangle_2 \}$$

$$= \frac{1}{2} (\mu_N/\hbar) \{ g_p \langle \alpha | \hat{s}_1 | \alpha \rangle + g_n \langle \alpha | \hat{s}_2 | \alpha \rangle + g_n \langle \alpha | \hat{s}_1 | \alpha \rangle + g_p \langle \alpha | \hat{s}_2 | \alpha \rangle \} \quad (131)$$

where we have carried out the spin and isospin inner products in the formal Dirac notation using

$$\langle p|p\rangle = \sum_{\eta} \langle p|\eta\rangle \langle \eta|p\rangle = 1; \quad \langle \alpha|\alpha\rangle = \sum_{\xi} \langle \alpha|\xi\rangle \langle \xi|\alpha\rangle = 1$$

and so forth so that in addition to $\langle p|p\rangle = 1$ and $\langle \alpha|\alpha\rangle = 1$ we have $\langle p|n\rangle=0$, $\langle n|p\rangle=0$, $\langle n|n\rangle=1$, $\langle \alpha|\beta\rangle=0$, $\langle \beta|\alpha\rangle=0$, and $\langle \beta|\beta\rangle=1$. Thus

$$\begin{aligned} \langle \psi_{01,11} | \vec{\mu} | \psi_{01,11} \rangle &= (\mu_N/\hbar) \{ (g_p + g_n) \langle \alpha | \vec{s} | \alpha \rangle \} \\ &= \frac{1}{2} \mu_N (g_p + g_n) e_z \end{aligned} \quad (132)$$

since

$$\langle \alpha | \vec{s} | \alpha \rangle = 0e_x + 0e_y + \frac{1}{2}\hbar e_z. \quad (133)$$

Indeed, considering only the $l=0$ term, the only contributions to the magnetic moment of the deuteron are the individual magnetic moments of the proton and neutron which add together to give a non-vanishing z component. The x and y components do vanish. As the texts point out this is not the correct result -- close, but not correct. Thus we must proceed to calculate the second term in (129) as a correction to (132).

Now we must evaluate $\langle \psi_{21,11} | \vec{\mu} | \psi_{21,11} \rangle$. There are three terms in $F_{21,11}$ which we must consider. Moreover, as we take the inner products the cross terms vanish so that what would appear to be nine scalar products (integrals over θ and ϕ) are actually only three non-vanishing terms. The first term $M_S = 1$ is analogous (129) which we just did for $F_{01,11}$ except for the Clebsch Gordon coefficient $C_2^0 = \sqrt{0.1}$. Therefore, carrying out the same steps we did above we find

$$\begin{aligned} & [C_2^0 Y_2^0]^* {}_1\langle \alpha | {}_2\langle \alpha | \{ \sqrt{\frac{1}{2}} \{ {}_1\langle p | {}_2\langle n | - {}_1\langle n | {}_2\langle p | \} \\ & (\mu_N/\hbar) \sqrt{\frac{1}{2}} \{ [g_p \vec{s}_1 + g_n \vec{s}_2] [C_0^0 Y_0^0] |\alpha\rangle_1 |\alpha\rangle_2 |p\rangle_1 |n\rangle_2 \\ & \quad - [g_n \vec{s}_1 + g_p \vec{s}_2] [C_2^0 Y_2^0] |\alpha\rangle_1 |\alpha\rangle_2 |n\rangle_1 |p\rangle_2 \} \\ & = \frac{1}{2} (\mu_N/\hbar) \{ g_p \langle \alpha | \vec{s}_1 | \alpha \rangle + g_n \langle \alpha | \vec{s}_2 | \alpha \rangle + g_n \langle \alpha | \vec{s}_1 | \alpha \rangle + g_p \langle \alpha | \vec{s}_2 | \alpha \rangle \} |C_0^0 Y_0^0|^2 \\ & = (\mu_N/\hbar) \{ (g_p + g_n) \langle \alpha | \vec{s}_1 | \alpha \rangle \} |C_2^0 Y_2^0|^2. \end{aligned} \quad (134)$$

Then doing the integrals over θ and ϕ we get for the first ($M_S=1$) term

$$(\mu_N/\hbar) \{ (g_p + g_n) \langle \alpha | \vec{s}_1 | \alpha \rangle |C_0^0|^2 \} = \mu_N \{ (g_p + g_n) (\frac{1}{2}) \} |C_2^0|^2 \quad (135)$$

The $M_S = -1$ term is similar to the $M_S = 1$ except that β replaces α and the orbital angular momentum $\vec{l} Y_2^2(\theta, \phi) \neq 0$. With $C_2^2 = \sqrt{0.6}$ we have

$$[C_2^2 Y_2^2]^* \langle \beta | \langle \beta | \{ \sqrt{\frac{1}{2}} \{ \langle p | \langle n | - \langle n | \langle p | \} \}$$

$$\begin{aligned} & (\mu_N/\hbar) \sqrt{\frac{1}{2}} \{ [g_p \vec{s}_1 + g_n \vec{s}_2 + \frac{1}{2} \vec{l}] [C_2^2 Y_2^2] |\beta\rangle_1 |\beta\rangle_2 |p\rangle_1 |n\rangle_2 \\ & \quad - [g_n \vec{s}_1 + g_p \vec{s}_2 + \frac{1}{2} \vec{l}] [C_2^2 Y_2^2] |\beta\rangle_1 |\beta\rangle_2 |n\rangle_1 |p\rangle_2 \} \\ &= \frac{1}{2} (\mu_N/\hbar) \{ [g_p \langle \beta | \vec{s}_1 | \beta \rangle + g_n \langle \beta | \vec{s}_2 | \beta \rangle \\ & \quad + g_n \langle \beta | \vec{s}_1 | \beta \rangle + g_p \langle \beta | \vec{s}_2 | \beta \rangle] |C_2^2 Y_2^2|^2 + |C_2^2|^2 (Y_2^{2*} \vec{l} Y_2^2) \} \\ &= (\mu_N/\hbar) \{ [(g_p + g_n) \langle \beta | \vec{s}_1 | \beta \rangle] |C_2^2 Y_0^0|^2 + \frac{1}{2} |C_2^2|^2 (Y_2^{2*} \vec{l} Y_2^2) \} \end{aligned}$$

and doing the integrals over θ and ϕ we get for the $M_S = -1$ term

$$\begin{aligned} & (\mu_N/\hbar) \{ [(g_p + g_n) \langle \beta | \vec{s}_1 | \beta \rangle] |C_2^2|^2 + \frac{1}{2} |C_2^2|^2 2\hbar e_z \} \\ &= \mu_N \{ (g_p + g_n) (-\frac{1}{2}) + 1 \} |C_2^2|^2. \quad (136) \end{aligned}$$

Finally we must do the $M_S = 0$ term. With $C_2^1 = -\sqrt{0.3}$,

$$\vec{\mu} [C_2^1 Y_2^1] \{ \sqrt{\frac{1}{2}} [|\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1] \} \{ \sqrt{\frac{1}{2}} [|p\rangle_1 |n\rangle_2 - |p\rangle_2 |n\rangle_1] \}$$

We look at the four terms individually

$$\frac{1}{2} \vec{\mu} \{ [C_2^1 Y_2^1] |\alpha\rangle_1 |\beta\rangle_2 |p\rangle_1 |n\rangle_2 = \quad (i)$$

$$(\mu_N/\hbar) \{ [g_p + 0] \vec{s}_1 + \frac{1}{2} \vec{l} + [0 + g_n] \vec{s}_2 + 0 \vec{l}_2 \} \{ [C_2^1 Y_2^1] |\alpha\rangle_1 |\beta\rangle_2 |p\rangle_1 |n\rangle_2 \}$$

$$\frac{1}{2} \vec{\mu} \{ (-[C_2^1 Y_2^1] |\alpha\rangle_1 |\beta\rangle_2 |n\rangle_1 |p\rangle_2) = \quad (ii)$$

$$(\mu_N/\hbar) \{ [0 + g_n] \vec{s}_1 + 0 \vec{l}_1 + [g_p + 0] \vec{s}_2 + \frac{1}{2} \vec{l} \} \{ (-[C_2^1 Y_2^1] |\alpha\rangle_1 |\beta\rangle_2 |n\rangle_1 |p\rangle_2) \}$$

$$\frac{1}{2} \vec{\mu} \{ [C_2^1 Y_2^1] |\beta\rangle_1 |\alpha\rangle_2 |p\rangle_1 |n\rangle_2 = \quad (iii)$$

$$\frac{(\mu_N/\hbar) \{ [g_p + 0] \vec{s}_1 + \frac{1}{2} \vec{l}_1 + [0 + g_n] \vec{s}_2 + 0 \vec{l}_2 \} [C_2^1 Y_2^1] (|\beta\rangle_1 |\alpha\rangle_2 |p\rangle_1 |n\rangle_2)}{\hline}$$

$$\frac{1}{2} \vec{\mu} \{ -[C_2^1 Y_2^1] |\beta\rangle_1 |\alpha\rangle_2 |n\rangle_1 |p\rangle_2 = \quad (iv)$$

$$\frac{(\mu_N/\hbar) \{ [0 + g_n] \vec{s}_1 + 0 \vec{l}_1 + [g_p + 0] \vec{s}_2 + \frac{1}{2} \vec{l}_2 \} (-[C_2^1 Y_2^1] |\beta\rangle_1 |\alpha\rangle_2 |n\rangle_1 |p\rangle_2)}{\hline}$$

Adding (i) + (ii) + (iii) + iv) and then taking the inner product we have

$$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta$$

$$\{ [C_2^1 Y_2^1]^* \{ \frac{1}{\sqrt{2}} [{}_1\langle\alpha| {}_2\langle\beta| + {}_1\langle\beta| {}_2\langle\alpha|] \} \{ \frac{1}{\sqrt{2}} [{}_1\langle p| {}_2\langle n| - {}_1\langle n| {}_2\langle p|] \} \}$$

$$\vec{\mu} [C_2^1 Y_2^1] \{ \frac{1}{\sqrt{2}} [|\alpha\rangle_1 |\beta\rangle_2 + |\alpha\rangle_2 |\beta\rangle_1] \} \{ \frac{1}{\sqrt{2}} [|p\rangle_1 |n\rangle_2 - |p\rangle_2 |n\rangle_1] \}$$

$$= \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta$$

$$\frac{1}{4} (\mu_N/\hbar) \{ [g_p \langle\alpha| \vec{s}_1 |\alpha\rangle + g_n \langle\beta| \vec{s}_2 |\beta\rangle] |C_2^1 Y_2^1|^2 + |C_2^1|^2 (Y_2^{1*} \frac{1}{2} \vec{l}_1 Y_2^1)$$

$$+ g_n [\langle\alpha| \vec{s}_1 |\alpha\rangle + g_p \langle\beta| \vec{s}_2 |\beta\rangle] |C_2^1 Y_2^1|^2 + |C_2^1|^2 (Y_2^{1*} \frac{1}{2} \vec{l}_2 Y_2^1)$$

$$+ g_p [\langle\beta| \vec{s}_1 |\beta\rangle + g_n \langle\alpha| \vec{s}_2 |\alpha\rangle] |C_2^1 Y_2^1|^2 + |C_2^1|^2 (Y_2^{1*} \frac{1}{2} \vec{l}_1 Y_2^1)$$

$$+ g_n [\langle\beta| \vec{s}_1 |\beta\rangle + g_p \langle\alpha| \vec{s}_2 |\alpha\rangle] |C_2^1 Y_2^1|^2 + |C_2^1|^2 (Y_2^{1*} \frac{1}{2} \vec{l}_2 Y_2^1) \}$$

$$= (\mu_N/\hbar) |C_2^1|^2 \frac{1}{2} \hbar e_z = \mu_N \left(\frac{1}{2}\right) |C_2^1|^2 \quad (137)$$

Then the sum of (135), (136) and (137) gives the final result for

$$\langle \psi_{21,11} | \vec{\mu} | \psi_{21,11} \rangle =$$

$$= \mu_N \{ (g_p + g_n) \left(\frac{1}{2}\right) \} |C_2^0|^2 + \mu_N \{ (g_p + g_n) \left(-\frac{1}{2}\right) + 1 \} |C_2^2|^2 + \mu_N \left\{ \frac{1}{2} \right\} |C_2^1|^2$$

$$= \mu_N \{ (g_p + g_n) \left[\frac{1}{2} |C_2^0|^2 - \frac{1}{2} |C_2^2|^2 \right] + |C_2^2|^2 + \frac{1}{2} |C_2^1|^2 \} \quad (138)$$

Now using the values of the Clebsch Gordon coefficients $|C_2^0|^2 = 0.1$, $|C_2^1|^2 = 0.3$ and $|C_2^2|^2 = 0.6$ we have that $\frac{1}{2}|C_2^0|^2 - \frac{1}{2}|C_2^2|^2 = -\frac{1}{4}$ and $|C_2^2|^2 + \frac{1}{2}|C_2^1|^2 = \frac{3}{4}$. Thus we obtain

$$\begin{aligned}\langle \psi_{21,11} | \mu | \psi_{21,11} \rangle &= \mu_N (g_p + g_n) \left[\frac{1}{2}|C_2^0|^2 - \frac{1}{2}|C_2^2|^2 \right] + |C_2^2|^2 + \frac{1}{2}|C_2^1|^2 \\ &= -\frac{1}{4} \mu_N (g_p + g_n) + \frac{3}{4} \mu_N\end{aligned}\quad (139)$$

And finally the magnetic moment of the deuteron is

$$\begin{aligned}\langle \Psi_0 | \vec{\mu} | \Psi_0 \rangle &= \cos^2 \omega \langle \psi_{01,11} | \vec{\mu} | \psi_{01,11} \rangle + \sin^2 \omega \langle \psi_{21,11} | \vec{\mu} | \psi_{21,11} \rangle \\ &= \langle \psi_{01,11} | \vec{\mu} | \psi_{01,11} \rangle + \sin^2 \omega [\langle \psi_{21,11} | \vec{\mu} | \psi_{21,11} \rangle - \langle \psi_{01,11} | \vec{\mu} | \psi_{01,11} \rangle] \\ &= \mu_N \left(\frac{1}{2} (g_p + g_n) \right) + \sin^2 \omega \left[-\frac{3}{4} \mu_N (g_p + g_n) + \frac{3}{4} \mu_N \right] \\ &= \frac{1}{2} \mu_N (g_p + g_n) \left\{ 1 - \frac{3}{2} \sin^2 \omega \right\} + \frac{3}{4} \mu_N \sin^2 \omega \\ &= \mu_N \left[\left(\frac{1}{2} g_p + \frac{1}{2} g_n \right) \left\{ 1 - \frac{3}{2} \sin^2 \omega \right\} + \frac{3}{4} \sin^2 \omega \right] \\ &= \mu_N \left[(\mu_p + \mu_n) \left\{ 1 - \frac{3}{2} \sin^2 \omega \right\} + \frac{3}{4} \sin^2 \omega \right]\end{aligned}\quad (140)$$

which is equation (4.40) on page 90 in Elton's book. Indeed, in Elton's text $\mu_p = 2.7927$ and $\mu_n = -1.9131$ are dimensionless quantities equal to $\frac{1}{2}g_p$ and $\frac{1}{2}g_n$ respectively and all magnetic quantities are in units of μ_N , the nuclear magneton.

So the modification of the magnetic moment due to the tensor term arises in two places, reducing the spin contribution and giving rise to an orbital angular momentum contribution. The two corrections are of order of a 6% reduction in the spin contribution and a 3% contribution due to the orbital angular momentum. We did not replace $\sin^2 \omega$ by ω^2 , as clearly this is not necessary, and a priori it is not clear that ω is small -- although in fact it turns out that $\omega \simeq 0.2$ and so $\omega^2 \simeq 0.04$. We now consider the electric quadrupole moment of the deuteron.

The electric quadrupole moment is by definition

$$Q = \frac{1}{e} \int_0^\infty q^2 dq \int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi \, [3q^2 \cos^2\theta - q^2] \rho(\vec{q}) \quad (141)$$

where the charge density $\rho(\vec{q})$ is the expectation value of the charge density operator. Here \vec{q} is a point in space with spherical coordinates denoted q, θ, ϕ . Indeed, \vec{q} is a parameter in the operator -- or equally true there are a non-denumerably infinite number of such charge density operators, one for each point in space. Indeed, the operator is

$$\hat{\rho}(\vec{r}_1, \vec{r}_2, \hat{i}_{1z}, \hat{i}_{2z}; \vec{q}) = e \{ \delta(\vec{r}_1 - \vec{q}) [\frac{1}{2}(\hat{i}_1 + \hat{i}_{1z})] + \delta(\vec{r}_2 - \vec{q}) [\frac{1}{2}(\hat{i}_2 + \hat{i}_{2z})] \} \quad (142)$$

where 1 and 2 are the nucleon particle labels and the isotopic spin operators insure that only the proton (for which $m_i = +\frac{1}{2}$) and not the neutron (for which $m_i = -\frac{1}{2}$) contribute to the charge density. The charge density is thus given by the expectation value

$$\rho(\vec{q}) = \langle \Psi | \hat{\rho}(\vec{r}_1, \vec{r}_2, \hat{i}_{1z}, \hat{i}_{2z}; \vec{q}) | \Psi \rangle \quad (143)$$

The expectation value involves the scalar product

$$\int_0^\infty r^2 dr \int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi \sum_{\xi_1} \sum_{\xi_2} \sum_{\eta_1} \sum_{\eta_2} \Psi_0(\vec{r}, \xi_1 \xi_2 \eta_1 \eta_2) \hat{\rho}(\dots; \vec{q}) \Psi_0(r, \xi_1 \xi_2 \eta_1 \eta_2) \quad (144)$$

We begin by noting the inner product over the isospin singlet state is:

$$[\frac{1}{\sqrt{2}}(|p\rangle_1 |n\rangle_2 - |n\rangle_1 |p\rangle_2)] \hat{\rho}(\vec{q}) [\frac{1}{\sqrt{2}}(|p\rangle_1 |n\rangle_2 - |n\rangle_1 |p\rangle_2)]$$

$$= \frac{1}{2} e \{ \delta(\vec{r}_1 - \vec{q}) + \delta(\vec{r}_2 - \vec{q}) \}$$

$$= \frac{1}{2} e \{ \delta(-\frac{1}{2}\vec{r} - \vec{q}) + \delta(\frac{1}{2}\vec{r} - \vec{q}) \}$$

$$= \frac{1}{2} e \{ 8 [\delta(\vec{r} + 2\vec{q}) + \delta(\vec{r} - 2\vec{q})] \}$$

where $8 = 1/[\frac{1}{2}]^3$.

★ We rewrite \vec{r}_1 and \vec{r}_2 in terms
 ★ of \vec{r} and \vec{R} , but understand $\vec{R}=\vec{0}$
 ★ Note that the 3 dimensional
 ★ $\delta(\lambda[\vec{r} - \vec{a}]) = \delta(\vec{r} - \vec{a})/\lambda^3$ and
 ★ $\delta(-\vec{r} - \vec{a}) = \delta(\vec{r} + \vec{a})$
 ★*****

Moreover since the charge density operator does not depend on the "ordinary" spin observables, the various terms which occur in Ψ are "diagonal" in the spin states -- i.e. they must "match up" in the bra and kets. All that remains then is to do the spatial integrals which [you would think] should be trivial because of the delta functions. However, we must be careful as the arguments of the delta functions are such that the vectors between the particles are twice the length of the distance to the point where the proton is. Indeed a typical term will involve

$$\int_0^\infty r^2 dr \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta R(r) Y_l^m(\theta, \phi)^* \hat{\rho}(\vec{q}) R(r) Y_l^m(\theta, \phi)$$

$$= \frac{1}{2} \cdot 8 \cdot e |R(2q)|^2 |Y_l^m(\pi - \theta_q, \pi + \phi_q)|^2 + |R(2q)|^2 |Y_l^m(\theta_q, \phi_q)|^2$$

$$= 8e |R(2q)|^2 |Y_l^m(\theta_q, \phi_q)|^2 \quad (145)$$

which is a function of the coordinates of the position \vec{q} . The two terms arise from the integration over the delta functions with $\vec{r} = -2\vec{q}$ in the first term and $\vec{r} = 2\vec{q}$ in the second term. Here we have recognized that the even spherical harmonics have even parity and so the two terms in the second line of (145) are equal for both the $l=0$ and the $l=2$ cases. Now we understand that the wavefunction to be used in the calculation is $\Psi_0 = \cos\omega \psi_{01,11} + \sin\omega \psi_{21,11}$ where $\psi_{01,11}$ and $\psi_{21,11}$ are given by (90) and (91) with the parameters having been optimized by the variational calculation of the ground state energy. We have terms

$$\rho(\vec{q}) = \cos^2\omega \langle \psi_{01,11} | \hat{\rho} | \psi_{01,11} \rangle + \sin^2\omega \langle \psi_{21,11} | \hat{\rho} | \psi_{21,11} \rangle +$$

$$\sin\omega\cos\omega [\langle \psi_{01,11} | \hat{\rho} | \psi_{21,11} \rangle + \langle \psi_{21,11} | \hat{\rho} | \psi_{01,11} \rangle]$$

$$= 8e \{ \cos^2\omega [|R_0(2q)|^2 |Y_0^0(\theta_q, \phi_q)|^2] \quad \begin{array}{l} \star \text{ from the "diagonal" } \psi_{01,11} \\ \star \text{ term} \end{array}$$

$$+ \sin^2\omega [|R_2(2q)|^2 \{ 0.1 |Y_2^0(\theta_q, \phi_q)|^2 \quad \begin{array}{l} \star \text{ from the "diagonal" } \psi_{21,11} \\ \star \text{ term; orthonormality of} \end{array}$$

$$+ 0.3 |Y_2^1(\theta_q, \phi_q)|^2 + 0.6 |Y_2^2(\theta_q, \phi_q)|^2 \}] \quad \begin{array}{l} \star \text{ spin functions leads to} \\ \star \text{ this sum of } |\dots|^2 \end{array}$$

$$+ \sin\omega\cos\omega [\sqrt{0.1} [R_0^*(2q)R_2(2q) Y_0^0(\theta_q, \phi_q)^* Y_2^0(\theta_q, \phi_q) \quad \begin{array}{l} \star \text{ cross term} \\ \star \text{ from the } \alpha_1\alpha_2 \\ \star \text{ spin factors.} \end{array}$$

$$+ R_2(2q)^* R_0(2q) Y_2^0(\theta_q, \phi_q)^* Y_0^0(\theta_q, \phi_q)] \} \quad (146)$$

where we recognize 0.1, 0.3, and 0.6 as the squares of the CG coefficients. Inserting the explicit expressions for the absolute squares of the spherical harmonics we find that the charge density

$$\begin{aligned}
 \rho(\vec{q}) &= 8e \left\{ \cos^2\omega \left[|R_0(2q)|^2 \frac{1}{4\pi} \right] \right. \\
 &+ \sin^2\omega |R_2(2q)|^2 \frac{1}{32\pi} \left\{ [3\cos^2\theta_q - 1]^2 + 18\sin^2\theta_q \cos^2\theta_q + 9\sin^4\theta_q \right\} \\
 &+ \sin\omega\cos\omega \left\{ \sqrt{0.1} \left[R_0(2q)R_2(2q) + R_2(2q)R_0(2q) \left[\frac{\sqrt{5}}{8\pi} \right] (3\cos^2\theta_q - 1) \right] \right\} \\
 &= 8e \left\{ \cos^2\omega \left[|R_0(2q)|^2 \frac{1}{4\pi} \right] \right. \\
 &+ \sin^2\omega |R_2(2q)|^2 \left\{ \frac{1}{32\pi} \{10 - 6\cos^2\theta_q\} \right. \\
 &+ \left. \sin\omega\cos\omega \left\{ \sqrt{0.1} \left[R_0(2q)R_2(2q) + R_2(2q)R_0(2q) \left[\frac{\sqrt{5}}{8\pi} \right] (3\cos^2\theta_q - 1) \right] \right\} \right\}
 \end{aligned} \tag{147}$$

where we have noted that

$$\begin{aligned}
 &9\cos^2\theta_q (1 - \sin^2\theta_q) - 6\cos^2\theta_q + 1 + 18\sin^2\theta_q \cos^2\theta_q + 9\sin^2\theta_q (1 - \cos^2\theta_q) \\
 &= 9 + 1 - 6\cos^2\theta_q = 10 - 6\cos^2\theta_q.
 \end{aligned} \tag{148}$$

First and foremost, we see that the overall charge density is not spherically symmetric. The first term ($l=0$ arising from $\psi_{01,11}$) is, by itself, spherically symmetric and as such does not contribute to the electric quadrupole moment. The next term ($l=2$ arising from $\psi_{21,11}$) is an oblate (hamburger bun) spheroid and the third term (the cross term) is a prolate (hot dog bun) spheroid. It is precisely the fact that the charge distribution is not spherically symmetric that the deuteron has an electric quadrupole moment.

Now we must evaluate

$$\begin{aligned}
 Q &= \frac{8e}{e} \int_0^\infty q^2 dq \int_0^\pi \sin\theta_q \int_0^{2\pi} d\phi_q [3\cos^2\theta_q - 1] q^2 \left\{ \cos^2\omega \left[|R_0(2q)|^2 \left[\frac{1}{4\pi} \right] \right. \right. \\
 &+ \sin^2\omega |R_2(2q)|^2 \left[\frac{1}{32\pi} \{10 - 6\cos^2\theta_q\} \right. \\
 &+ \left. \left. \sin\omega\cos\omega \left\{ \sqrt{0.1} \left[R_0(2q)R_2(2q) + R_2(2q)R_0(2q) \left[\frac{\sqrt{5}}{8\pi} \right] (3\cos^2\theta_q - 1) \right] \right\} \right] \right\}
 \end{aligned}$$

We let the new dummy variables of integration be $r = 2q$ and thus arrive at the expression given in Elton, for indeed

$$q = \frac{1}{2}r \Rightarrow q^2 dq = \left[\frac{1}{2}\right]^3 r^2 dr \quad \text{and} \quad q^2 = \left[\frac{1}{2}\right]^2 r^2$$

Thus we need to evaluate

$$Q = \frac{1}{4} \int_0^\infty r^2 dr \int_0^\pi \sin\theta \int_0^{2\pi} d\phi \left[3\cos^2\theta_q - 1 \right] r^2 \left\{ \cos^2\omega \left[|R_0(r)|^2 \frac{1}{4\pi} \right] \right. \\ \left. + \sin^2\omega |R_2(r)|^2 \left\{ \frac{1}{32\pi} (10 - 6\cos^2\theta_q) \right\} \right. \\ \left. + \sin\omega\cos\omega \left[\sqrt{0.1} \{ R_0(r)R_2(r) + R_2(r)R_0(r) \} \left[-\frac{\sqrt{5}}{8\pi} \right] (3\cos^2\theta_q - 1) \right] \right\} \quad (149)$$

which is how Elton get the factor of $\frac{1}{4}$. Evaluating the integrals we have

$$Q = \frac{1}{4} \left\{ 0 + \sin^2\omega \left[\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi (3\cos^2\theta - 1)(10 - 6\cos^2\theta) \right] \right. \\ \left. \times \frac{1}{32\pi} \int_0^\infty r^4 dr |R_2(r)|^2 \right. \\ \left. + [\sqrt{0.1}] \sin\omega\cos\omega \left[\int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi (3\cos^2\theta - 1)(3\cos^2\theta - 1) \right] \right. \\ \left. \times \frac{\sqrt{5}}{8\pi} \int_0^\infty r^4 dr \{ R_0^*(r) R_2(r) + R_2^*(r) R_0(r) \} \right\}$$

Therefore the electric quadrupole moment of the deuteron is

$$Q = -\frac{1}{20} \int_0^\infty r^4 dr |R_2(r)|^2 + \\ + \frac{1}{2\sqrt{50}} \int_0^\infty r^4 dr \{ R_0(r)^* R_2(r) + R_2(r)^* R_0(r) \}$$

which (for real radial functions) is the result on page 89 in Elton. Note that in Elton $R_0(r) \equiv u(r)/r$ and $R_2(r) \equiv v(r)/r$. Once we have found the parameters in the radial functions by optimizing the ground state energy we are able to find the electric quadrupole moment.