J. Condensed Matter Nucl. Sci. 34 (2021) 110–131

Research Article

Reduction of the HD/^{3}He Phonon–Nuclear Matrix Element

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Abstract

In the previous work, a relativistic phonon–nuclear interaction was found which mediates transitions between internal nuclear states when a phonon is exchanged. We are of the opinion that this interaction provides a foundation for many of the anomalies reported in experiments in Condensed Matter Nuclear Science. In this work, we report progress toward the development of an approximate calculation of the phonon–nuclear coupling matrix element for HD/^{3}He transitions. A construction consistent with the generalized Pauli principle is given for the dominant ^{2}S configuration of the ^{3}He ground state, and for four molecular HD nuclear wave functions with one unit of angular momentum, which are coupled to consistent with the selection rules for the interaction. A reduction of the spin, isospin, and angular momentum components of the matrix elements was carried out using a brute force Mathematica calculation. With these results it becomes possible to develop an evaluation of the radial integrals needed for a quantification of the phonon–nuclear matrix elements.

Keywords: Phonon-nuclear interaction, HD/^{3}He transition, theoretical models, spin and isospin reduction, phonon-nuclear matrix element

1. Introduction

For excess heat in PdD we have proposed that the first step of the coherent mechanism involves excitation transfer where the 24 MeV associated with the D_2/^{4}He transition is transferred to a reasonably stable highly excited state in a nucleus that makes up the surrounding lattice [1]. To model this process we require an estimate for the associated phonon–nuclear matrix element. Some years ago following the identification of the relativistic phonon–nuclear interaction, an attempt was made to evaluate the matrix element making use of a Pauli reduction [2]. Since that time it became understood that a much better approach would be to focus on the phonon–nuclear interaction [3], and to develop matrix element calculations on a standard footing much like other matrix elements. In support of this effort, a nonrelativistic reduction of the relativistic phonon–nuclear interaction has been reported in the special case of the long range one-pion exchange potential based on pseudovector coupling [4]. This interaction should play an important role in models based on the chiral effective field theory potentials currently in use in nuclear physics [5–7]. It should

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also provide us with a tool with which we can begin developing approximate estimates for some of the important phonon–nuclear interaction matrix elements.

Due to issues involved in the Pauli reduction, we are motivated to develop a new calculation for the $D_2/^4He$ phonon–nuclear interaction matrix element. Such a calculation is a bit complicated due to it being a 4-body problem. A similar problem that is simpler is the calculation of the $HD/^3He$ phonon–nuclear matrix element, which involves working with a 3-body problem. The $HD/^3He$ transition is important in its own right, as it would be involved in the first step for excess heat production in light water experiments [1]. If excitation transfer of the large 24 MeV quantum associated with the $D_2/^4He$ transition to host metal nuclei is responsible for some of the low-level energetic nuclear products that have been reported, then we should expect an analogous emission at lower energy due to excitation transfer of a 5.5-MeV quantum from the $HD/^3He$ transition [8].

In this work, our focus is on the reduction of the spin, isospin, and angular momentum matrix elements associated with the $HD/^3He$ phonon–nuclear matrix element. This could be done making use of the standard machinery associated with Racah algebra. Due to the relative simplicity of the 3-body problem, it is possible to carry out the reduction by brute force using Mathematica—an approach we made use of in the calculation that follows.

To develop an accurate description of the ^3He nucleus one needs to include a 3-body ^2S ground-state configuration along with a set of excited states [9]. There are four relevant HD states molecular states for which matrix elements are of interest. In a complete calculation, we would require matrix elements for transitions between the four HD states and all of the states needed for ^3He. As our interest at this point is in developing an estimate for the phonon–nuclear matrix element, we will restrict the calculation to include only the ^2S ground state ^3He configuration and the ^3S ground state of the deuteron.

2. Construction of the ^{3}He Ground State

An important first step in the

$$[321]_{RST} \;=\; [111]_R[321]_{ST} \;=\; [111]_R\frac{1}{\sqrt{2}}\bigg([211]_S[121]_T - [121]_S[211]_T\bigg), \tag{1}$$

where the group theoretical approach used here is discussed in Chaudhary's thesis [10]. In this construction $[111]_R$ is the fully symmetric spatial wave function

$$[111]_R \;=\; \frac{1}{6}\bigg(f(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)+f(\mathbf{r}_1,\mathbf{r}_3,\mathbf{r}_2)+f(\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_3)+f(\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_1)+f(\mathbf{r}_3,\mathbf{r}_1,\mathbf{r}_2)+f(\mathbf{r}_3,\mathbf{r}_2,\mathbf{r}_1)\bigg). \tag{2}$$

We work with the $M_T = 1/2, M_J = M_S = 1/2$ state, for which we can write

$$\begin{aligned}[211]_S \;&=\; \frac{1}{\sqrt{6}}\bigg(\downarrow_1\uparrow_2 + \uparrow_1\downarrow_2\bigg)\uparrow_3 - \sqrt{\frac{2}{3}}\uparrow_1\uparrow_2\downarrow_3,\\ [121]_S \;&=\; \frac{1}{\sqrt{2}}\bigg(\downarrow_1\uparrow_2 - \uparrow_1\downarrow_2\bigg)\uparrow_3,\end{aligned} \tag{3}$$

$$\begin{aligned}[211]_T \;&=\; \frac{1}{\sqrt{6}}\bigg(n_1p_2+p_1n_2\bigg)p_3 - \sqrt{\frac{2}{3}}p_1p_2n_3,\\ [121]_T \;&=\; \frac{1}{\sqrt{2}}\bigg(n_1p_2-p_1n_2\bigg)p_3.\end{aligned} \tag{4}$$

We can put these together and write

$$
\begin{aligned}
[321]_{ST} \;=\; & \frac{1}{\sqrt{2}}\Big([211]_S[121]_T - [121]_S[211]_T\Big) \\
=\; & \frac{1}{\sqrt{2}}\Bigg(\frac{1}{\sqrt{6}}\Big(\downarrow_1\uparrow_2 + \uparrow_1\downarrow_2\Big)\uparrow_3 - \sqrt{\frac{2}{3}}\uparrow_1\uparrow_2\downarrow_3\Bigg)\frac{1}{\sqrt{2}}\Big(n_1p_2 - p_1n_2\Big)p_3 \\
& -\frac{1}{\sqrt{2}}\Big(\downarrow_1\uparrow_2 - \uparrow_1\downarrow_2\Big)\uparrow_3\left(\frac{1}{\sqrt{6}}\Big(n_1p_2 + p_1n_2\Big)p_3 - \sqrt{\frac{2}{3}}p_1p_2n_3\right) \\
=\; & \frac{1}{\sqrt{6}}\Big((n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 - (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 + (p\downarrow)_1(p\uparrow)_2(n\uparrow)_3 \\
& -(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 + (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big).
\end{aligned}
\tag{5}
$$

A reduction into product states where individual particle quantum numbers are made explicit is required for the Mathematica calculations.

3. The Molecular HD States

There are four molecular HD states for which the selection rules are satisfied. These include

$$
\begin{aligned}
& \left|HD\left(L=1, S=\frac{1}{2}\right)J=\frac{3}{2}\right\rangle, \qquad \left|HD\left(L=1, S=\frac{3}{2}\right)J=\frac{3}{2}\right\rangle, \\
& \left|HD\left(L=1, S=\frac{1}{2}\right)J=\frac{1}{2}\right\rangle, \qquad \left|HD\left(L=1, S=\frac{3}{2}\right)J=\frac{1}{2}\right\rangle.
\end{aligned}
\tag{6}
$$

There is in addition a state with $J = \frac{5}{2}$, but there would be no coupling to it at lowest order since the selection rules are not satisfied.

Because of the Wigner–Eckart theorem, it is possible to determine the matrix element for all of the transitions between the substates given a nonzero evaluation of one of the transitions. Consequently, we only require a construction of one substate associated with each of these. As was the case for the ^{3}He ^{2}S configuration in the previous section, our goal is to develop wave functions written in terms of sums of products of individual terms with well-defined spin and isospin that are suitable for use in a brute force Mathematica calculation.

3.1. Construction of a $\left|\left(L=1, S=\frac{1}{2}\right)J=\frac{3}{2}\right\rangle$ state

For the $J = \frac{3}{2}$ states the construction is simplest in the case of the highest M_J. In this case we can write

$$
\left|\left(L=1, S=\frac{1}{2}\right), J=\frac{3}{2}, M_J=\frac{3}{2}\right\rangle \;=\; \left|L=1, M_L=1\right\rangle\left|S=\frac{1}{2}, M_S=\frac{1}{2}\right\rangle,
\tag{7}
$$

where the first term on the right is associated with the molecular rotation, and the second term is associated with the spin. Consequently, we can focus on the spin and isospin part of the wave function and write

$$\left|T=\frac{1}{2}, M_T=\frac{1}{2}, S=\frac{1}{2}, M_S=\frac{1}{2}\right\rangle$$

$$= \sqrt{\frac{2}{3}}\psi_D(M_S=1)\psi_p(m_s=-1/2) - \sqrt{\frac{1}{3}}\psi_D(M_S=0)\psi_p(m_s=1/2)$$

$$= \sqrt{\frac{2}{3}}\left\{\left(\frac{1}{\sqrt{2}}(p_1n_2-n_1p_2)\uparrow_1\uparrow_2\right)\left(p_3\downarrow_3\right)\right\}$$

$$-\sqrt{\frac{1}{3}}\left\{\frac{1}{2}\Big((p\uparrow)_1(n\downarrow)_2-(n\uparrow)_1(p\downarrow)_2+(p\downarrow)_1(n\uparrow)_2-(n\downarrow)_1(p\uparrow)_2\Big)(p\uparrow)_3\right\}$$

$$= \frac{1}{\sqrt{3}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3-(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big)$$

$$-\frac{1}{\sqrt{12}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3-(n\uparrow)_1(p\downarrow)_2(p\uparrow)_3+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3-(n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big). \tag{8}$$

Prior to antisymmetrization we can write

$$\left|\left(L=1, S=\frac{1}{2}\right), J=\frac{3}{2}, M_J=\frac{3}{2}\right\rangle =$$

$$-\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3-(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21})$$

$$+\frac{1}{\sqrt{24}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3-(n\uparrow)_1(p\downarrow)_2(p\uparrow)_3+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3-(n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21}), \tag{9}$$

where $\phi_D(r_{21})$ is the relative deuteron wave function, which in this case involves particles 1 and 2. The function $-f(r_{3|21})(x_{3|21}+iy_{3|21})$ is the product of the molecular HD wave function between the proton (particle 3) and the deuteron (with a center of mass position midway between particles 1 and 2) and the spherical harmonic for one unit of rotational motion.

After antisymmetrization we have

$$\left|\left(L=1, S=\frac{1}{2}\right), J=\frac{3}{2}, M_J=\frac{3}{2}\right\rangle =$$

$$-\frac{1}{\sqrt{18}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3-(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21})$$

$$+\frac{1}{\sqrt{72}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3-(n\uparrow)_1(p\downarrow)_2(p\uparrow)_3+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3-(n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21})$$

$$-\frac{1}{\sqrt{18}}\Big((p\downarrow)_1(p\uparrow)_2(n\uparrow)_3-(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{32})f(r_{1|32})(x_{1|32}+iy_{1|32})$$

$$+\frac{1}{\sqrt{72}}\Big((p\uparrow)_1(p\uparrow)_2(n\downarrow)_3-(p\uparrow)_1(n\uparrow)_2(p\downarrow)_3+(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3-(p\uparrow)_1(n\downarrow)_2(p\uparrow)_3\Big)\phi_D(r_{32})f(r_{1|32})(x_{1|32}+iy_{1|32})$$
$$-\frac{1}{\sqrt{18}}\Big((n\uparrow)_1(p\downarrow)_2(p\uparrow)_3-(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3\Big)\phi_D(r_{31})f(r_{2|31})(x_{2|31}+iy_{2|31})$$
$$+\frac{1}{\sqrt{72}}\Big((n\downarrow)_1(p\uparrow)_2(p\uparrow)_3-(p\downarrow)_1(p\uparrow)_2(n\uparrow)_3+(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3-(p\uparrow)_1(p\uparrow)_2(n\downarrow)_3\Big)\phi_D(r_{31})f(r_{2|31})(x_{2|31}+iy_{2|31}). \tag{10}$$

3.2. Construction of a $\left|\left(L=1,S=\frac{3}{2}\right)J=\frac{3}{2}\right\rangle$ state

Once again the simplest construction is for the state with maximum M_J, so we can write

$$\left|\left(L=1,S=\frac{3}{2}\right),J=\frac{3}{2},M_J=\frac{3}{2}\right\rangle = \left|L=1,M_L=1\right\rangle\left|S=\frac{3}{2},M_S=\frac{1}{2}\right\rangle\left\langle 1,1,\frac{3}{2},\frac{1}{2}\middle|\frac{3}{2}\frac{3}{2}\right\rangle$$
$$+\left|L=1,M_L=0\right\rangle\left|S=\frac{3}{2},M_S=\frac{3}{2}\right\rangle\left\langle 1,0,\frac{3}{2},\frac{3}{2}\middle|\frac{3}{2}\frac{3}{2}\right\rangle. \tag{11}$$

We can evaluate the Clebsch–Gordan coefficients to obtain

$$\left|\left(L=1,S=\frac{3}{2}\right),J=\frac{3}{2},M_J=\frac{3}{2}\right\rangle = \sqrt{\frac{2}{5}}\left|L=1,M_L=1\right\rangle\left|S=\frac{3}{2},M_S=\frac{1}{2}\right\rangle$$
$$-\sqrt{\frac{3}{5}}\left|L=1,M_L=0\right\rangle\left|S=\frac{3}{2},M_S=\frac{3}{2}\right\rangle. \tag{12}$$

For the $M_S=3/2$ state we can write

$$\left|T=\frac{1}{2},M_T=\frac{1}{2},S=\frac{3}{2},M_S=\frac{3}{2}\right\rangle = \psi_D(M_S=1)\psi_p(m_s=1/2)$$
$$= \left(\frac{1}{\sqrt{2}}(p_1n_2-n_1p_2)\uparrow_1\uparrow_2\right)(p\uparrow)_3 =$$
$$\frac{1}{\sqrt{2}}\Big((p\uparrow)_1(n\uparrow)_2(p\uparrow)_3-(n\uparrow)_1(p\uparrow)_2(p\uparrow)_3\Big). \tag{13}$$

For the $M_S=1/2$ state we have

$$\left|T=\frac{1}{2},M_T=\frac{1}{2},S=\frac{3}{2},M_s=\frac{1}{2}\right\rangle$$
$$= \sqrt{\frac{1}{3}}\psi_D(M_S=1)\psi_p(m_s=-1/2)+\sqrt{\frac{2}{3}}\psi_D(M_S=0)\psi_p(m_s=1/2)$$
$$= \sqrt{\frac{1}{3}}\left\{\left(\frac{1}{\sqrt{2}}(p_1n_2-n_1p_2)\uparrow_1\uparrow_2\right)\left(p_3\downarrow_3\right)\right\}$$
$$+\sqrt{\frac{2}{3}}\left\{\frac{1}{2}\Big((p\uparrow)_1(n\downarrow)_2-(n\uparrow)_1(p\downarrow)_2+(p\downarrow)_1(n\uparrow)_2-(n\downarrow)_1(p\uparrow)_2\Big)(p\uparrow)_3\right\}$$

$$
= \frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big)
$$

$$
+\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big). \tag{14}
$$

For the relevant angular momentum states we will use

$$
\begin{aligned}
|L=1, M_L=1\rangle &\rightarrow -\frac{1}{\sqrt{2}}(x_{3|21}+iy_{3|21}) \\
|L=1, M_L=0\rangle &\rightarrow z_{3|21}
\end{aligned} \tag{15}
$$

since the remainder of the order 1 spherical harmonic is included in f. We can make use of these formulas to write (prior to antisymmetrization)

$$
\begin{aligned}
&\left|\left(L=1, S=\frac{3}{2}\right), J=\frac{3}{2}, M_J=\frac{3}{2}\right\rangle = \\
&-\sqrt{\frac{2}{5}}\frac{1}{\sqrt{12}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 + (p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 \\
&+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21}) \\
&-\sqrt{\frac{3}{5}}\frac{1}{\sqrt{2}}\Big((p\uparrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{21})f(r_{3|21})z_{3|21}
\end{aligned} \tag{16}
$$

If we antisymmetrize we can write

$$
\begin{aligned}
&\left|\left(L=1, S=\frac{3}{2}\right), J=\frac{3}{2}, M_J=\frac{3}{2}\right\rangle = \\
&-\sqrt{\frac{1}{90}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 + (p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 \\
&+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21}) \\
&-\frac{1}{\sqrt{10}}\Big((p\uparrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{21})f(r_{3|21})z_{3|21} \\
&-\sqrt{\frac{1}{90}}\Big((p\downarrow)_1(p\uparrow)_2(n\uparrow)_3 - (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 + (p\uparrow)_1(p\uparrow)_2(n\downarrow)_3 - (p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 \\
&+(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3 - (p\uparrow)_1(n\downarrow)_2(p\uparrow)_3\Big)\phi_D(r_{32})f(r_{1|32})(x_{1|32}+iy_{1|32}) \\
&-\frac{1}{\sqrt{10}}\Big((p\uparrow)_1(p\uparrow)_2(n\uparrow)_3 - (p\uparrow)_1(n\uparrow)_2(p\uparrow)_3\Big)\phi_D(r_{32})f(r_{1|32})z_{1|32} \\
&-\sqrt{\frac{1}{90}}\Big((n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 - (p\uparrow)_1(p\downarrow)_2(n\uparrow)_3 + (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3 - (p\downarrow)_1(p\uparrow)_2(n\uparrow)_3 \\
&+(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 - (p\uparrow)_1(p\uparrow)_2(n\downarrow)_3\Big)\phi_D(r_{31})f(r_{2|31})(x_{2|31}+iy_{2|31}) \\
&-\frac{1}{\sqrt{10}}\Big((n\uparrow)_1(p\uparrow)_2(p\uparrow)_3 - (p\uparrow)_1(p\uparrow)_2(n\uparrow)_3\Big)\phi_D(r_{31})f(r_{2|31})z_{2|31}
\end{aligned} \tag{17}
$$

3.3. Construction of a $\left|\left(L=1, S=\frac{1}{2}\right) J=\frac{1}{2}\right\rangle$ state

Somewhat arbitrarily we choose to work with the $M_J=\frac{1}{2}$ state, which is

$$\left|\left(L=1, S=\frac{1}{2}\right), J=\frac{1}{2}, M_J=\frac{1}{2}\right\rangle = \left|L=1, M_L=1\right\rangle\left|S=\frac{1}{2}, M_S=-\frac{1}{2}\right\rangle\left\langle 1,1,\frac{1}{2},-\frac{1}{2}\middle|\frac{1}{2}\frac{1}{2}\right\rangle$$
$$+\left|L=1, M_L=0\right\rangle\left|S=\frac{1}{2}, M_S=\frac{1}{2}\right\rangle\left\langle 1,0,\frac{1}{2},\frac{1}{2}\middle|\frac{1}{2}\frac{1}{2}\right\rangle \tag{18}$$

This evaluates to

$$\left|\left(L=1, S=\frac{1}{2}\right), J=\frac{1}{2}, M_J=\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|L=1, M_L=1\right\rangle\left|S=\frac{1}{2}, M_S=-\frac{1}{2}\right\rangle$$
$$-\sqrt{\frac{1}{3}}\left|L=1, M_L=0\right\rangle\left|S=\frac{1}{2}, M_S=\frac{1}{2}\right\rangle \tag{19}$$

For the spin doublet $M_S=1/2$ state we can write

$$\left|T=\frac{1}{2}, M_T=\frac{1}{2}, S=\frac{1}{2}, M_S=\frac{1}{2}\right\rangle$$
$$= \sqrt{\frac{2}{3}}\psi_D(M_S=1)\psi_p(m_s=-1/2) - \sqrt{\frac{1}{3}}\psi_D(M_S=0)\psi_p(m_s=1/2)$$
$$= \sqrt{\frac{2}{3}}\left\{\left(\frac{1}{\sqrt{2}}(p_1 n_2 - n_1 p_2)\uparrow_1\uparrow_2\right)\left(p_3\downarrow_3\right)\right\}$$
$$-\sqrt{\frac{1}{3}}\left\{\frac{1}{2}\Big((p\uparrow)_1(n\downarrow)_2-(n\uparrow)_1(p\downarrow)_2+(p\downarrow)_1(n\uparrow)_2-(n\downarrow)_1(p\uparrow)_2\Big)(p\uparrow)_3\right\}$$
$$= \frac{1}{\sqrt{3}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3-(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big)$$
$$-\frac{1}{\sqrt{12}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3-(n\uparrow)_1(p\downarrow)_2(p\uparrow)_3+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3-(n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big) \tag{20}$$

For the spin doublet $M_S=-1/2$ state we can write

$$\left|T=\frac{1}{2}, M_T=\frac{1}{2}, S=\frac{1}{2}, M_S=-\frac{1}{2}\right\rangle$$
$$= \sqrt{\frac{1}{3}}\psi_D(M_S=0)\psi_p(m_s=-1/2) - \sqrt{\frac{2}{3}}\psi_D(M_S=-1)\psi_p(m_s=1/2)$$
$$= \sqrt{\frac{1}{3}}\left\{\frac{1}{2}\Big((p\uparrow)_1(n\downarrow)_2-(n\uparrow)_1(p\downarrow)_2+(p\downarrow)_1(n\uparrow)_2-(n\downarrow)_1(p\uparrow)_2\Big)(p\downarrow)_3\right\}$$
$$-\sqrt{\frac{2}{3}}\left\{\left(\frac{1}{\sqrt{2}}(p_1 n_2 - n_1 p_2)\downarrow_1\downarrow_2\right)(p\uparrow)_3\right\}$$
$$= \frac{1}{\sqrt{12}}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3-(n\uparrow)_1(p\downarrow)_2(p\downarrow)_3+(p\downarrow)_1(n\uparrow)_2(p\downarrow)_3-(n\downarrow)_1(p\uparrow)_2(p\downarrow)_3\Big)$$
$$-\frac{1}{\sqrt{3}}\Big((p\downarrow)_1(n\downarrow)_2(p\uparrow)_3-(n\downarrow)_1(p\downarrow)_2(p\uparrow)_3\Big) \tag{21}$$

We can make use of these results to write

$$\left| \left(L=1, S=\frac{1}{2}\right), J=\frac{1}{2}, M_J=\frac{1}{2} \right\rangle =$$

$$\sqrt{\frac{2}{3}}\Big(-\frac{1}{\sqrt{2}}(x_{3|21}+iy_{3|21})\Big)\Big\{ \frac{1}{\sqrt{12}}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\downarrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\downarrow)_3 \Big)$$

$$-\frac{1}{\sqrt{3}}\Big((p\downarrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\downarrow)_2(p\uparrow)_3 \Big)\Big\}$$

$$-\sqrt{\frac{1}{3}}z_{3|21}\Big\{ \frac{1}{\sqrt{3}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 \Big)$$

$$-\frac{1}{\sqrt{12}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3 \Big)\Big\} \tag{22}$$

This can be expanded to give

$$\left| \left(L=1, S=\frac{1}{2}\right), J=\frac{1}{2}, M_J=\frac{1}{2} \right\rangle =$$

$$-\frac{1}{6}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\downarrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\downarrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21})$$

$$+\frac{1}{3}\Big((p\downarrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\downarrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21})$$

$$-\frac{1}{3}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})z_{3|21}$$

$$+\frac{1}{6}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})z_{3|21} \tag{23}$$

We can antisymmetrize to obtain

$$\left| \left(L=1, S=\frac{1}{2}\right), J=\frac{1}{2}, M_J=\frac{1}{2} \right\rangle =$$

$$-\frac{1}{\sqrt{108}}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\downarrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\downarrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21})$$

$$+\frac{1}{\sqrt{27}}\Big((p\downarrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\downarrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21})$$

$$-\frac{1}{\sqrt{27}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})z_{3|21}$$

$$+\frac{1}{\sqrt{108}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})z_{3|21}$$

$$-\frac{1}{\sqrt{108}}\Big((p\downarrow)_1(p\uparrow)_2(n\downarrow)_3 - (p\downarrow)_1(n\uparrow)_2(p\downarrow)_3 + (p\downarrow)_1(p\downarrow)_2(n\uparrow)_3 - (p\downarrow)_1(n\downarrow)_2(p\uparrow)_3 \Big)\phi_D(r_{32})f(r_{1|32})(x_{1|32}+iy_{1|32})$$

$$+\frac{1}{\sqrt{27}}\Big((p\uparrow)_1(p\downarrow)_2(n\downarrow)_3 - (p\uparrow)_1(n\downarrow)_2(p\downarrow)_3 \Big)\phi_D(r_{32})f(r_{1|32})(x_{1|32}+iy_{1|32})$$

$$-\frac{1}{\sqrt{27}}\Big((p\downarrow)_1(p\uparrow)_2(n\uparrow)_3 - (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{32})f(r_{1|32})z_{1|32}$$

$$+\frac{1}{\sqrt{108}}\Big((p\uparrow)_1(p\uparrow)_2(n\downarrow)_3-(p\uparrow)_1(n\uparrow)_2(p\downarrow)_3+(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3-(p\uparrow)_1(n\downarrow)_2(p\uparrow)_3\Big)\phi_D(r_{32})f(r_{1|32})z_{1|32}$$
$$-\frac{1}{\sqrt{108}}\Big((n\downarrow)_1(p\downarrow)_2(p\uparrow)_3-(p\downarrow)_1(p\downarrow)_2(n\uparrow)_3+(n\uparrow)_1(p\downarrow)_2(p\downarrow)_3-(p\uparrow)_1(p\downarrow)_2(n\downarrow)_3\Big)\phi_D(r_{31})f(r_{2|31})(x_{2|31}+iy_{2|31})$$
$$+\frac{1}{\sqrt{27}}\Big((n\downarrow)_1(p\uparrow)_2(p\downarrow)_3-(p\downarrow)_1(p\uparrow)_2(n\downarrow)_3\Big)\phi_D(r_{31})f(r_{2|31})(x_{2|31}+iy_{2|31})$$
$$-\frac{1}{\sqrt{27}}\Big((n\uparrow)_1(p\downarrow)_2(p\uparrow)_3-(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3\Big)\phi_D(r_{31})f(r_{2|31})z_{2|31}$$
$$+\frac{1}{\sqrt{108}}\Big((n\downarrow)_1(p\uparrow)_2(p\uparrow)_3-(p\downarrow)_1(p\uparrow)_2(n\uparrow)_3+(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3-(p\uparrow)_1(p\uparrow)_2(n\downarrow)_3\Big)\phi_D(r_{31})f(r_{2|31})z_{2|31} \quad (24)$$

3.4. Construction of a $\left|\left(L=1,S=\frac{3}{2}\right)J=\frac{1}{2}\right\rangle$ state

We again work with a state with $M_J = \frac{1}{2}$, for which we can write

$$\begin{aligned}\left|\left(L=1,S=\frac{3}{2}\right),J=\frac{1}{2},M_J=\frac{1}{2}\right\rangle &= \Big|L=1,M_L=1\Big\rangle\Big|S=\frac{3}{2},M_S=-\frac{1}{2}\Big\rangle\Big\langle 1,1,\frac{3}{2},-\frac{1}{2}\Big|\frac{1}{2}\frac{1}{2}\Big\rangle\\ &+\Big|L=1,M_L=0\Big\rangle\Big|S=\frac{3}{2},M_S=\frac{1}{2}\Big\rangle\Big\langle 1,0,\frac{3}{2},\frac{1}{2}\Big|\frac{1}{2}\frac{1}{2}\Big\rangle\\ &+\Big|L=1,M_L=-1\Big\rangle\Big|S=\frac{3}{2},M_S=\frac{3}{2}\Big\rangle\Big\langle 1,0,\frac{3}{2},\frac{3}{2}\Big|\frac{1}{2}\frac{1}{2}\Big\rangle\\ &= \sqrt{\frac{1}{6}}\Big|L=1,M_L=1\Big\rangle\Big|S=\frac{3}{2},M_S=-\frac{1}{2}\Big\rangle\\ &-\sqrt{\frac{1}{3}}\Big|L=1,M_L=0\Big\rangle\Big|S=\frac{3}{2},M_S=\frac{1}{2}\Big\rangle\\ &+\sqrt{\frac{1}{2}}\Big|L=1,M_L=-1\Big\rangle\Big|S=\frac{3}{2},M_S=\frac{3}{2}\Big\rangle.\end{aligned} \quad (25)$$

For the different spin states we recall that

$$\begin{aligned}\Big|T=\frac{1}{2},M_T=\frac{1}{2},S=\frac{3}{2},M_S=\frac{3}{2}\Big\rangle &= \psi_D(M_S=1)\psi_p(m_s=1/2)\\ &= \left(\frac{1}{\sqrt{2}}(p_1n_2-n_1p_2)\uparrow_1\uparrow_2\right)(p\uparrow)_3 =\\ &\frac{1}{\sqrt{2}}\Big((p\uparrow)_1(n\uparrow)_2(p\uparrow)_3-(n\uparrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\end{aligned} \quad (26)$$

$$\Big|T=\frac{1}{2},M_T=\frac{1}{2},S=\frac{3}{2},M_s=\frac{1}{2}\Big\rangle$$
$$=\sqrt{\frac{1}{3}}\psi_D(M_S=1)\psi_p(m_s=-1/2)+\sqrt{\frac{2}{3}}\psi_D(M_S=0)\psi_p(m_s=1/2)$$
$$=\sqrt{\frac{1}{3}}\left\{\left(\frac{1}{\sqrt{2}}(p_1n_2-n_1p_2)\uparrow_1\uparrow_2\right)\Big(p_3\downarrow_3\Big)\right\}$$

$$+\sqrt{\frac{2}{3}}\left\{\frac{1}{2}\Big((p\uparrow)_1(n\downarrow)_2-(n\uparrow)_1(p\downarrow)_2+(p\downarrow)_1(n\uparrow)_2-(n\downarrow)_1(p\uparrow)_2\Big)(p\uparrow)_3\right\}$$

$$=\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3-(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big)$$

$$+\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3-(n\uparrow)_1(p\downarrow)_2(p\uparrow)_3+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3-(n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big) \tag{27}$$

$$\left|T=\frac{1}{2},M_T=\frac{1}{2},S=\frac{3}{2},M_s=-\frac{1}{2}\right\rangle$$

$$=\sqrt{\frac{2}{3}}\psi_D(M_S=0)\psi_p(m_s=-1/2)+\sqrt{\frac{1}{3}}\psi_D(M_S=-1)\psi_p(m_s=1/2)$$

$$=\sqrt{\frac{2}{3}}\left\{\frac{1}{2}\Big((p\uparrow)_1(n\downarrow)_2-(n\uparrow)_1(p\downarrow)_2+(p\downarrow)_1(n\uparrow)_2-(n\downarrow)_1(p\uparrow)_2\Big)(p\downarrow)_3\right\}$$

$$+\sqrt{\frac{2}{3}}\left\{\left(\frac{1}{\sqrt{2}}(p_1n_2-n_1p_2)\downarrow_1\downarrow_2\right)(p\uparrow)_3\right\}$$

$$=\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3-(n\uparrow)_1(p\downarrow)_2(p\downarrow)_3+(p\downarrow)_1(n\uparrow)_2(p\downarrow)_3-(n\downarrow)_1(p\uparrow)_2(p\downarrow)_3\Big)$$

$$+\frac{1}{\sqrt{6}}\Big((p\downarrow)_1(n\downarrow)_2(p\uparrow)_3-(n\downarrow)_1(p\downarrow)_2(p\uparrow)_3\Big). \tag{28}$$

For the three angular momentum states we have

$$|L=1,M_L=1\rangle \ \rightarrow\ -\frac{1}{\sqrt{2}}(x_{3|21}+iy_{3|21})$$

$$|L=1,M_L=0\rangle \ \rightarrow\ z_{3|21}$$

$$|L=1,M_L=-1\rangle \ \rightarrow\ \frac{1}{\sqrt{2}}(x_{3|21}-iy_{3|21}). \tag{29}$$

We can put these together and write

$$\left|\left(L=1,S=\frac{3}{2}\right),J=\frac{1}{2},M_J=\frac{1}{2}\right\rangle =$$

$$\sqrt{\frac{1}{6}}\Big(-\frac{1}{\sqrt{2}}(x_{3|21}+iy_{3|21})\Big)\left\{\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3-(n\uparrow)_1(p\downarrow)_2(p\downarrow)_3+(p\downarrow)_1(n\uparrow)_2(p\downarrow)_3-(n\downarrow)_1(p\uparrow)_2(p\downarrow)_3\Big)\right.$$

$$\left.+\frac{1}{\sqrt{6}}\Big((p\downarrow)_1(n\downarrow)_2(p\uparrow)_3-(n\downarrow)_1(p\downarrow)_2(p\uparrow)_3\Big)\right\}$$

$$-\sqrt{\frac{1}{3}}z_{3|21}\left\{\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3-(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3\Big)\right.$$

$$\left.+\frac{1}{\sqrt{6}}\Big((p\uparrow)_1(n\downarrow)_2(p\uparrow)_3-(n\uparrow)_1(p\downarrow)_2(p\uparrow)_3+(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3-(n\downarrow)_1(p\uparrow)_2(p\uparrow)_3\Big)\right\}$$

$$+\sqrt{\frac{1}{2}}\Big(\frac{1}{\sqrt{2}}(x_{3|21}-iy_{3|21})\Big)\frac{1}{\sqrt{2}}\Big((p\uparrow)_1(n\uparrow)_2(p\uparrow)_3-(n\uparrow)_1(p\uparrow)_2(p\uparrow)_3\Big). \tag{30}$$

This we can rewrite as

$$
\begin{aligned}
&\left| \left(L=1, S=\frac{3}{2}\right), J=\frac{1}{2}, M_J=\frac{1}{2} \right\rangle = \\
&-\sqrt{\frac{1}{72}}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\downarrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\downarrow)_3 \\
&\quad +(p\downarrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\downarrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21}) \\
&-\sqrt{\frac{1}{18}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 + (p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 \\
&\quad +(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})z_{3|21} \\
&+\frac{1}{\sqrt{8}}\Big((p\uparrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}-iy_{3|21}).
\end{aligned} \tag{31}
$$

Antisymmetrization leads to

$$
\begin{aligned}
&\left| \left(L=1, S=\frac{3}{2}\right), J=\frac{1}{2}, M_J=\frac{1}{2} \right\rangle = \\
&-\sqrt{\frac{1}{216}}\Big((p\uparrow)_1(n\downarrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\downarrow)_3 + (p\downarrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\downarrow)_3 \\
&\quad +(p\downarrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\downarrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}+iy_{3|21}) \\
&-\sqrt{\frac{1}{54}}\Big((p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\downarrow)_3 + (p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\downarrow)_2(p\uparrow)_3 \\
&\quad +(p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\downarrow)_1(p\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})z_{3|21} \\
&+\frac{1}{\sqrt{24}}\Big((p\uparrow)_1(n\uparrow)_2(p\uparrow)_3 - (n\uparrow)_1(p\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{21})f(r_{3|21})(x_{3|21}-iy_{3|21}) \\
&-\sqrt{\frac{1}{216}}\Big((p\downarrow)_1(p\uparrow)_2(n\downarrow)_3 - (p\downarrow)_1(n\uparrow)_2(p\downarrow)_3 + (p\downarrow)_1(p\downarrow)_2(n\uparrow)_3 - (p\downarrow)_1(n\downarrow)_2(p\uparrow)_3 \\
&\quad +(p\uparrow)_1(p\downarrow)_2(n\downarrow)_3 - (p\uparrow)_1(n\downarrow)_2(p\downarrow)_3 \Big)\phi_D(r_{32})f(r_{1|32})(x_{1|32}+iy_{1|32}) \\
&-\sqrt{\frac{1}{54}}\Big((p\downarrow)_1(p\uparrow)_2(n\uparrow)_3 - (p\downarrow)_1(n\uparrow)_2(p\uparrow)_3 + (p\uparrow)_1(p\uparrow)_2(n\downarrow)_3 - (p\uparrow)_1(n\uparrow)_2(p\downarrow)_3 \\
&\quad +(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3 - (p\uparrow)_1(n\downarrow)_2(p\uparrow)_3 \Big)\phi_D(r_{32})f(r_{1|32})z_{1|32} \\
&+\frac{1}{\sqrt{24}}\Big((p\uparrow)_1(p\uparrow)_2(n\uparrow)_3 - (p\uparrow)_1(n\uparrow)_2(p\uparrow)_3 \Big)\phi_D(r_{32})f(r_{1|32})(x_{1|32}-iy_{1|32}) \\
&-\sqrt{\frac{1}{216}}\Big((n\downarrow)_1(p\downarrow)_2(p\uparrow)_3 - (p\downarrow)_1(p\downarrow)_2(n\uparrow)_3 + (n\uparrow)_1(p\downarrow)_2(p\downarrow)_3 - (p\uparrow)_1(p\downarrow)_2(n\downarrow)_3 \\
&\quad +(n\downarrow)_1(p\uparrow)_2(p\downarrow)_3 - (p\downarrow)_1(p\uparrow)_2(n\downarrow)_3 \Big)\phi_D(r_{31})f(r_{2|31})(x_{2|31}+iy_{2|31})
\end{aligned}
$$

$$-\sqrt{\frac{1}{54}}\bigg((n\uparrow)_1(p\downarrow)_2(p\uparrow)_3-(p\uparrow)_1(p\downarrow)_2(n\uparrow)_3+(n\downarrow)_1(p\uparrow)_2(p\uparrow)_3-(p\downarrow)_1(p\uparrow)_2(n\uparrow)_3$$

$$+(n\uparrow)_1(p\uparrow)_2(p\downarrow)_3-(p\uparrow)_1(p\uparrow)_2(n\downarrow)_3\bigg)\phi_D(r_{31})f(r_{2|31})z_{2|31}$$

$$+\frac{1}{\sqrt{24}}\bigg((n\uparrow)_1(p\uparrow)_2(p\uparrow)_3-(p\uparrow)_1(p\uparrow)_2(n\uparrow)_3\bigg)\phi_D(r_{31})f(r_{2|31})(x_{2|31}-iy_{2|31}). \tag{32}$$

4. Normalization for the Molecular States

Before a systematic evaluation of the matrix elements for the phonon–nuclear interaction, we need to consider the normalization of the molecular state wave functions. Although our focus here is on the reduction of the phonon–nuclear matrix elements, the normalization will be of interest when the matrix elements are evaluated.

For the different cases Mathematica gives

$$\left\langle \left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\middle|\left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\right\rangle =$$

$$\bigg\langle\frac{1}{36}(-r_{21}^2+2r_{31}^2+2r_{32}^2)\phi_D^2(r_{21})f^2(r_{3|21})+\frac{1}{36}(2r_{21}^2-r_{31}^2+2r_{32}^2)\phi_D^2(r_{31})f^2(r_{2|31})$$

$$+\frac{1}{36}(2r_{21}^2+2r_{31}^2-r_{32}^2)\phi_D^2(r_{32})f^2(r_{1|32})+\frac{1}{144}(r_{21}^2+r_{31}^2-5r_{32}^2)\phi_D(r_{21})\phi_D(r_{31})f(r_{3|21})f(r_{2|31})$$

$$+\frac{1}{144}(r_{21}^2-5r_{31}^2+r_{32}^2)\phi_D(r_{21})\phi_D(r_{32})f(r_{3|21})f(r_{1|32})+\frac{1}{144}(-5r_{21}^2+r_{31}^2+r_{32}^2)\phi_D(r_{31})\phi_D(r_{32})f(r_{2|31})f(r_{1|32})\bigg\rangle. \tag{33}$$

We can take advantage of the symmetry to write this as

$$\left\langle \left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\middle|\left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\right\rangle =$$

$$= \bigg\langle\frac{1}{36}(-r_{21}^2+2r_{31}^2+2r_{32}^2)\phi_D^2(r_{21})f^2(r_{3|21})+\frac{1}{144}(r_{21}^2+r_{31}^2-5r_{32}^2)\phi_D(r_{21})\phi_D(r_{31})f(r_{3|21})f(r_{2|31})\bigg\rangle$$

$$+\quad(1\to3)\quad+\quad(2\to3). \tag{34}$$

For the other cases we have

$$\left\langle \left(L=1,S=\frac{3}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\middle|\left(L=1,S=\frac{3}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\right\rangle =$$

$$\bigg\langle\frac{1}{36}(-r_{21}^2+2r_{31}^2+2r_{32}^2)\phi_D^2(r_{21})f^2(r_{3|21})+\frac{1}{72}(-r_{21}^2-r_{31}^2+5r_{32}^2)\phi_D(r_{21})\phi_D(r_{31})f(r_{3|21})f(r_{2|31})\bigg\rangle$$

$$+\quad(1\to3)\quad+\quad(2\to3) \tag{35}$$

$$\left\langle \left(L=1, S=\frac{1}{2}\right) J=\frac{1}{2}, M_J=\frac{1}{2} \middle| \left(L=1, S=\frac{1}{2}\right) J=\frac{1}{2}, M_J=\frac{1}{2} \right\rangle \ =$$

$$\left\langle \frac{1}{36}(-r_{21}^2+2r_{31}^2+2r_{32}^2)\phi_D^2(r_{21})f^2(r_{3|21}) + \frac{1}{144}(r_{21}^2+r_{31}^2-5r_{32}^2)\phi_D(r_{21})\phi_D(r_{31})f(r_{3|21})f(r_{2|31}) \right\rangle$$

$$+ \quad (1\rightarrow 3) \quad + \quad (2 \rightarrow 3) \tag{36}$$

$$\left\langle \left(L=1, S=\frac{3}{2}\right) J=\frac{1}{2}, M_J=\frac{1}{2} \middle| \left(L=1, S=\frac{3}{2}\right) J=\frac{1}{2}, M_J=\frac{1}{2} \right\rangle \ =$$

$$\left\langle \frac{1}{36}(-r_{21}^2+2r_{31}^2+2r_{32}^2)\phi_D^2(r_{21})f^2(r_{3|21}) + \frac{1}{72}(-r_{21}^2-r_{31}^2+5r_{32}^2)\phi_D(r_{21})\phi_D(r_{31})f(r_{3|21})f(r_{2|31}) \right\rangle$$

$$+ \quad (1\rightarrow 3) \quad + \quad (2 \rightarrow 3). \tag{37}$$

The lowest-order contribution is the same in all cases as expected. The symmetry of the terms in the integral in each case provides a check on the construction of the molecular wave functions. The cross terms present do show a difference between configurations, but these are expected to be small.

5. One-pion exchange part of the phonon–nuclear interaction

We have discussed previously the lowest-order contribution to the phonon–nuclear interaction, which can be written as [3]

$$\hat{H}_{int} \ = \ \frac{1}{2Mc}\sum_{j<k}\left[\beta_j \boldsymbol{\alpha}_j + \beta_k \boldsymbol{\alpha}_k, \hat{V}_{jk}\right]\cdot \hat{\mathbf{P}}. \tag{38}$$

Recently, we documented the nonrelativistic reduction of this for the special case of the one-pion exchange potential with pseudovector coupling (as used in chiral effective field theory potentials) [4]

$$\left(\hat{H}'_{int}(j,k)\right)_{NR} \ = \ -\frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_j\cdot\mathbf{p}_j, \left[\boldsymbol{\sigma}_j\cdot\mathbf{P}, \hat{V}_{jk}^{(NR)}\right]\right] - \frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_k\cdot\mathbf{p}_k, \left[\boldsymbol{\sigma}_k\cdot\mathbf{P}, \hat{V}_{jk}^{(NR)}\right]\right] \tag{39}$$

with

$$\hat{V}_{jk}^{(NR)} \ = \ -\left(\frac{f_{\pi NN}}{m_\pi}\right)^2 (\boldsymbol{\tau}_k\cdot\boldsymbol{\tau}_j)\boldsymbol{\sigma}_k\cdot\int\frac{\mathbf{k}\mathbf{k}}{(m_\pi c^2)^2+\hbar^2c^2|\mathbf{k}|^2}e^{i\mathbf{k}\cdot(\mathbf{r}_k-\mathbf{r}_j)}\frac{d^3\mathbf{k}}{(2\pi)^3}\cdot\boldsymbol{\sigma}_j. \tag{40}$$

After carrying out the integrations in $\mathbf{k}$ we end up with a contact potential, a central potential, and a tensor potential. The long range part of the interaction involves the central and tensor potentials which in the absence of a regulator are given by

$$\hat{V}_{jk}^{(central)}(r) \;=\; \frac{1}{3}\frac{f_{\pi NN}^2}{4\pi}\mu_\pi c^2(\boldsymbol{\tau}_j\cdot\boldsymbol{\tau}_k)(\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k)\frac{e^{-\kappa r}}{\kappa r} \tag{41}$$

$$\hat{V}_{jk}^{(tensor)}(r) \;=\; \frac{f_{\pi NN}^2}{4\pi}\mu_\pi c^2(\boldsymbol{\tau}_j\cdot\boldsymbol{\tau}_k)\left(\frac{(\boldsymbol{\sigma}_j\cdot\mathbf{r})(\boldsymbol{\sigma}_k\cdot\mathbf{r})}{r^2}-\frac{\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k}{3}\right)\left(1+\frac{3}{\kappa r}+\frac{3}{\kappa^2 r^2}\right). \tag{42}$$

We can use these to develop expressions for the central and tensor contributions to the phonon–nuclear interaction

$$\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(central)} \;=\; -\frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_j\cdot\mathbf{p}_j,\left[\boldsymbol{\sigma}_j\cdot\mathbf{P},\hat{V}_{jk}^{(central)}\right]\right]-\frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_k\cdot\mathbf{p}_k,\left[\boldsymbol{\sigma}_k\cdot\mathbf{P},\hat{V}_{jk}^{(central)}\right]\right] \tag{43}$$

$$\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(tensor)} \;=\; -\frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_j\cdot\mathbf{p}_j,\left[\boldsymbol{\sigma}_j\cdot\mathbf{P},\hat{V}_{jk}^{(tensor)}\right]\right]-\frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_k\cdot\mathbf{p}_k,\left[\boldsymbol{\sigma}_k\cdot\mathbf{P},\hat{V}_{jk}^{(tensor)}\right]\right]. \tag{44}$$

6. Central potential contribution

We have used the wave functions outline above to reduce the phonon–nuclear interaction in the case of contributions from the central potential. Results for the different cases are listed in this section.

6.1. HD $\left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2}$ case

$$\left\langle \mathrm{HD}\left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\right|\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(central)}\left|{}^3\mathrm{He}\;J=\frac{1}{2},M_J=\frac{1}{2}\right\rangle \;=$$
$$\frac{i\hbar(P_x-iP_y)}{4Mmc^2}\frac{1}{2\sqrt{3}}\left\langle\phi_D(r_{21})f(r_{3|21})\right|-4\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}-4\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}$$
$$+5\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}+3\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}$$
$$-2\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}+3\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}$$
$$+5\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}+2\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}$$
$$+\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_C(r_{31})\right)+\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_C(r_{32})\right)\left|u(r_{21},r_{31},r_{32})\right\rangle$$
$$+\quad(1\to 3)\quad+\quad(2\to 3) \tag{45}$$

6.2. HD $\left(L=1,S=\frac{3}{2}\right)$ $J=\frac{3}{2}$ case

$$\left\langle \text{HD}\left(L=1,S=\frac{3}{2}\right)J=\frac{3}{2},M_J=\frac{3}{2}\middle|\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(central)}\middle|{}^3\text{He}\,J=\frac{1}{2},M_J=\frac{1}{2}\right\rangle =$$

$$\begin{aligned}
&\frac{i\hbar(P_x-iP_y)}{4Mmc^2}\frac{1}{2}\sqrt{\frac{5}{3}}\Big\langle\phi_D(r_{21})f(r_{3|21})\Big|-2\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}-2\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}+3\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+2\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}+3\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\\
&+\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}-2\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\\
&+2\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_C(r_{31})\right)+2\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_C(r_{32})\right)\Big|u(r_{21},r_{31},r_{32})\Big\rangle\\
&\quad+\quad(1\rightarrow 3)\quad+\quad(2\rightarrow 3)
\end{aligned}\tag{46}$$

6.3. HD $\left(L=1,S=\frac{1}{2}\right)$ $J=\frac{1}{2}$ case

$$\left\langle \text{HD}\left(L=1,S=\frac{1}{2}\right)J=\frac{1}{2},M_J=\frac{1}{2}\middle|\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(central)}\middle|{}^3\text{He}\,J=\frac{1}{2},M_J=\frac{1}{2}\right\rangle =$$

$$\begin{aligned}
&-\frac{i\hbar P_z}{4Mmc^2}\frac{1}{6\sqrt{2}}\Big\langle\phi_D(r_{21})f(r_{3|21})\Big|8\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}+8\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&-\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}+15\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+16\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}+15\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\\
&-\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)V_C(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}-16\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\\
&+4\frac{1}{6}(-r_{21}^2+3r_{31}^2+r_{32}^2)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_C(r_{31})\right)+4\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_C(r_{32})\right)\Big|u(r_{21},r_{31},r_{32})\Big\rangle\\
&\quad+\quad(1\rightarrow 3)\quad+\quad(2\rightarrow 3)
\end{aligned}\tag{47}$$

6.4. HD $\left(L=1,S=\frac{3}{2}\right)$ $J=\frac{1}{2}$ case

$$\left\langle \text{HD}\left(L=1,S=\frac{3}{2}\right)J=\frac{1}{2},M_J=\frac{1}{2}\middle|\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(central)}\middle|{}^3\text{He}\,J=\frac{1}{2},M_J=\frac{1}{2}\right\rangle =$$

$$\begin{aligned}
&\frac{i\hbar P_z}{4Mmc^2}\frac{2}{3}\Big\langle\phi_D(r_{21})f(r_{3|21})\Big|5\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}+5\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+2\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}-2\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}
\end{aligned}$$

$$
+2\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)V_C(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}+2\frac{1}{3}(r_{31}^2-r_{32}^2)V_C(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}
$$
$$
+\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)\left(\frac{d}{dr_{31}}V_C(r_{31})\right)+\frac{1}{6}(-r_{21}^2+r_{31}^2+3r_{32}^2)\left(\frac{d}{dr_{32}}V_C(r_{32})\right)\bigg|u(r_{21},r_{31},r_{32})\bigg\rangle
$$
$$
+\quad (1\rightarrow 3)\quad +\quad (2\rightarrow 3). \tag{48}
$$

6.5. Central potential definition

In these expressions we have used $V_C(r)$ consistent with

$$
\hat{V}_{jk}^{(central)}(r) \;=\; (\boldsymbol{\tau}_j\cdot\boldsymbol{\tau}_k)(\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k)V_C(r). \tag{49}
$$

7. Tensor potential contribution

The wave functions presented above have been used for the reduction of the contribution associated with the tensor interaction. Results for the different cases are given below.

7.1. HD $\left(L=1,S=\frac{1}{2}\right)\ J=\frac{3}{2}$ case

$$
\left\langle \mathrm{HD}\left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2}M_J=\frac{1}{2}\right|\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(tensor)}\left|{}^3\mathrm{He}\ J=\frac{1}{2}M_J=\frac{1}{2}\right\rangle
$$
$$
=\ \frac{i\hbar(P_x-iP_y)}{4Mmc^2}\frac{1}{12\sqrt{3}}\bigg\langle\phi_D(r_{21})f(r_{3|21})\bigg|
$$
$$
2\left(\frac{r_{21}^4+3r_{31}^4+3r_{32}^4-4r_{21}^2r_{32}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}
$$
$$
+2\left(\frac{r_{21}^4+3r_{31}^4+3r_{32}^4-4r_{21}^2r_{31}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}
$$
$$
-2\left(\frac{3r_{21}^4-5r_{31}^4+3r_{32}^4-6r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2+2r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}
$$
$$
+5\left(-r_{21}^2+3r_{31}^2+r_{32}^2\right)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_T(r_{31})\right)+15\left(\frac{-r_{21}^2+3r_{31}^2+r_{32}^2}{r_{31}^2}\right)V_T(r_{31})
$$
$$
+8\left(-r_{21}^2+3r_{31}^2+r_{32}^2\right)V_T(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}
$$
$$
-2\left(\frac{3r_{21}^4+3r_{31}^4-5r_{32}^4-6r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2+2r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}
$$
$$
+5\left(-r_{21}^2+r_{31}^2+3r_{32}^2\right)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_T(r_{32})\right)+15\left(\frac{-r_{21}^2+r_{31}^2+3r_{32}^2}{r_{32}^2}\right)V_T(r_{32})
$$
$$
+8\left(-r_{21}^2+r_{31}^2+3r_{32}^2\right)V_T(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\bigg|u(r_{21},r_{31},r_{32})\bigg\rangle
$$

$$
\begin{aligned}
&+\frac{i\hbar(P_x-iP_y)}{4Mmc^2}\frac{1}{12\sqrt{3}}\Big\langle \phi_D(r_{31})f(r_{2|31})\Big| \\
&5\left(3r_{21}^2-r_{31}^2+r_{32}^2\right)\frac{1}{r_{21}}\left(\frac{d}{dr_{21}}V_T(r_{21})\right)+15\left(\frac{3r_{21}^2-r_{31}^2+r_{32}^2}{r_{21}^2}\right)V_T(r_{21}) \\
&+8\left(3r_{21}^2-r_{31}^2+r_{32}^2\right)V_T(r_{21})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&-2\left(\frac{-5r_{21}^4+3r_{31}^4+3r_{32}^4-6r_{21}^2r_{31}^2+2r_{21}^2r_{32}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&+2\left(\frac{3r_{21}^4+r_{31}^4+3r_{32}^4-6r_{21}^2r_{32}^2-4r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&+2\left(\frac{3r_{21}^4+r_{31}^4+3r_{32}^4-4r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}} \\
&-2\left(\frac{3r_{21}^4+3r_{31}^4-5r_{32}^4-6r_{21}^2r_{31}^2+2r_{21}^2r_{32}^2-6r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&+5\left(r_{21}^2-r_{31}^2+3r_{32}^2\right)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_T(r_{32})\right)+15\left(\frac{r_{21}^2-r_{31}^2+3r_{32}^2}{r_{32}^2}\right)V_T(r_{32}) \\
&+8\left(r_{21}^2-r_{31}^2+3r_{32}^2\right)V_T(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\Big|u(r_{21},r_{31},r_{32})\Big\rangle \\
&+\frac{i\hbar(P_x-iP_y)}{4Mmc^2}\frac{1}{12\sqrt{3}}\Big\langle \phi_D(r_{32})f(r_{1|32})\Big| \\
&5\left(3r_{21}^2+r_{31}^2-r_{32}^2\right)\frac{1}{r_{21}}\left(\frac{d}{dr_{21}}V_T(r_{21})\right)+15\left(\frac{3r_{21}^2+r_{31}^2-r_{32}^2}{r_{21}^2}\right)V_T(r_{21}) \\
&+8\left(3r_{21}^2+r_{31}^2-r_{32}^2\right)V_T(r_{21})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&-2\left(\frac{-5r_{21}^4+3r_{31}^4+3r_{32}^4+2r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\Bigg\} \\
&+5\left(r_{21}^2+3r_{31}^2-r_{32}^2\right)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_T(r_{31})\right)+15\left(\frac{r_{21}^2+3r_{31}^2-5r_{32}^2}{r_{31}^2}\right)V_T(r_{31}) \\
&+8\left(r_{21}^2+3r_{31}^2-r_{32}^2\right)V_T(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&-2\left(\frac{3r_{21}^4-5r_{31}^4+3r_{32}^4+2r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2-6r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}} \\
&+2\left(\frac{3r_{21}^4+3r_{31}^4+r_{32}^4-6r_{21}^2r_{31}^2-4r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&+2\left(\frac{3r_{21}^4+3r_{31}^4+r_{32}^4-6r_{21}^2r_{31}^2-4r_{21}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\Big|u(r_{21},r_{31},r_{32})\Big\rangle.
\end{aligned}
\tag{50}
$$

This contribution is composed of three sets of terms which differ only in numbering. We can write this as

$$
\left\langle \mathrm{HD}\left(L=1,S=\frac{1}{2}\right)J=\frac{3}{2}M_J=\frac{1}{2}\right|\left(\hat{H}'_{int}(j,k)\right)^{(tensor)}_{NR}\left|^3\mathrm{He}\ J=\frac{1}{2}M_J=\frac{1}{2}\right\rangle
$$

$$
\begin{aligned}
&= \frac{i\hbar(P_x - iP_y)}{4Mmc^2}\frac{1}{12\sqrt{3}}\Big\langle \phi_D(r_{21})f(r_{3|21})\Big| \\
&2\left(\frac{r_{21}^4 + 3r_{31}^4 + 3r_{32}^4 - 4r_{21}^2r_{32}^2 - 6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&+2\left(\frac{r_{21}^4 + 3r_{31}^4 + 3r_{32}^4 - 4r_{21}^2r_{31}^2 - 6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}} \\
&-2\left(\frac{3r_{21}^4 - 5r_{31}^4 + 3r_{32}^4 - 6r_{21}^2r_{31}^2 - 6r_{21}^2r_{32}^2 + 2r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&+5\Big(-r_{21}^2 + 3r_{31}^2 + r_{32}^2\Big)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_T(r_{31})\right) + 15\left(\frac{-r_{21}^2 + 3r_{31}^2 + r_{32}^2}{r_{31}^2}\right)V_T(r_{31}) \\
&+8\Big(-r_{21}^2 + 3r_{31}^2 + r_{32}^2\Big)V_T(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&-2\left(\frac{3r_{21}^4 + 3r_{31}^4 - 5r_{32}^4 - 6r_{21}^2r_{31}^2 - 6r_{21}^2r_{32}^2 + 2r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&+5\Big(-r_{21}^2 + r_{31}^2 + 3r_{32}^2\Big)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_T(r_{32})\right) + 15\left(\frac{-r_{21}^2 + r_{31}^2 + 3r_{32}^2}{r_{32}^2}\right)V_T(r_{32}) \\
&+8\Big(-r_{21}^2 + r_{31}^2 + 3r_{32}^2\Big)V_T(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\Big|u(r_{21}, r_{31}, r_{32})\Big\rangle \\
&+ \quad (1 \to 3) \quad + \quad (2 \to 3)
\end{aligned} \tag{51}
$$

7.2. HD $\left(L = 1, S = \frac{3}{2}\right)$ $J = \frac{3}{2}$ case

$$
\begin{aligned}
&\Big\langle \mathrm{HD}\left(L = 1, S = \frac{3}{2}\right)J = \frac{3}{2}M_J = \frac{1}{2}\Big|\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(tensor)}\Big|^3\mathrm{He}\ J = \frac{1}{2}M_J = \frac{1}{2}\Big\rangle \\
&= -\frac{i\hbar(P_x - iP_y)}{4Mmc^2}\frac{1}{24\sqrt{15}}\Big\langle \phi_D(r_{21})f(r_{3|21})\Big| \\
&8\left(\frac{r_{21}^4 + 3r_{31}^4 + 3r_{32}^4 - 4r_{21}^2r_{32}^2 - 6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&+8\left(\frac{r_{21}^4 + 3r_{31}^4 + 3r_{32}^4 - 4r_{21}^2r_{31}^2 - 6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}} \\
&-7\left(\frac{3r_{21}^4 - 5r_{31}^4 + 3r_{32}^4 - 6r_{21}^2r_{31}^2 - 6r_{21}^2r_{32}^2 + 2r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&+10\Big(-r_{21}^2 + 3r_{31}^2 + r_{32}^2\Big)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_T(r_{31})\right) + 30\left(\frac{-r_{21}^2 + 3r_{31}^2 + r_{32}^2}{r_{31}^2}\right)V_T(r_{31}) \\
&+40\Big(-r_{21}^2 + 3r_{31}^2 + r_{32}^2\Big)V_T(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&+3\left(\frac{3r_{21}^4 + 7r_{31}^4 + 3r_{32}^4 - 10r_{21}^2r_{31}^2 - 6r_{21}^2r_{32}^2 + 6r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}
\end{aligned}
$$

$$
\begin{aligned}
&-7\left(\frac{3r_{21}^4+3r_{31}^4-5r_{32}^4-6r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2+2r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\\
&+3\left(\frac{3r_{21}^4+3r_{31}^4+7r_{32}^4-6r_{21}^2r_{31}^2-10r_{21}^2r_{32}^2+6r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+10\left(\frac{-r_{21}^2+r_{31}^2+3r_{32}^2}{r_{32}^2}\right)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_T(r_{32})\right)+30\left(\frac{-r_{21}^2+r_{31}^2+3r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\\
&+40\left(-r_{21}^2+r_{31}^2+3r_{32}^2\right)V_T(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\Big|u(r_{21},r_{31},r_{32}\Big\rangle\\
&+\quad(1\rightarrow 3)\quad+\quad(2\rightarrow 3)
\end{aligned}
\tag{52}
$$

7.3. HD $\left(L=1,S=\frac{1}{2}\right)$ $J=\frac{1}{2}$ case

$$
\begin{aligned}
&\left\langle \mathrm{HD}\left(L=1,S=\frac{1}{2}\right)J=\frac{1}{2}M_J=\frac{1}{2}\right|\left(\hat{H}'_{int}(j,k)\right)_{NR}^{(tensor)}\Big|^3\mathrm{He}\ J=\frac{1}{2}M_J=\frac{1}{2}\Big\rangle\\
&=\ -\frac{i\hbar P_z}{4Mmc^2}\frac{1}{18\sqrt{2}}\Big\langle\phi_D(r_{21})f(r_{3|21})\Big|\\
&-2\left(\frac{r_{21}^4+3r_{31}^4+3r_{32}^4-4r_{21}^2r_{31}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\\
&-2\left(\frac{r_{21}^4+3r_{31}^4+3r_{32}^4-4r_{21}^2r_{32}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+3\left(\frac{3r_{21}^4+7r_{31}^4+3r_{32}^4-10r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2+6r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\\
&+\left(\frac{-3r_{21}^4+5r_{31}^4-3r_{32}^4+6r_{21}^2r_{31}^2+6r_{21}^2r_{32}^2-2r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\\
&+10\left(-r_{21}^2+3r_{31}^2+r_{32}^2\right)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_T(r_{31})\right)+30\left(\frac{-r_{21}^2+3r_{31}^2+r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\\
&+16\left(-r_{21}^2+3r_{31}^2+r_{32}^2\right)V_T(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+\left(\frac{-3r_{21}^4-3r_{31}^4+5r_{32}^4+6r_{21}^2r_{31}^2+6r_{21}^2r_{32}^2-2r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\\
&+3\left(\frac{3r_{21}^4+3r_{31}^4+7r_{32}^4-6r_{21}^2r_{31}^2-10r_{21}^2r_{32}^2+6r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\\
&+10\left(-r_{21}^2+r_{31}^2+3r_{32}^2\right)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_T(r_{32})\right)+30\left(\frac{-r_{21}^2+r_{31}^2+3r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\\
&+16\left(-r_{21}^2+r_{31}^2+3r_{32}^2\right)V_T(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\Big|u(r_{21},r_{31},r_{32})\Big\rangle\\
&+\quad(1\rightarrow 3)\quad+\quad(2\rightarrow 3)
\end{aligned}
\tag{53}
$$

7.4. HD $\left(L=1, S=\frac{3}{2}\right) J=\frac{1}{2}$ case

$$
\begin{aligned}
&\left\langle \mathrm{HD}\left(L=1,S=\frac{3}{2}\right)J=\frac{1}{2}M_J=\frac{1}{2}\right|\left(\hat{H}'_{int}(j,k)\right)^{(tensor)}_{NR}\left|^3\mathrm{He}\ J=\frac{1}{2}M_J=\frac{1}{2}\right\rangle \\
&= -\frac{i\hbar P_z}{4Mmc^2}\frac{1}{36}\left\langle \phi_D(r_{21})f(r_{3|21})\right| \\
&+8\left(\frac{r_{21}^4+3r_{31}^4+3r_{32}^4-4r_{21}^2r_{32}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&8\left(\frac{r_{21}^4+3r_{31}^4+3r_{32}^4-4r_{21}^2r_{31}^2-6r_{31}^2r_{32}^2}{r_{21}^2}\right)V_T(r_{21})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}} \\
&\left(\frac{3r_{21}^4-5r_{31}^4+3r_{32}^4-6r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2+2r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&-2\left(r_{21}^2-3r_{31}^2-r_{32}^2\right)\frac{1}{r_{31}}\left(\frac{d}{dr_{31}}V_T(r_{31})\right)-6\left(\frac{r_{21}^2-3r_{31}^2-r_{32}^2}{r_{31}^2}\right)V_T(r_{31}) \\
&+8\left(-r_{21}^2+3r_{31}^2+r_{32}^2\right)V_T(r_{31})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&+3\left(\frac{3r_{21}^4+7r_{31}^4+3r_{32}^4-10r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2+6r_{31}^2r_{32}^2}{r_{31}^2}\right)V_T(r_{31})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}} \\
&+\left(\frac{3r_{21}^4+3r_{31}^4-5r_{32}^4-6r_{21}^2r_{31}^2-6r_{21}^2r_{32}^2+2r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}} \\
&+3\left(\frac{3r_{21}^4+3r_{31}^4+7r_{32}^4-6r_{21}^2r_{31}^2-10r_{21}^2r_{32}^2+6r_{31}^2r_{32}^2}{r_{32}^2}\right)V_T(r_{32})\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}} \\
&-2\left(r_{21}^2-r_{31}^2-3r_{32}^2\right)\frac{1}{r_{32}}\left(\frac{d}{dr_{32}}V_T(r_{32})\right)-6\left(\frac{r_{21}^2-r_{31}^2-3r_{32}^2}{r_{32}^2}\right)V_T(r_{32}) \\
&+8\left(-r_{21}^2+r_{31}^2+3r_{32}^2\right)V_T(r_{32})\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\left|u(r_{21},r_{31},r_{32})\right\rangle \\
&+\ (1\rightarrow 3)\ +\ (2\rightarrow 3)
\end{aligned}
\tag{54}
$$

7.5. Tensor potential definition

For these expressions, we have used $V_T(r)$ defined to be consistent with

$$
\hat{V}_{jk}^{(tensor)}(r) \;=\; (\boldsymbol{\tau}_j\cdot\boldsymbol{\tau}_k)\left(\frac{(\boldsymbol{\sigma}_j\cdot\mathbf{r})(\boldsymbol{\sigma}_k\cdot\mathbf{r})}{r^2}-\frac{\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_k}{3}\right)V_T(r) \tag{55}
$$

8. Wigner–Eckart theorem

The Wigner–Eckart theorem can be written as

$$\langle jm|T_q^{(k)}|j'm'\rangle \;=\; \langle j'm'kq|jm\rangle\langle j||T^{(k)}||j'\rangle \tag{56}$$

where $\langle jm|T_q^{(k)}|j'm'\rangle$ is a (normal) matrix element similar to what we are working with in the reductions above, and where $\langle j||T^{(q)}||j'\rangle$ is a reduced matrix element which depends on the configurations but not on the sublevels. The term $\langle j'm'kq|jm\rangle$ is a Clebsch–Gordan coefficient which gives the coupling to the different sublevels based on the order k of the tensor interaction.

This can be used to determine the reduced matrix element for a transition through

$$\langle j||T^{(k)}||j'\rangle \;=\; \frac{\langle jm|T_q^{(k)}|j'm'\rangle}{\langle j'm'kq|jm\rangle.} \tag{57}$$

For us this allows for a consistency check for the Mathematica calculations (and was used as a tool to debug the model). We developed a set of additional nuclear states, including the $M_J = -\frac{1}{2}$ state of the ^{3}He nucleus, as well as four additional molecular HD states, and used these to test for consistency with the Wigner–Eckart theorem. Tests were carried out both for the central contribution and for the tensor contribution to the lowest order phonon–nuclear interaction matrix elements. In all cases we found consistency.

9. Discussion

The relativistic phonon–nuclear interaction is relatively simple in form written as

$$\hat{H}_{int} \;=\; \frac{1}{2Mc}\sum_{j<k}\left[\beta_j\boldsymbol{\alpha}_j + \beta_k\boldsymbol{\alpha}_k, \hat{V}_{jk}\right]\cdot\hat{\mathbf{P}}. \tag{58}$$

The nonrelativistic reduction for the one-pion exchange potential is a bit more complicated

$$\left(\hat{H}'_{int}(j,k)\right)_{NR} \;=\; -\frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_j\cdot\mathbf{p}_j, \left[\boldsymbol{\sigma}_j\cdot\mathbf{P}, \hat{V}_{jk}^{(NR)}\right]\right] - \frac{1}{4Mmc^2}\left[\boldsymbol{\sigma}_k\cdot\mathbf{p}_k, \left[\boldsymbol{\sigma}_k\cdot\mathbf{P}, \hat{V}_{jk}^{(NR)}\right]\right]. \tag{59}$$

As is apparent from the results above, the implementation of this interaction for the relatively simple 3-body problem associated with the HD/^{3}He single-phonon transition is pretty complicated.

What remains to be done is to evaluate the radial integrals associated with the matrix elements presented above. In the case of simple approximate models for the deuteron wave function, molecular HD wave function, and ^{3}He nucleus this should be straightforward. A more sophisticated treatment might involve the use of a more realistic ^{3}He wave function, along with correlation effects for the molecular and deuteron wave functions when the proton and deuteron are close. The question of how much contribution comes from short range interactions remains to be dealt with.

Working with a brute force Mathematica calculation turned out to be useful in this calculation. There were some technical issues to be dealt with, as we learned that Mathematica does better when a big calculation is split up into smaller pieces. The calculations for the central potential contribution took on the order of minutes, and the calculations for the tensor potential terms took on the order of hours.

We are interested in the extension of this kind of calculation for the D_2/^{4}He phonon–nuclear coupling matrix elements. Conceptually, it would be very similar. On the other hand, the matrices will be much larger, which suggests that the calculations will be much slower. Due to the importance of the associated matrix element in the field, we are motivated to try such a calculation in the future.

A summary of this calculation was presented at ICCF22.

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