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A New Treatment of 2N and 3N Bound States in Three Dimensions

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Abstract The direct treatment of the Faddeev equation for the three-boson system in 3 dimensions is generalized to nucleons. The one Faddeev equation for identical bosons is replaced by a strictly finite set of coupled equations for scalar functions which depend only on 3 variables. The spin-momentum dependence occurring as scalar products in 2N and 3N forces accompanied by scalar functions is supplemented by a corresponding expansion of the Faddeev amplitudes. After removing the spin degrees of freedom by suitable operations only scalar expressions depending on momenta remain. The corresponding steps are performed for the deuteron leading to two coupled equations.

1 Introduction

With the advent of chiral three-nucleon (3N) forces at $N^3\text{LO}$ (1; 2) which have a rich spin and momentum structure, the calculation of the 3N system based on standard partial wave representations is rather tedious. Moreover, for higher angular momenta it is a challenging task to reliably control the numerical accuracy (3). For a system of three bosons a numerical treatment working directly with momentum vectors for bound and scattering states including model three-boson forces turned out to be very feasible (4; 5; 6; 7). Therefore, we suggest to also formulate the Faddeev equation for the 3N system directly with vector variables. Our proposed

Dedicated to Prof. W. Plessas on the occasion of his 60th birthday.

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formulation is an alternative to Ref. (8), where spin and iso-spin couplings are explicitly carried out. The key ingredient thereby is an operator representation of the ^3He wave function given long time ago by (9) and later on modified and strictly re-derived from the complete partial wave representation (10). Thus, the idea is to represent 2N t-operators, the 3N forces and the Faddeev components of the 3N wave function as products of scalar functions with scalar products of spin operators and momentum vectors. Furthermore, by suitable operations one removes the spin operators leading to relations among scalar functions of momentum vectors only.

In Sect. 2 we consider the deuteron as warm-up exercise, whereas the central topic, the treatment of the 3N Faddeev equation, is given in Sect. 3. We end with a brief summary and outlook in Sect. 4.

2 The Deuteron

The deuteron momentum wave function has the well known operator form (see for instance (11; 12))

$$\begin{aligned}\Psi_{m_d} &= \left[\phi_1(p) + \left(\sigma_{(2)} \cdot \mathbf{p} \, \sigma_{(3)} \cdot \mathbf{p} - \frac{1}{3} p^2 \right) \phi_2(p) \right] |1m_d\rangle \\ &\equiv \sum_{k=1}^2 \phi_k(p) b_k(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}) |1m_d\rangle,\end{aligned}\quad (1)$$

where $|1m_d\rangle$ describes the state in which two spin 1/2 states are coupled to total spin 1 and magnetic quantum number m_d . The scalar functions $\phi_1(p)$ describes the spherical part of the wave function. Applying a tensor operator to the scalar function $\phi_2(p)$ generates its non-spherical part. We label the two nucleons as particles 2 and 3, and the operator $\sigma_{(i)}$ ($i=2,3$), represents the corresponding spin operators.

As is well known, rotational-, parity-, and time reversal-invariance restrict any NN potential V to be formed with six terms (13), so that the most general NN force has the form

$$V(\mathbf{p}, \mathbf{p}') = \sum_{j=1}^6 v_j(\mathbf{p}, \mathbf{p}') w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}'), \quad (2)$$

with $v_j(\mathbf{p}, \mathbf{p}')$ being scalar functions. The spin-momentum scalar operators $w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}')$ are given by

$$\begin{aligned}w_1 &= 1 \\ w_2 &= (\sigma_{(2)} + \sigma_{(3)}) \cdot (\mathbf{p} \times \mathbf{p}') \\ w_3 &= \sigma_{(2)} \cdot (\mathbf{p} \times \mathbf{p}') \, \sigma_{(3)} \cdot (\mathbf{p} \times \mathbf{p}') \\ w_4 &= \sigma_{(2)} \cdot (\mathbf{p} + \mathbf{p}') \, \sigma_{(3)} \cdot (\mathbf{p} + \mathbf{p}') \\ w_5 &= \sigma_{(2)} \cdot (\mathbf{p} - \mathbf{p}') \, \sigma_{(3)} \cdot (\mathbf{p} - \mathbf{p}') \\ w_6 &= \sigma_{(2)} \cdot \sigma_{(3)}\end{aligned}\quad (3)$$

and represent the maximum possible set of invariant operators. On the energy shell, w_6 can be expressed as a linear combination of w_3 , w_4 , and w_5 , leading to the well known Wolfenstein representation of the elastic NN scattering amplitude (13). Using these operators the Schrödinger equation in integral form reads

$$\begin{aligned}
 & \left[\phi_1(p) + \left(\sigma_{(2)} \cdot \mathbf{p} \, \sigma_{(3)} \cdot \mathbf{p} - \frac{1}{3} p^2 \right) \phi_2(p) \right] |1m_d\rangle \\
 &= \frac{1}{E_d - \frac{p^2}{m}} \int d^3 p' \sum_{j=1}^6 v_j(\mathbf{p}, \mathbf{p}') w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \\
 & \quad \times \left[\phi_1(p') + \left(\sigma_{(2)} \cdot \mathbf{p}' \, \sigma_{(3)} \cdot \mathbf{p}' - \frac{1}{3} p'^2 \right) \phi_2(p') \right] |1m_d\rangle. \quad (4)
 \end{aligned}$$

We remove the spin dependence by projecting from the left with $\langle 1m_d | b_k(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p})$ and summing over m_d . This leads to

$$\begin{aligned}
& \sum_{m_d=-1}^1 \langle 1m_d | b_k(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}) \sum_{k'=1}^2 \phi_{k'}(p) b_{k'}(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}) | 1m_d \rangle \\
&= \frac{1}{E_d - \frac{p^2}{m}} \sum_{m_d=-1}^1 \int d^3 p' \sum_{j=1}^6 v_j(\mathbf{p}, \mathbf{p}') \langle 1m_d | b_k(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \\
&\quad \times \sum_{k''=1}^2 \phi_{k''}(p') b_{k''}(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}') | 1m_d \rangle . \tag{5}
\end{aligned}$$

If we define the scalar objects

$$\begin{aligned}
A_{kk'}(p) &\equiv \sum_{m_d=-1}^1 \langle 1m_d | b_k(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}) b_{k'}(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}) | 1m_d \rangle \tag{6} \\
B_{kjk''}(\mathbf{p}, \mathbf{p}') &\equiv \sum_{m_d=-1}^1 \langle 1m_d | b_k(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') b_{k''}(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}') | 1m_d \rangle
\end{aligned}$$

which can be calculated once for all we obtain

$$\sum_{k'=1}^2 A_{kk'}(p) \phi_{k'}(p) = \frac{1}{E_d - \frac{p^2}{m}} \int d^3 p' \sum_{j=1}^6 v_j(\mathbf{p}, \mathbf{p}') \sum_{k''=1}^2 B_{kjk''}(\mathbf{p}, \mathbf{p}') \phi_{k''}(p') . \tag{8}$$

This is a set of two coupled equations for the s- and d-wave components $\phi_1(p)$ and $\phi_2(p)$. The summation over m_d guarantees the scalar nature of $A_{kk'}(p)$ and $B_{kjk''}(\mathbf{p}, \mathbf{p}')$. Expressions for $A_{kk'}(p)$ and $B_{kjk''}(\mathbf{p}, \mathbf{p}')$ are given in the Appendix.

The azimuthal angle can be trivially integrated out, leading to the final form of the deuteron equation

$$\sum_{k'=1}^2 A_{kk'}(p) \phi_{k'}(p) = \frac{2\pi}{E_d - \frac{p^2}{m}} \sum_{k''=1}^2 \int_0^\infty dp' p'^2 \phi_{k''}(p') \int_{-1}^1 dx \sum_{j=1}^6 v_j(p, p', x) B_{kjk''}(p, p', x) \tag{9}$$

where $x \equiv \hat{\mathbf{p}} \cdot \hat{\mathbf{p}}'$.

3 The 3N Bound State

The Faddeev equation for the 3N bound state reads

$$\psi = G_0 t P \psi + (1 + G_0 t) G_0 V^{(1)} (1 + P) \psi, \tag{10}$$

where G_0 is the free propagator, t the NN t -operator for nucleons 2 and 3, the permutation operator

$P = P_{12}P_{23} + P_{13}P_{23}$. The term $V^{(1)}$ is that part of the 3N force, which is symmetrical under exchange of nucleons 2 and 3. The choice of the subsystem pair 2, 3 is of course arbitrary. The Faddeev component is given by ψ , and the total 3N state is then $\Psi = (1 + P)\psi$.

We introduce the three possible 3N isospin states

$$\begin{aligned} |\gamma_0\rangle &= |0 \frac{1}{2}\rangle \frac{1}{2} \\ |\gamma_1\rangle &= |1 \frac{1}{2}\rangle \frac{1}{2} \\ |\gamma_2\rangle &= |1 \frac{1}{2}\rangle \frac{3}{2}, \end{aligned} \quad (11)$$

with the notation that the 2N subsystem isospin is either 0 or 1 and coupled with the isospin of the third nucleon to the total isospins $T = 1/2$ or $3/2$.

We expand the Faddeev component ψ , the 2N t-matrix t , and $V^{(1)}$ as

$$\psi = \sum_{\gamma} |\gamma\rangle \psi_{\gamma} \equiv \sum_{iT} |t \frac{1}{2}\rangle T \psi_{iT} \quad (12)$$

$$t = \sum_{\gamma, \gamma'} |\gamma\rangle t_{\gamma, \gamma'} \langle \gamma| \quad (13)$$

$$V^{(1)} = \sum_{\gamma, \gamma'} |\gamma\rangle V_{\gamma, \gamma'}^{(1)} \langle \gamma|. \quad (14)$$

Then projecting Eq. (10) from the left, we obtain

$$\psi_{\gamma} = G_0 \sum_{\gamma', \gamma''} t_{\gamma, \gamma'} \langle \gamma' | P | \gamma'' \rangle \psi_{\gamma''} + \sum_{\gamma', \gamma'', \gamma'''} \langle \gamma | (1 + G_0 t) | \gamma' \rangle G_0 V_{\gamma', \gamma''}^{(1)} \langle \gamma'' | (1 + P) | \gamma''' \rangle \psi_{\gamma'''} \quad (15)$$

We neglect the change of the total 2N isospin and the change of the total 3N isospin in the 3NF and define

$$t_{\gamma, \gamma'} \equiv \delta_{iT' T'} t_{iT T'} \quad (16)$$

$$V_{\gamma, \gamma'}^{(1)} \equiv \delta_{T T'} V_{iT' T'}^{(1)}. \quad (17)$$

Furthermore (14),

$$\langle \gamma | P | \gamma' \rangle = \delta_{T T'} P_{iT' T} = \delta_{T T'} F_{iT' T} (P_{12}^{sm} P_{23}^{sm} + (-)^{t+t'} P_{13}^{sm} P_{23}^{sm}), \quad (18)$$

where $F_{iT' T}$ are geometrical factors and P_{ij}^{sm} acts only in spin and momentum space.

Inserting all that into Eq. (15) yields

$$\begin{aligned} \psi_{iT} &= G_0 \sum_{T'} t_{iT T'} \sum_{i'} F_{iT' T'} (P_{12}^{sm} P_{23}^{sm} + (-)^{t+t'} P_{13}^{sm} P_{23}^{sm}) \psi_{i' T'} \\ &+ \sum_{T'} (\delta_{T T'} + G_0 t_{iT T'}) G_0 \sum_{i'} V_{iT' T'}^{(1)} \\ &\times \sum_{i''} (\delta_{i' i''} + F_{i' i'' T'} (P_{12}^{sm} P_{23}^{sm} + (-)^{t'+t''} P_{13}^{sm} P_{23}^{sm})) \psi_{i'' T'}. \end{aligned} \quad (19)$$

The charge independence and charge symmetry breaking in the 2N force leads to the coupling of total isospin $T = 1/2$ and $3/2$.

In the space spanned by the two Jacobi momenta $\mathbf{p}$ and $\mathbf{q}$ we encounter the off-shell NN t -matrix

$$\langle \mathbf{p}\mathbf{q} | t_{TT'} | \mathbf{p}'\mathbf{q}' \rangle = \delta(\mathbf{q} - \mathbf{q}') t_{TT'}(\mathbf{p}, \mathbf{p}', E_q) \quad (20)$$

with $E_q \equiv E - \frac{3}{4m}q^2$ and the matrices for the permutations (15)

$$\begin{aligned} \langle \mathbf{p}\mathbf{q} | P_{12}^{sm} P_{23}^{sm} | \mathbf{p}'\mathbf{q}' \rangle &= \delta(\mathbf{p} - \pi(\mathbf{q}, \mathbf{q}')) \delta(\mathbf{p}' - \pi'(\mathbf{q}, \mathbf{q}')) P_{12}^s P_{23}^s \\ \langle \mathbf{p}\mathbf{q} | P_{13}^{sm} P_{23}^{sm} | \mathbf{p}'\mathbf{q}' \rangle &= \delta(\mathbf{p} + \pi(\mathbf{q}, \mathbf{q}')) \delta(\mathbf{p}' + \pi'(\mathbf{q}, \mathbf{q}')) P_{13}^s P_{23}^s \end{aligned} \quad (21)$$

with

$$\pi(\mathbf{q}, \mathbf{q}') = \frac{1}{2}\mathbf{q} + \mathbf{q}' \quad (22)$$

$$\pi'(\mathbf{q}, \mathbf{q}') = \mathbf{q} + \frac{1}{2}\mathbf{q}'. \quad (23)$$

Consequently with $\psi_{iT}(\mathbf{p}, \mathbf{q}) \equiv \langle \mathbf{p}\mathbf{q} | \psi_{iT} \rangle$ we get

$$\begin{aligned} \psi_{iT}(\mathbf{p}, \mathbf{q}) &= \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 q' \\ &\times \sum_{T'} \left(t_{TT'}(\mathbf{p}, \pi(\mathbf{q}, \mathbf{q}'), E_q) P_{12}^s P_{23}^s \sum_{T''} F_{TT''} \psi_{T''}(\pi'(\mathbf{q}, \mathbf{q}'), \mathbf{q}') \right. \\ &+ (-)^{t+t'} t_{TT'}(\mathbf{p}, -\pi(\mathbf{q}, \mathbf{q}'), E_q) P_{13}^s P_{23}^s \sum_{T''} F_{TT''} \psi_{T''}(-\pi'(\mathbf{q}, \mathbf{q}'), \mathbf{q}') \Big) \\ &+ \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 p' d^3 q' \sum_{T'} V_{TT'}^{(1)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \psi_{T'}(\mathbf{p}', \mathbf{q}') \\ &+ \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' t_{TT'}(\mathbf{p}, \mathbf{p}', E_q) \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \\ &\times \sum_{T''} \int d^3 p'' d^3 q'' V_{TT''}^{(1)}(\mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') \psi_{T''}(\mathbf{p}'', \mathbf{q}'') \\ &+ \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 q' d^3 q'' \\ &\times \sum_{T'} \left(V_{TT'}^{(1)}(\mathbf{p}, \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{12}^s P_{23}^s \sum_{T''} F_{TT''} \psi_{T''}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \right. \\ &+ (-)^{t'+t''} V_{TT'}^{(1)}(\mathbf{p}, \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{13}^s P_{23}^s \sum_{T''} F_{TT''} \psi_{T''}(-\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Big) \\ &+ \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' t_{TT'}(\mathbf{p}, \mathbf{p}', E_q) \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \\ &\times \int d^3 q' d^3 q'' \sum_{T''} \left(V_{TT''}^{(1)}(\mathbf{p}', \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{12}^s P_{23}^s \sum_{T'''} F_{TT'''} \psi_{T'''}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \right. \\ &+ (-)^{t'+t''} V_{TT''}^{(1)}(\mathbf{p}', \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{13}^s P_{23}^s \\ &\times \sum_{T'''} F_{TT'''} \psi_{T'''}(-\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Big). \end{aligned} \quad (24)$$

The antisymmetry of the Faddeev component under exchange of particles 2 and 3 imposes the condition

$$(-)^t P_{23}^{sm} \psi_{iT} = \psi_{iT} \quad (25)$$

which in momentum space reads

$$(-)^t P_{23}^s \psi_{iT}(-\mathbf{p}, \mathbf{q}) = \psi_{iT}(\mathbf{p}, \mathbf{q}). \quad (26)$$

Thus ψ_{0T} (ψ_{1T}) is even (odd) under exchange of particles 2 and 3 in spin and momenta.

This relation can be used to simplify Eq. (24). We regard

$$P_{13}^s P_{23}^s \psi_{iT}(-\mathbf{p}, \mathbf{q}) = P_{23}^s P_{12}^s P_{23}^s \psi_{iT}(-\mathbf{p}, \mathbf{q}) = P_{23}^s P_{12}^s P_{23}^s (-)^t \psi_{iT}(\mathbf{p}, \mathbf{q}) \quad (27)$$

which turns Eq. (24) into

$$\begin{aligned} \psi_{iT}(\mathbf{p}, \mathbf{q}) = & \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 q' \\ & \times \sum_{T'} (t_{iTT'}(\mathbf{p}, \pi(\mathbf{q}, \mathbf{q}'), E_q) + (-)^t t_{iTT'}(\mathbf{p}, -\pi(\mathbf{q}, \mathbf{q}'), E_q) P_{23}^s) \\ & \times P_{12}^s P_{23}^s \sum_{T'} F_{iT'T'} \psi_{iT'}(\pi'(\mathbf{q}, \mathbf{q}'), \mathbf{q}') \\ & + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 p' d^3 q' \sum_{T'} V_{iT'T}^{(1)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \psi_{iT'}(\mathbf{p}', \mathbf{q}') \\ & + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' t_{iTT'}(\mathbf{p}, \mathbf{p}', E_q) \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \\ & \times \sum_{T'} \int d^3 p'' d^3 q'' V_{iT'T'}^{(1)}(\mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') \psi_{iT'}(\mathbf{p}'', \mathbf{q}'') \\ & + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 q' d^3 q'' \\ & \times \sum_{T'} (V_{iT'T}^{(1)}(\mathbf{p}, \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') + (-)^t V_{iT'T}^{(1)}(\mathbf{p}, \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{23}^s) \\ & \times P_{12}^s P_{23}^s \sum_{T''} F_{iT'T''} \psi_{iT''}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \\ & + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' t_{iTT'}(\mathbf{p}, \mathbf{p}', E_q) \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \\ & \times \int d^3 q' d^3 q'' \\ & \times \sum_{T'} (V_{iT'T'}^{(1)}(\mathbf{p}', \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') + (-)^t V_{iT'T'}^{(1)}(\mathbf{p}', \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{23}^s) \\ & \times P_{12}^s P_{23}^s \sum_{T''} F_{iT'T''} \psi_{iT''}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}''). \end{aligned} \quad (28)$$

We now come to the decisive points. In Ref. (10) we derived the operator form of the 3N bound state wave function based on the complete set of partial wave states.

Exactly the same arguments can be applied to the Faddeev components $\psi_{iT}(\mathbf{p}, \mathbf{q})$. Thus, in the notation of Ref. (10) one can write

$$\psi_{iT}(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^8 \phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) O_i |\chi^m\rangle = \sum_{i=1}^8 \tilde{\phi}_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) |\chi_i\rangle, \quad (29)$$

where $|\chi^m\rangle = |(0\frac{1}{2})\frac{1}{2}m\rangle$ is a specific state in which the three spin-1/2 states are coupled to the total angular momentum quantum numbers of the 3N bound state.

The functions $\phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q})$ are scalar functions and the operators O_i are given as

$$\begin{aligned} O_1 &= 1 \\ O_2 &= \sigma(23) \cdot \sigma_{(1)} \\ O_3 &= \sigma_{(1)} \cdot (\hat{\mathbf{p}} \times \hat{\mathbf{q}}) \\ O_4 &= \sigma(23) \cdot \hat{\mathbf{p}} \times \hat{\mathbf{q}} \\ O_5 &= \sigma(23) \cdot \hat{\mathbf{q}} \sigma_{(1)} \cdot \hat{\mathbf{p}} \\ O_6 &= \sigma(23) \cdot \hat{\mathbf{p}} \sigma_{(1)} \cdot \hat{\mathbf{q}} \\ O_7 &= \sigma(23) \cdot \hat{\mathbf{p}} \sigma_{(1)} \cdot \hat{\mathbf{p}} \\ O_8 &= \sigma(23) \cdot \hat{\mathbf{q}} \sigma_{(1)} \cdot \hat{\mathbf{q}}. \end{aligned} \quad (30)$$

Here $\sigma(23) \equiv \frac{1}{2}(\sigma_{(2)} - \sigma_{(3)})$. These operators create all possible spin states.

The second expansion in Eq. (29) is based on

$$\begin{aligned} \chi_1 &= |\chi^m\rangle \\ \chi_2 &= \frac{1}{\sqrt{3}} \sigma(23) \cdot \sigma_{(1)} |\chi^m\rangle \\ \chi_3 &= \sqrt{\frac{3}{2}} \frac{1}{i} \sigma_{(1)} \cdot \hat{\mathbf{p}} \times \hat{\mathbf{q}} |\chi^m\rangle \\ \chi_4 &= \frac{1}{\sqrt{2}} \left(i \sigma(23) \times (\hat{\mathbf{p}} \times \hat{\mathbf{q}}) - \sigma_{(1)} \times \sigma(23) \cdot (\hat{\mathbf{p}} \times \hat{\mathbf{q}}) \right) |\chi^m\rangle \\ \chi_5 &= \frac{1}{i} \left(\sigma(23) - \frac{i}{2} \sigma_{(1)} \times \sigma(23) \right) \times (\hat{\mathbf{p}} \times \hat{\mathbf{q}}) |\chi^m\rangle \\ \chi_6 &= \sqrt{\frac{3}{2}} \left(\sigma(23) \cdot \hat{\mathbf{p}} \sigma_{(1)} \cdot \hat{\mathbf{p}} - \frac{1}{3} \sigma(23) \cdot \sigma_{(1)} \right) |\chi^m\rangle \\ \chi_7 &= \sqrt{\frac{3}{2}} \left(\sigma(23) \cdot \hat{\mathbf{q}} \sigma_{(1)} \cdot \hat{\mathbf{q}} - \frac{1}{3} \sigma(23) \cdot \sigma_{(1)} \right) |\chi^m\rangle \\ \chi_8 &= \frac{3}{2} \frac{1}{\sqrt{5}} \left(\sigma(23) \cdot \hat{\mathbf{q}} \sigma_{(1)} \cdot \hat{\mathbf{p}} + \sigma(23) \cdot \hat{\mathbf{p}} \sigma_{(1)} \cdot \hat{\mathbf{q}} - \frac{2}{3} \hat{\mathbf{p}} \cdot \hat{\mathbf{q}} \sigma(23) \cdot \sigma_{(1)} \right) |\chi^m\rangle. \end{aligned} \quad (31)$$

One can express the $|\chi_i\rangle$ in terms of the $O_i |\chi^m\rangle$ and vice versa. Furthermore, we use the most general operator structure of the NN t-matrix $t_{TT'}(\mathbf{p}, \mathbf{p}', E_q)$, which is given by

$$t_{TT'}(\mathbf{p}, \mathbf{p}', E_q) = \sum_{j=1}^6 t_{TT'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}'). \quad (32)$$

Here the matrix elements $t_{TT'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q)$ are scalar functions and the operators $w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}')$ are given in Eq. (3).

Next, the 3NF operator $V_{tt'T}^{(1)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}')$ also allows for an expansion

$$V_{tt'T}^{(1)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') = \sum_l v_{tt'T}^{(l)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \quad (33)$$

with a strictly finite number of terms. In the context of chiral effective field theory 3NF's have been worked out up to N³LO (1; 2; 16), where the expressions can be found. As an example we provide the operators Ω_l for the 2π -exchange (17; 18)

$$V^{(1)} = \frac{\sigma_{(2)} \cdot \mathbf{Q} \sigma_{(3)} \cdot \mathbf{Q}'}{(Q^2 + m_\pi^2)(Q'^2 + m_\pi^2)} (A + B\mathbf{Q} \cdot \mathbf{Q}') \tau(2) \cdot \tau(3) + C\sigma_{(1)} \cdot (\mathbf{Q} \times \mathbf{Q}') \tau(1) \cdot (\tau(2) \times \tau(3)), \quad (34)$$

where $\mathbf{Q}$ and $\mathbf{Q}'$ are momentum transfers of nucleons 2 and 3. Using (18)

$$\begin{aligned} \langle \left(t \frac{1}{2}\right) T | \tau(2) \cdot \tau(3) | \left(t' \frac{1}{2}\right) T \rangle &= -\delta_{tt'} 6(-)^t \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & t \\ \frac{1}{2} & \frac{1}{2} & 1 \end{Bmatrix} \quad (35) \\ \langle \left(t \frac{1}{2}\right) T | \tau(1) \cdot (\tau(2) \times \tau(3)) | \left(t' \frac{1}{2}\right) T \rangle &= i36\sqrt{(2t+1)(2t'+1)}(-)^{t'+\frac{1}{2}+T} \\ &\quad \times \begin{Bmatrix} \frac{1}{2} & t' & T \\ t & \frac{1}{2} & 1 \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 1 \\ \frac{1}{2} & \frac{1}{2} & t \\ \frac{1}{2} & \frac{1}{2} & t' \end{Bmatrix} \quad (36) \end{aligned}$$

one obtains

$$V_{tt'T}^{(1)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') = v_{tt'T}^{(1)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \cdot \mathbf{1} + v_{tt'T}^{(2)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \sigma_{(1)} \cdot ((\mathbf{p} - \mathbf{p}') \times (\mathbf{q} - \mathbf{q}')) \quad (37)$$

with $\mathbf{Q}, \mathbf{Q}'$ expressed in terms of the Jacobi momenta. This defines a subset of the Ω_l operators with the accompanying scalar functions $v_{tt'T}^{(l)}$.

Now we insert Eqs. (29), (32) and (33) into Eq. (28) and obtain

$$\begin{aligned}
& \sum_{i=1}^8 \phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) O_i(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) |\chi^m\rangle \\
&= \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 q' \sum_{T'} \sum_{j=1}^6 \left(t_{iT'T'}^{(j)}(\mathbf{p}, \pi(\mathbf{q}, \mathbf{q}'), E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \pi(\mathbf{q}, \mathbf{q}')) \right. \\
&\quad \left. + (-)^t t_{iT'T'}^{(j)}(\mathbf{p}, -\pi(\mathbf{q}, \mathbf{q}'), E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, -\pi(\mathbf{q}, \mathbf{q}')) P_{23}^s \right) \\
&\quad \times \sum_{t'} F_{t't'T'} \sum_{k=1}^8 \phi_{t't'T'}^{(k)}(\pi'(\mathbf{q}, \mathbf{q}'), \mathbf{q}') P_{12}^s P_{23}^s O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \pi'(\mathbf{q}, \mathbf{q}'), \mathbf{q}') |\chi^m\rangle \\
&\quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 p' d^3 q' \sum_{t'} \sum_l v_{t't'T}^{(l)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \\
&\quad \times \sum_{k=1}^8 \phi_{t'T}^{(k)}(\mathbf{p}', \mathbf{q}') O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}') |\chi^m\rangle \\
&\quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' \sum_{j=1}^6 \left(t_{iT'T'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \right. \\
&\quad \times \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \sum_{t'} \int d^3 p'' d^3 q'' \sum_l v_{t't'T'}^{(l)}(\mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') \\
&\quad \times \sum_{k=1}^8 \phi_{t'T'}^{(k)}(\mathbf{p}'', \mathbf{q}'') O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}'', \mathbf{q}'') |\chi^m\rangle \\
&\quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 q' d^3 q'' \\
&\quad \times \sum_{t'} \left(\sum_l v_{t't'T}^{(l)}(\mathbf{p}, \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \right. \\
&\quad \left. + (-)^{t'} \sum_l v_{t't'T}^{(l)}(\mathbf{p}, \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{23}^s \right) \\
&\quad \times \sum_{t''} F_{t't''T} \sum_{k=1}^8 \phi_{t't''T}^{(k)}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{12}^s P_{23}^s O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') |\chi^m\rangle \\
&\quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' \sum_{j=1}^6 \left(t_{iT'T'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \right. \\
&\quad \times \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \int d^3 q' d^3 q'' \\
&\quad \times \sum_{t'} \left(\sum_l v_{t't'T'}^{(l)}(\mathbf{p}', \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \right. \\
&\quad \left. + (-)^{t'} \sum_l v_{t't'T'}^{(l)}(\mathbf{p}', \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{23}^s \right) \\
&\quad \times \sum_{t''} F_{t't''T} \sum_{k=1}^8 \phi_{t't''T}^{(k)}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{12}^s P_{23}^s O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') |\chi^m\rangle. \quad (38)
\end{aligned}$$

This can be further simplified by using

$$P_{12}^s P_{23}^s O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) |\chi^m\rangle = -\frac{1}{2} O_k(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \mathbf{p}, \mathbf{q}) (1 + \sigma_{(23)} \cdot \sigma_{(1)}) |\chi^m\rangle \quad (39)$$

which turns Eq. (38) into

$$\begin{aligned} & \sum_{i=1}^8 \phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) O_i(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) |\chi^m\rangle \\ &= \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m} q^2} \int d^3 q' \sum_{T'} \sum_{j=1}^6 \left(t_{TT'}^{(j)}(\mathbf{p}, \boldsymbol{\pi}(\mathbf{q}, \mathbf{q}'), E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \boldsymbol{\pi}(\mathbf{q}, \mathbf{q}')) \right. \\ & \quad \left. + (-)^T t_{TT'}^{(j)}(\mathbf{p}, -\boldsymbol{\pi}(\mathbf{q}, \mathbf{q}'), E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, -\boldsymbol{\pi}(\mathbf{q}, \mathbf{q}')) P_{23}^s \right) \\ & \quad \times \sum_{t'} F_{t'T'} \sum_{k=1}^8 \phi_{t'T}^{(k)}(\boldsymbol{\pi}'(\mathbf{q}, \mathbf{q}'), \mathbf{q}') \left(-\frac{1}{2} \right) O_k(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \boldsymbol{\pi}'(\mathbf{q}, \mathbf{q}'), \mathbf{q}') \\ & \quad \times (1 + \sigma_{(23)} \cdot \sigma_{(1)}) |\chi^m\rangle \\ & \quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m} q^2} \int d^3 p' d^3 q' \sum_{t'} \sum_l v_{t'T}^{(l)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \\ & \quad \times \sum_{k=1}^8 \phi_{t'T}^{(k)}(\mathbf{p}', \mathbf{q}') O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}') |\chi^m\rangle \\ & \quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m} q^2} \sum_{T'} \int d^3 p' \sum_{j=1}^6 t_{TT'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m} q'^2} \\ & \quad \times \sum_{t'} \int d^3 p'' d^3 q'' \sum_l v_{t'T}^{(l)}(\mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') \\ & \quad \times \sum_{k=1}^8 \phi_{t'T}^{(k)}(\mathbf{p}'', \mathbf{q}'') O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}'', \mathbf{q}'') |\chi^m\rangle \\ & \quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m} q^2} \int d^3 q' d^3 q'' \\ & \quad \times \sum_{t'} \left(\sum_l v_{t'T}^{(l)}(\mathbf{p}, \mathbf{q}, \boldsymbol{\pi}(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \boldsymbol{\pi}(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \right. \\ & \quad \left. + (-)^{t'} \sum_l v_{t'T}^{(l)}(\mathbf{p}, \mathbf{q}, -\boldsymbol{\pi}(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, -\boldsymbol{\pi}(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{23}^s \right) \\ & \quad \times \sum_{t''} F_{t''T} \sum_{k=1}^8 \phi_{t''T}^{(k)}(\boldsymbol{\pi}'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \left(-\frac{1}{2} \right) O_k(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \boldsymbol{\pi}'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \\ & \quad \times (1 + \sigma_{(23)} \cdot \sigma_{(1)}) |\chi^m\rangle \\ & \quad + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m} q^2} \sum_{T'} \int d^3 p' \sum_{j=1}^6 t_{TT'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \\ & \quad \times \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m} q'^2} \int d^3 q' d^3 q'' \\ & \quad \times \sum_{t'} \left(\sum_l v_{t'T}^{(l)}(\mathbf{p}', \mathbf{q}, \boldsymbol{\pi}(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, \boldsymbol{\pi}(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \right. \end{aligned}$$

$$\begin{aligned}
& + (-)^{t'} \sum_l v_{t't'}^{(l)}(\mathbf{p}', \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \Omega_l(\sigma_{(1)}, \sigma_{(2)} \sigma_{(3)} \mathbf{p}', \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') P_{23}^s) \\
& \times \sum_{t''} F_{t't''T'} \sum_{k=1}^8 \phi_{t''T'}^{(k)}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') (-\frac{1}{2}) O_k(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \\
& \times (1 + \sigma(23) \cdot \sigma_{(1)}) |\chi^m\rangle.
\end{aligned} \tag{40}$$

Analogous to Eq. (5) in case of the deuteron we now project from the left with $\langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q})$ and sum over m . This leads to the following definitions, which are all scalars

$$C_{ki}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) = \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) O_i(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) | \chi^m \rangle \quad (41)$$

$$D_{kjk'}(\mathbf{p}\mathbf{q}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = -\frac{1}{2} \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}') \\ \times O_{k'}(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \mathbf{p}'', \mathbf{q}'') (1 + \sigma(23) \cdot \sigma_{(1)}) | \chi^m \rangle \quad (42)$$

$$D'_{kjk'}(\mathbf{p}\mathbf{q}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = \frac{1}{2} \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}') \\ \times O_{k'}(\sigma_{(3)}, \sigma_{(2)}, \sigma_{(1)}, \mathbf{p}'', \mathbf{q}'') (1 - \sigma(23) \cdot \sigma_{(1)}) | \chi^m \rangle \quad (43)$$

$$E_{klk'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}\mathbf{p}'\mathbf{q}', \mathbf{p}'\mathbf{q}') = \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) \\ \times \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') O_{k'}(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}') | \chi^m \rangle \quad (44)$$

$$F_{kjl k'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{p}', \mathbf{p}'\mathbf{q}\mathbf{p}''\mathbf{q}'', \mathbf{p}''\mathbf{q}'') = \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \\ \times \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') O_{k'}(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \mathbf{p}'', \mathbf{q}'') \\ \times (1 + \sigma(23) \cdot \sigma_{(1)}) | \chi^m \rangle \quad (45)$$

$$G_{klk'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}\mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = -\frac{1}{2} \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \\ \times O_{k'}(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \mathbf{p}'', \mathbf{q}'') (1 + \sigma(23) \cdot \sigma_{(1)}) | \chi^m \rangle \quad (46)$$

$$G'_{klk'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}\mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = \frac{1}{2} \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \\ \times O_{k'}(\sigma_{(3)}, \sigma_{(2)}, \sigma_{(1)}, \mathbf{p}'', \mathbf{q}'') (1 - \sigma(23) \cdot \sigma_{(1)}) | \chi^m \rangle \quad (47)$$

$$H_{kjl k'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{p}', \mathbf{p}'\mathbf{q}\mathbf{p}''\mathbf{q}'', \mathbf{p}'''\mathbf{q}''') = -\frac{1}{2} \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \\ \times \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') O_{k'}(\sigma_{(2)}, \sigma_{(3)}, \sigma_{(1)}, \mathbf{p}''', \mathbf{q}''') \\ \times (1 + \sigma(23) \cdot \sigma_{(1)}) | \chi^m \rangle \quad (48)$$

$$H'_{kjl k'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{p}', \mathbf{p}'\mathbf{q}\mathbf{p}''\mathbf{q}'', \mathbf{p}'''\mathbf{q}''') = \frac{1}{2} \sum_m \langle \chi^m | O_k(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) w_j(\sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{p}') \\ \times \Omega_l(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') O_{k'}(\sigma_{(3)}, \sigma_{(2)}, \sigma_{(1)}, \mathbf{p}''', \mathbf{q}''') \\ \times (1 - \sigma(23) \cdot \sigma_{(1)}) | \chi^m \rangle . \quad (49)$$

Using these expressions we end up with the final form of the Faddeev equation

$$\sum_{i=1}^8 C_{ki}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) \phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) = \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3q' \\ \times \sum_{T'} \sum_{k'=1}^6 \sum_{j=1}^6 \left(t_{iT T'}^{(j)}(\mathbf{p}, \pi(\mathbf{q}, \mathbf{q}'), E_q) D_{kjk'}(\mathbf{p}\mathbf{q}, \mathbf{p}\pi(\mathbf{q}, \mathbf{q}'), \pi'(\mathbf{q}, \mathbf{q}')\mathbf{q}') \right. \\ \left. + (-)^t t_{iT T'}^{(j)}(\mathbf{p}, -\pi(\mathbf{q}, \mathbf{q}'), E_q) D'_{kjk'}(\mathbf{p}\mathbf{q}, \mathbf{p}(-\pi(\mathbf{q}, \mathbf{q}')), \pi'(\mathbf{q}, \mathbf{q}')\mathbf{q}') \right) \\ \times \sum_{T'} F_{T' T'} \phi_{T' T'}^{(k')}(\pi'(\mathbf{q}, \mathbf{q}')\mathbf{q}')$$

$$\begin{aligned}
& + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 p' d^3 q' \sum_{i'} \sum_l v_{i'T}^{(l)}(\mathbf{p}, \mathbf{q}, \mathbf{p}', \mathbf{q}') \sum_{k'=1}^8 E_{klk'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}\mathbf{p}'\mathbf{q}', \mathbf{p}'\mathbf{q}') \phi_{i'T}^{(k')}(\mathbf{p}', \mathbf{q}') \\
& + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' \sum_{j=1}^6 t_{iTT'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q) \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \\
& \times \sum_{i''} \int d^3 p'' d^3 q'' \sum_l v_{i''T'}^{(l)}(\mathbf{p}', \mathbf{q}, \mathbf{p}'', \mathbf{q}'') \sum_{k'=1}^8 F_{kjl k'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{p}', \mathbf{p}'\mathbf{q}\mathbf{p}''\mathbf{q}'', \mathbf{p}''\mathbf{q}'') \phi_{i''T'}^{(k')}(\mathbf{p}'', \mathbf{q}'') \\
& + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \int d^3 q' d^3 q'' \\
& \times \sum_{i'} \left(\sum_l v_{i'T}^{(l)}(\mathbf{p}, \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \sum_{k'=1}^8 G_{klk'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}\pi(\mathbf{q}', \mathbf{q}'')\mathbf{q}'', \pi'(\mathbf{q}', \mathbf{q}'')\mathbf{q}'') \right. \\
& + (-)^{i'} \sum_l v_{i'T}^{(l)}(\mathbf{p}, \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \sum_{k'=1}^8 G'_{klk'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}(-\pi(\mathbf{q}', \mathbf{q}'')\mathbf{q}'', \pi'(\mathbf{q}', \mathbf{q}'')\mathbf{q}'') \\
& \times \sum_{i''} F_{i'i''T} \phi_{i''T}^{(k')}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \\
& + \frac{1}{E - \frac{p^2}{m} - \frac{3}{4m}q^2} \sum_{T'} \int d^3 p' \sum_{j=1}^6 t_{iTT'}^{(j)}(\mathbf{p}, \mathbf{p}', E_q) \frac{1}{E - \frac{p'^2}{m} - \frac{3}{4m}q^2} \int d^3 q' d^3 q'' \\
& \times \sum_{i'} \left(\sum_l v_{i'T'}^{(l)}(\mathbf{p}', \mathbf{q}, \pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \sum_{k'=1}^8 H_{kjl k'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{p}', \mathbf{p}'\mathbf{q}\pi(\mathbf{q}', \mathbf{q}'')\mathbf{q}'', \pi'(\mathbf{q}', \mathbf{q}'')\mathbf{q}'') \right. \\
& + (-)^{i'} \sum_l v_{i'T'}^{(l)}(\mathbf{p}', \mathbf{q}, -\pi(\mathbf{q}', \mathbf{q}''), \mathbf{q}'') \\
& \times \sum_{k'=1}^8 H'_{kjl k'}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{p}', \mathbf{p}'\mathbf{q}(-\pi(\mathbf{q}', \mathbf{q}'')\mathbf{q}'', \pi'(\mathbf{q}', \mathbf{q}'')\mathbf{q}'') \\
& \times \sum_{i''} F_{i'i''T'} \phi_{i''T'}^{(k')}(\pi'(\mathbf{q}', \mathbf{q}''), \mathbf{q}'').
\end{aligned} \tag{50}$$

The first part of Eq. (50) refers to NN forces only and provides the bulk of the binding energy. The remaining parts refer to the action of the 3NF and its interplay with NN forces.

It should be stressed, that the momenta only occur in scalar expressions (41)–(49) which has to be determined only once. For selected examples we refer to the Appendix.

Due to the expansion of Eq. (29) the number of coupled equations to solve is strictly finite. There at most three 3N isospin states and therefore the number of equations is $N = 3 \times 8 = 24$. If one neglects charge independence and charge symmetry breaking in the 2N system then $N = 8$ (see also (8)). Moreover, as has been documented in (10; 19) only very few out of the 8 components are dominant in the expansion of the full ^3He state. We expect that a similar reduction takes place also for the Faddeev amplitude.

If one neglects the 3NF only the first part in Eq. (50) is present. The big question at present, however, is to investigate the contribution of the N³LO 3NF's, which are parameter free and therefore the full set has to be treated.

The final remark refers to symmetry requirements for the unknown scalar amplitudes $\phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q})$. They follow from Eq. (26) and the expansion given in Eq. (29):

$$\begin{aligned} P_{23}^s \psi_{iT}(-\mathbf{p}, \mathbf{q}) &= \sum_{i=1}^8 \phi_{iT}^{(i)}(-\mathbf{p}, \mathbf{q}) O_i(\sigma_{(1)}, \sigma_{(3)}, \sigma_{(2)}, -\mathbf{p}, \mathbf{q}) P_{23}^s |\chi^m\rangle \\ &= (-)^t \sum_{i=1}^8 \phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) O_i(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) |\chi^m\rangle. \end{aligned} \quad (51)$$

The operators O_2, O_3, O_7 and O_8 are odd under exchange of particles 2 and 3, whereas O_1, O_4, O_5 and O_6 are even.

Furthermore, $P_{23}^s |\chi^m\rangle = -|\chi^m\rangle$ leading to

$$\sum_{i=1}^8 \phi_{iT}^{(i)}(-\mathbf{p}, \mathbf{q}) O_i(\sigma_{(1)}, \sigma_{(3)}, \sigma_{(2)}, -\mathbf{p}, \mathbf{q}) P_{23}^s |\chi^m\rangle = (-)^{t+1} \sum_{i=1}^8 \phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) O_i(\sigma_{(1)}, \sigma_{(2)}, \sigma_{(3)}, \mathbf{p}, \mathbf{q}) |\chi^m\rangle. \quad (52)$$

Now we use the symmetry properties of the operators O_i and get

$$\begin{aligned} &\left(\phi_{iT}^{(1)}(-\mathbf{p}, \mathbf{q}) O_1 - \phi_{iT}^{(2)}(-\mathbf{p}, \mathbf{q}) O_2 - \phi_{iT}^{(3)}(-\mathbf{p}, \mathbf{q}) O_3 + \phi_{iT}^{(4)}(-\mathbf{p}, \mathbf{q}) O_4 \right. \\ &\quad \left. + \phi_{iT}^{(5)}(-\mathbf{p}, \mathbf{q}) O_5 + \phi_{iT}^{(6)}(-\mathbf{p}, \mathbf{q}) O_6 - \phi_{iT}^{(7)}(-\mathbf{p}, \mathbf{q}) O_7 - \phi_{iT}^{(8)}(-\mathbf{p}, \mathbf{q}) O_8 \right) |\chi^m\rangle \\ &= (-)^{t+1} \sum_{i=1}^8 \phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q}) O_i |\chi^m\rangle. \end{aligned} \quad (53)$$

This is fulfilled if the scalar functions obey

$$\begin{aligned} \phi_{iT}^{(1)}(-\mathbf{p}, \mathbf{q}) &= (-)^{t+1} \phi_{iT}^{(1)}(\mathbf{p}, \mathbf{q}) \\ \phi_{iT}^{(2)}(-\mathbf{p}, \mathbf{q}) &= (-)^t \phi_{iT}^{(2)}(\mathbf{p}, \mathbf{q}) \\ \phi_{iT}^{(3)}(-\mathbf{p}, \mathbf{q}) &= (-)^t \phi_{iT}^{(3)}(\mathbf{p}, \mathbf{q}) \\ \phi_{iT}^{(4)}(-\mathbf{p}, \mathbf{q}) &= (-)^{t+1} \phi_{iT}^{(4)}(\mathbf{p}, \mathbf{q}) \\ \phi_{iT}^{(5)}(-\mathbf{p}, \mathbf{q}) &= (-)^{t+1} \phi_{iT}^{(5)}(\mathbf{p}, \mathbf{q}) \\ \phi_{iT}^{(6)}(-\mathbf{p}, \mathbf{q}) &= (-)^{t+1} \phi_{iT}^{(6)}(\mathbf{p}, \mathbf{q}) \\ \phi_{iT}^{(7)}(-\mathbf{p}, \mathbf{q}) &= (-)^t \phi_{iT}^{(7)}(\mathbf{p}, \mathbf{q}) \\ \phi_{iT}^{(8)}(-\mathbf{p}, \mathbf{q}) &= (-)^t \phi_{iT}^{(8)}(\mathbf{p}, \mathbf{q}). \end{aligned} \quad (54)$$

Our standard manner (20) to solve the 3N bound state Faddeev equation is by iteration and using a Lanczos type algorithm, which requires a choice of initial amplitudes $\phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q})$. In order to guarantee the Fermi character for the 3N system, the symmetry requirements given in Eq. (54) have to be imposed for the initial amplitudes. It is not difficult to explicitly demonstrate that the coupled set of equations (50) conserves this symmetry requirement during the iteration provided the numerics is reliably under control. In Ref. (10) it

is documented that the $\hat{\mathbf{p}} \cdot \hat{\mathbf{q}}$ dependence of the corresponding scalar functions for the full ${}^3\text{He}$ state is rather weak. This suggests to use a Legendre expansion for that angular dependence, which would directly guarantee the symmetry requirements.

It might be advantageous to replace the operators O_i by the second form of expansion given in Eq. (29) which is directly related to a partial wave expansion. Ref. (10) documents numerically that only very few terms dominate this expansion. It can be easily checked also for the Faddeev amplitudes which of the two expansions are more efficient, since solutions for realistic forces are available in partial wave form and from there the scalar functions $\phi(\mathbf{p}, \mathbf{q})$ and $\tilde{\phi}(\mathbf{p}, \mathbf{q})$ can be generated as laid out in Ref. (10).

4 Summary and Outlook

Using an expansion of the Faddeev amplitudes in products of scalar functions $\phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q})$ with products of scalar expressions in spin and momenta as well as corresponding expansions of the NN t -operator and 3N forces, the Faddeev equations for the 3N bound state can be reformulated into a strictly finite set of coupled equations for the amplitudes $\phi_{iT}^{(i)}(\mathbf{p}, \mathbf{q})$, which only depend on three variables. The single corresponding equation for three bosons has been solved reliably (4; 5). For three nucleons this turns now into a coupled set of equations, which can be solved with modern computing resources.

In case of 3N scattering one standard form of Faddeev equations is (21)

$$T|\Phi\rangle = tP|\Phi\rangle + tPG_0|\Phi\rangle + (1 + tG_0)V^{(1)}(1 + P)|\Phi\rangle + (1 + tG_0)V^{(1)}(1 + P)G_0T|\Phi\rangle \quad (55)$$

We expect that a generalization of the operator expansion for the NN t -operator can be found for $T|\Phi\rangle$ as well. However, like for the system of three boson, these scalar functions will depend on 5 variables (6): $|\mathbf{p}|$, $|\mathbf{q}|$, $\hat{\mathbf{p}} \cdot \hat{\mathbf{q}}_0$, $\hat{\mathbf{q}} \cdot \hat{\mathbf{q}}_0$, and $(\widehat{\mathbf{q}_0 \times \mathbf{q}}) \cdot (\widehat{\mathbf{q}_0 \times \mathbf{p}})$, where $\mathbf{q}_0$ is the initial projectile momentum. The numerical treatment is thus more demanding with respect to interpolations compared to the 3N bound state. But again, this has been already mastered (6; 7) for 3 boson scattering well into the GeV region.

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Appendix: Selected Scalar Functions

Below we provide expressions for 2N scalar functions $A_{kk'}(p)$ and $B_{kjk''}(\mathbf{p}, \mathbf{p}')$:

$$A_{11'}(p) = 3 \quad (56)$$

$$A_{12'}(p) = A_{21'}(p) = 0 \quad (57)$$

$$A_{22'}(p) = \frac{8}{3} p^4 \quad (58)$$

$$B_{111}(\mathbf{p}, \mathbf{p}') = B_{161}(\mathbf{p}, \mathbf{p}') = 3 \quad (59)$$

$$B_{211}(\mathbf{p}, \mathbf{p}') = B_{121}(\mathbf{p}, \mathbf{p}') = B_{221}(\mathbf{p}, \mathbf{p}') = B_{261}(\mathbf{p}, \mathbf{p}') = 0 \quad (60)$$

$$B_{131}(\mathbf{p}, \mathbf{p}') = (\mathbf{p} \times \mathbf{p}')^2 \quad (61)$$

$$B_{141}(\mathbf{p}, \mathbf{p}') = (\mathbf{p} + \mathbf{p}')^2 \quad (62)$$

$$B_{151}(\mathbf{p}, \mathbf{p}') = (\mathbf{p} - \mathbf{p}')^2 \quad (63)$$

$$B_{231}(\mathbf{p}, \mathbf{p}') = -p^2(p'^2 - (\mathbf{p} \cdot \mathbf{p}')^2) - \frac{1}{3}p^2(\mathbf{p} \times \mathbf{p}')^2 \quad (64)$$

$$B_{241}(\mathbf{p}, \mathbf{p}') = 3(p^2 + \mathbf{p} \cdot \mathbf{p}')^2 - (\mathbf{p} \times \mathbf{p}')^2 - \frac{1}{3}p^2(\mathbf{p} + \mathbf{p}')^2 \quad (65)$$

$$B_{251}(\mathbf{p}, \mathbf{p}') = 3(p^2 - \mathbf{p} \cdot \mathbf{p}')^2 - (\mathbf{p} \times \mathbf{p}')^2 - \frac{1}{3}p^2(\mathbf{p} - \mathbf{p}')^2 \quad (66)$$

Expression for the scalar functions B_{1j2} are obtained from B_{2j1} replacing $\mathbf{p} \leftrightarrow \mathbf{p}'$.

$$B_{212}(\mathbf{p}, \mathbf{p}') = B_{262}(\mathbf{p}, \mathbf{p}') = 3(\mathbf{p} \cdot \mathbf{p}')^2 - (\mathbf{p} \times \mathbf{p}')^2 - \frac{1}{3}p^2p'^2 \quad (67)$$

$$B_{222}(\mathbf{p}, \mathbf{p}') = -8i\mathbf{p} \cdot \mathbf{p}' (\mathbf{p} \times \mathbf{p}')^2 \quad (68)$$

$$B_{232}(\mathbf{p}, \mathbf{p}') = \frac{1}{9}(-27(\mathbf{p} \times \mathbf{p}')^4 + p^2p'^2(\mathbf{p} \times \mathbf{p}')^2 + 3p'^2(\mathbf{p} \times (\mathbf{p} \times \mathbf{p}'))^2 + 3p^2(\mathbf{p}' \times (\mathbf{p}' \times \mathbf{p}))^2 + 9(\mathbf{p} \cdot \mathbf{p}')^2(\mathbf{p} \times \mathbf{p}')^2) \quad (69)$$

$$B_{242}(\mathbf{p}, \mathbf{p}') = \frac{10}{9}p^2p'^2(\mathbf{p} + \mathbf{p}')^2 - p^2(p'^2 + \mathbf{p} \cdot \mathbf{p}')^2 - p'^2(p^2 + \mathbf{p} \cdot \mathbf{p}')^2 + \frac{1}{3}(p^2 + p'^2)(\mathbf{p} \times \mathbf{p}')^2 \quad (70)$$

$$B_{252}(\mathbf{p}, \mathbf{p}') = \frac{10}{9}p^2p'^2(\mathbf{p} - \mathbf{p}')^2 - p^2(p'^2 - \mathbf{p} \cdot \mathbf{p}')^2 - p'^2(p^2 - \mathbf{p} \cdot \mathbf{p}')^2 + \frac{1}{3}(p^2 + p'^2)(\mathbf{p} \times \mathbf{p}')^2 \quad (71)$$

The 3N scalar functions $C_{ki}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q})$ are symmetrical in k and i indices. The diagonal values are:

$$C_{11}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) = 2 \quad (72)$$

$$C_{22}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) = 6 \quad (73)$$

$$C_{33}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) = C_{44}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) = 2(\hat{\mathbf{p}} \times \hat{\mathbf{q}})^2 \quad (74)$$

$$C_{55}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) = C_{66}(\mathbf{p}\mathbf{q}, \mathbf{p}\mathbf{q}) = 2\hat{\mathbf{p}}^2\hat{\mathbf{q}}^2 \quad (75)$$

$$C_{77}(\mathbf{pq}, \mathbf{pq}) = 2\hat{\mathbf{p}}^2\hat{\mathbf{p}}^2 \quad (76)$$

$$C_{88}(\mathbf{pq}, \mathbf{pq}) = 2\hat{\mathbf{q}}^2\hat{\mathbf{q}}^2 \quad (77)$$

The nonvanishing nondiagonal values are:

$$C_{25}(\mathbf{pq}, \mathbf{pq}) = C_{26}(\mathbf{pq}, \mathbf{pq}) = 2\hat{\mathbf{p}} \cdot \hat{\mathbf{q}} \quad (78)$$

$$C_{27}(\mathbf{pq}, \mathbf{pq}) = 2\hat{\mathbf{p}}^2 \quad (79)$$

$$C_{28}(\mathbf{pq}, \mathbf{pq}) = 2\hat{\mathbf{q}}^2 \quad (80)$$

$$C_{56}(\mathbf{pq}, \mathbf{pq}) = C_{78}(\mathbf{pq}, \mathbf{pq}) = 2(\hat{\mathbf{p}} \cdot \hat{\mathbf{q}})^2 \quad (81)$$

$$C_{57}(\mathbf{pq}, \mathbf{pq}) = C_{67}(\mathbf{pq}, \mathbf{pq}) = 2\hat{\mathbf{p}}^2\hat{\mathbf{p}} \cdot \hat{\mathbf{q}} \quad (82)$$

$$C_{58}(\mathbf{pq}, \mathbf{pq}) = C_{68}(\mathbf{pq}, \mathbf{pq}) = 2\hat{\mathbf{q}}^2\hat{\mathbf{p}} \cdot \hat{\mathbf{q}} \quad (83)$$

Some other arbitrarily chosen 3N scalar functions $D_{kjk'}(\mathbf{pq}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'')$, $D'_{kjk'}(\mathbf{pq}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'')$ and $H_{kjl k'}(\mathbf{pq}, \mathbf{pp}', \mathbf{p}'\mathbf{qp}''\mathbf{q}'', \mathbf{p}'''\mathbf{q}''')$ are:

$$D_{211}(\mathbf{pq}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = -3 \quad (84)$$

$$D_{222}(\mathbf{pq}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = D_{243}(\mathbf{pq}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = 0 \quad (85)$$

$$D'_{211}(\mathbf{pq}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = -3 \quad (86)$$

$$D'_{222}(\mathbf{pq}, \mathbf{p}'\mathbf{q}', \mathbf{p}''\mathbf{q}'') = 0 \quad (87)$$

$$H_{2223}(\mathbf{pq}, \mathbf{pp}', \mathbf{p}'\mathbf{qp}''\mathbf{q}'', \mathbf{p}'''\mathbf{q}''') = 0 \quad (88)$$

$$\begin{aligned} H_{6528}(\mathbf{pq}, \mathbf{pp}', \mathbf{p}'\mathbf{qp}''\mathbf{q}'', \mathbf{p}'''\mathbf{q}''') &= i\hat{\mathbf{p}} \cdot (\mathbf{p} - \mathbf{p}') \times (\mathbf{p}''' - \mathbf{q}''') \\ &\quad - \frac{1}{2}i(\hat{\mathbf{p}} \times ((\mathbf{p} - \mathbf{p}') \times \mathbf{p}''')) \cdot ((\mathbf{p} - \mathbf{p}') \times \mathbf{q}''') \\ &\quad - \frac{1}{2}i(\hat{\mathbf{p}} \times ((\mathbf{p} - \mathbf{p}') \times \mathbf{q}''')) \cdot ((\mathbf{p} - \mathbf{p}') \times \mathbf{p}''') \end{aligned} \quad (89)$$

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