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A new way to perform partial wave decompositions of few-nucleon forces

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Abstract. We formulate a general and exact method of partial wave decomposition (PWD) of any nucleon-nucleon (NN) potential and any three-nucleon (3N) force. The approach allows one to efficiently use symbolic algebra software to generate the interaction dependent part of the program code calculating the interaction. We demonstrate the feasibility of this approach for the one-boson exchange BonnB potential, a recent nucleon-nucleon chiral force and the chiral two-pion-exchange three-nucleon force. In all cases very good agreement between the new and the traditional PWD is found. The automated PWD offered by the new approach is of the utmost importance in view of future applications of numerous chiral N³LO contributions to the 3N force in three nucleon calculations.

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1 Introduction

The standard way to set up calculations of two- and three-nucleon systems is a partial wave decomposition (PWD). Especially at low energies, i.e. below the pion production threshold, this procedure is still most commonly used, despite the advent of the approaches which use a direct three-dimensional notation [1, 2, 3, 4].

Recently we proposed a formulation of the two- and three-nucleon system [5, 6], which is based on scalar spin-momentum operators and accompanying scalar functions depending only on the momenta of the system. This formulation is based on the most general operator structure a nuclear force given in momentum space can have. The two- and three-nucleon equations are obtained by carrying out traces over the spin-momentum operators building the nuclear force. The same approach can be used to obtain partial wave projected matrix elements of the potential and the transition operators. Taking traces of spin-momentum operators lends itself to the use of symbolic algebra software to obtain general expressions for those matrix elements.

In this work we demonstrate that by algebraic operations general expressions for the partial wave decompo-

sition of any nucleon-nucleon (NN) potential can be obtained. This method will be presented in Sec. 2, and explicit expressions for calculating specific matrix elements of NN potentials are given in an appendix. Numerical comparisons between our suggested methods and the standards partial wave decomposition using recent chiral NN forces [7] and the one-boson-exchange NN potential BonnB [8] are presented in Sec. 3. In Sec. 4 we demonstrate that the same method can be extended to the PWD of a three-nucleon force. As a numerical example given in Sec. 5 we take the two-pion-exchange (TPE) chiral NNLO three-nucleon force. Finally we conclude in Sec. 6.

2 Partial wave decomposition of the NN potential

We start, as in Ref. [6], by projecting the NN potential on the two-nucleon (2N) isospin states $|(\frac{1}{2}, \frac{1}{2})tm_t\rangle \equiv |tm_t\rangle$. Furthermore, we assume that there is no isospin mixing but allow for charge independence and charge symmetry breaking, and thus for a dependence on m_t :

$$\langle t'm'_t|V|tm_t\rangle = \delta_{t't}\delta_{m'_tm_t}V^{tm_t}. \quad (1)$$

It is well known that the most general form of the NN force, which is invariant under rotations, parity and time reversal can be expressed by six scalar spin-momentum operators [10], which we choose as

$$\begin{aligned}
w_1(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}) &= 1, \\
w_2(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}) &= \boldsymbol{\sigma}(1) \cdot \boldsymbol{\sigma}(2), \\
w_3(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}) &= i(\boldsymbol{\sigma}(1) + \boldsymbol{\sigma}(2)) \cdot (\mathbf{p} \times \mathbf{p}'), \\
w_4(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}) &= \boldsymbol{\sigma}(1) \cdot (\mathbf{p} \times \mathbf{p}') \boldsymbol{\sigma}(2) \cdot (\mathbf{p} \times \mathbf{p}'), \\
w_5(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}) &= \boldsymbol{\sigma}(1) \cdot (\mathbf{p}' + \mathbf{p}) \boldsymbol{\sigma}(2) \cdot (\mathbf{p}' + \mathbf{p}), \\
w_6(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}) &= \boldsymbol{\sigma}(1) \cdot (\mathbf{p}' - \mathbf{p}) \boldsymbol{\sigma}(2) \cdot (\mathbf{p}' - \mathbf{p}).
\end{aligned} \tag{2}$$

Thus the isospin projected potential can be expressed as

$$V^{tm_t}(\mathbf{p}', \mathbf{p}) = \sum_{i=1}^6 f_i(\mathbf{p}', \mathbf{p}) w_i(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}). \tag{3}$$

The expansion coefficient here are scalar functions $f_i(\mathbf{p}', \mathbf{p})$ that depend on two vector momenta \mathbf{p}' and \mathbf{p} , more specifically on the magnitudes of the vectors and the cosine of the relative angle between them. In order to determine the functions f_i , we evaluate the spin dependence analytically by taking traces with the operators of Eq. (2) and thus arrive at a system of six coupled linear equations

$$\sum_{j=1}^6 \text{Tr}(w_i w_j) f_j = \text{Tr}(V^{tm_t} w_i), \quad i = 1, 2, \dots, 6, \tag{4}$$

which has a unique solution provided that $\mathbf{p}' \neq \mathbf{p}$. (When $\mathbf{p}' = \mathbf{p}$ only five out of the six operators w_i are sufficient, since w_2 is linearly dependent on w_4 , w_5 , and w_6 .)

Our task is to obtain matrix elements of V^{tm_t} in the basis of states $|p(ls)jm_j\rangle$, where the relative angular momentum l and the total spin s are coupled to the total angular momentum j with its projection m_j . When calculating NN observables one usually sums angular momenta j up to a certain j_{max} at which the calculation is converged. For calculations of NN observables below the pion production threshold convergence is reached for $j_{max} \leq 8$.

To obtain the potential matrix element in the basis $|p(ls)jm_j\rangle$, the four-fold integral

$$\begin{aligned}
\langle p'(l's)jm_j | V^{tm_t} | p(ls)jm_j \rangle &= \\
&= \int d\hat{p}' \int d\hat{p} \sum_{m'_i} c(l', s, j; m'_i, m_j - m'_i, m_j) \\
&\quad \times \sum_{m_i} c(l, s, j; m_i, m_j - m_i, m_j) Y_{l' m'_i}^*(\theta', \phi') Y_{l m_i}(\theta, \phi) \\
&\quad \times \langle s m_j - m'_i | V^{tm_t}(\mathbf{p}', \mathbf{p}) | s m_j - m_i \rangle
\end{aligned} \tag{5}$$

needs to be evaluated. Here $c(l, s, j; m_i, m_j - m_i, m_j)$ are the standard Clebsch-Gordan coefficients, and $Y_{l m_i}(\theta, \phi)$ the spherical harmonics calculated for the angles corresponding to the directions of the momenta \mathbf{p}' and \mathbf{p} . This quantity does not actually depend on m_j , so instead of Eq. (5) we can calculate

$$H(l', l, s, j) \equiv \frac{1}{2j+1} \sum_{m_j=-j}^j \langle p'(l's)jm_j | V | p(ls)jm_j \rangle. \tag{6}$$

Since now the integrand is a scalar, it is possible to reduce the number of integrals to one:

$$\begin{aligned}
H(l', l, s, j) &= 8\pi^2 \int_{-1}^1 d(\cos \theta') \frac{1}{2j+1} \sum_{m_j=-j}^j \\
&\quad \times \sum_{m'_i=-l'}^{l'} c(l', s, j; m'_i, m_j - m'_i, m_j) \\
&\quad \times \sum_{m_i=-l}^l c(l, s, j; m_i, m_j - m_i, m_j) \\
&\quad \times Y_{l' m'_i}(\theta', 0) Y_{l m_i}^*(0, 0) \\
&\quad \times \langle s m_j - m'_i | V(\mathbf{p}', \mathbf{p}) | s m_j - m_i \rangle.
\end{aligned} \tag{7}$$

In the NN system we can choose the z-axis to be

$$\mathbf{p} = (0, 0, p). \tag{8}$$

Then the direction of the vector \mathbf{p}' is given as

$$\mathbf{p}' = (p' \sin \theta', 0, p' \cos \theta'). \tag{9}$$

Most importantly however, the matrix element in the 2N spin space,

$$\begin{aligned}
\langle s m_j - m'_i | V(\mathbf{p}', \mathbf{p}) | s m_j - m_i \rangle &= \\
\langle s m_j - m'_i | \sum_{i=1}^6 f_i(\mathbf{p}', \mathbf{p}, x) & \\
w_i(\boldsymbol{\sigma}(1), \boldsymbol{\sigma}(2), \mathbf{p}', \mathbf{p}) | s m_j - m_i \rangle &
\end{aligned} \tag{10}$$

can be calculated analytically¹. The three sums in Eq. (7) over m_j , m'_i and m_i can be written out explicitly so the integrand over $x \equiv \cos \theta'$ can be prepared *once* for all NN potentials that are represented in the form of Eq. (3). The resulting expression is given in terms of p , p' , x and the expansion coefficients $f(i) \equiv f_i(\mathbf{p}', \mathbf{p}, x)$. As example, evaluating Eq. (7) for the 1S_0 channel leads to

$$\begin{aligned}
H(0, 0, 0, 0) &= 2\pi \int_{-1}^1 dx \left(f(1) - 3f(2) + f(4)p^2 p'^2 (x^2 - 1) \right. \\
&\quad \left. - f(5)(p^2 + p'^2 + 2pp'x) \right. \\
&\quad \left. - f(6)(p^2 + p'^2 - 2pp'x) \right).
\end{aligned} \tag{11}$$

Further examples are collected in Appendix A.

¹ For this calculation symbolic software like *Mathematica* © [11] proves very useful. Here it is particularly simple with the concept of the Kronecker product which makes such matrix elements simple matrix elements in the four-dimensional space.

3 Application of the new method to the 2N potential

In this section we want to give two examples a PWD of an NN potential based on our new method and compare with results obtained in the traditional way. First we consider the one-boson exchange potential BonnB [8]. Here we use the operator form of this potential presented in [6]. In Figs. 1–6 we show matrix elements $\langle p'(l's)jm_j | V^{tm_t} | p_0(ls)jm_j \rangle$ for several partial waves for a fixed value of $p_0 = 1 \text{ fm}^{-1}$ as a function of the momentum p' . In Figs. 1 through 3 selected partial wave projected potential amplitudes for the BonnB potential are shown. The agreement of the matrix elements calculated with our operator based formulation and the original PWD based on a helicity formulation [9] is excellent. That is not too surprising, in both cases the numerical accuracy is determined by the integration over $\cos \theta'$.

As second example we take the neutron-proton version of the chiral NNLO potential [7] and use the same set of the parameters as given in [6]. In Figs. 4–6 selected partial wave projected potential amplitudes are shown for this potential. Again, the agreement between the two methods is excellent.

4 Extension to Three-Nucleon Forces

The arguments used in Sec. 2 for the 2N potential can be applied to any three-nucleon (3N) force. Now we use the 3N states $|pq\beta\rangle$ [12] in the so-called LS -coupling

$$|pq\beta\rangle \equiv |pq(l\lambda)L(s\frac{1}{2})S(LS)JM_J\rangle | (t\frac{1}{2})Tm_T \rangle, \quad (12)$$

where the quantum numbers for the relative angular momenta l (within the pair (23)) and λ (between the pair (23) and nucleon 1) are coupled to the total angular momentum L . In the spin space the spin of the (23) pair is coupled with the spin $\frac{1}{2}$ of nucleon 1 to the total spin S . Finally L and S are coupled to the total 3N angular momentum J with the projection M_J . The isospin 3N state, where we couple the total isospin of the (23) subsystem t with the isospin $\frac{1}{2}$ of the third nucleon to the total 3N isospin T with the projection m_T , is constructed in the same way as the 3N spin state. Since we want the states $|pq\beta\rangle$ to be antisymmetric with respect to the exchange of particles 2 and 3, we require additionally that $(-1)^{l+s+t} = -1$.

We start with the eight-dimensional integral

$$\begin{aligned} & \langle p'q'(l'\lambda')L'(s'\frac{1}{2})S'(L'S')JM_J | \\ & \quad V^{3N} | pq(l\lambda)L(s\frac{1}{2})S(LS)JM_J \rangle \\ &= \int d\hat{p}' \int d\hat{q}' \int d\hat{p} \int d\hat{q} \\ & \quad \sum_{m_{L'}} c(L', S', J; m_{L'}, M_J - m_{L'}, M_J) \\ & \quad \sum_{m_L} c(L, S, J; m_L, M_J - m_L, M_J) \\ & \quad \mathcal{Y}_{l',\lambda'}^{*L',m_{L'}}(\hat{p}', \hat{q}') \mathcal{Y}_{l,\lambda}^{L,m_L}(\hat{p}, \hat{q}) \\ & \langle (s\frac{1}{2})S'M_J - m_{L'} | V^{3N}(\mathbf{p}', \mathbf{q}', \mathbf{p}, \mathbf{q}) | (s\frac{1}{2})S'M_J - m_L \rangle, \end{aligned} \quad (13)$$

where

$$\begin{aligned} \mathcal{Y}_{l,\lambda}^{L,m_L}(\hat{p}, \hat{q}) &\equiv \sum_{m_l=-l}^l c(l, \lambda, L; m_l, m_L - m_l, m_L) \\ &\quad \times Y_{l,m_l}(\hat{p}) Y_{\lambda,m_L-m_l}(\hat{q}). \end{aligned} \quad (14)$$

This quantity is independent of M_J , and instead of Eq. (13) we can calculate

$$\begin{aligned} & G(l', \lambda', L', s', S', l, \lambda, L, s, S, J) \\ & \equiv \frac{1}{2J+1} \sum_{M_J=-J}^J \langle p'q'(l'\lambda')L'(s'\frac{1}{2})S'(L'S')JM_J | \\ & \quad V^{3N} | pq(l\lambda)L(s\frac{1}{2})S(LS)JM_J \rangle. \end{aligned} \quad (15)$$

Since the integrand is now a scalar, it is possible to reduce the number of integrals from eight to five. Namely we take first $\hat{p} = \hat{z}$ and then consider all scalar products among the \hat{p} , \hat{q} , \hat{p}' and \hat{q}' unit vectors. They depend on the following quantities: θ_q , $\theta_{p'}$, $\theta_{q'}$, $\phi_{p'} - \phi_q$, $\phi_{q'} - \phi_q$ and $\phi_{p'} - \phi_{q'}$. Since the last three are not independent, it is possible to set additionally $\phi_q = 0$. Of course, taking $\hat{p} = \hat{z}$ and $\phi_q = 0$ is only one possibility. The best choice (from the computational point of view) of the five integration variables might depend on the form of $V^{3N}(\mathbf{p}', \mathbf{q}', \mathbf{p}, \mathbf{q})$, which is an operator in the 3N spin space. This quantity G has to be multiplied by the matrix element of isospin operator \hat{I}

$$\langle (t\frac{1}{2})T'm_T' | \hat{I} | (t\frac{1}{2})Tm_T \rangle, \quad (16)$$

which can be worked out exactly, independent from the momentum and spin spaces.

5 Numerical example for a 3N force

We consider just one example of the 3N force: a two-pion-exchange contribution to the chiral NNLO 3N force as given in [13], V_{TPE}^{3NF} . In particular we take the part of V_{TPE}^{3NF} which is symmetric under the exchange of nucleons 2 and 3

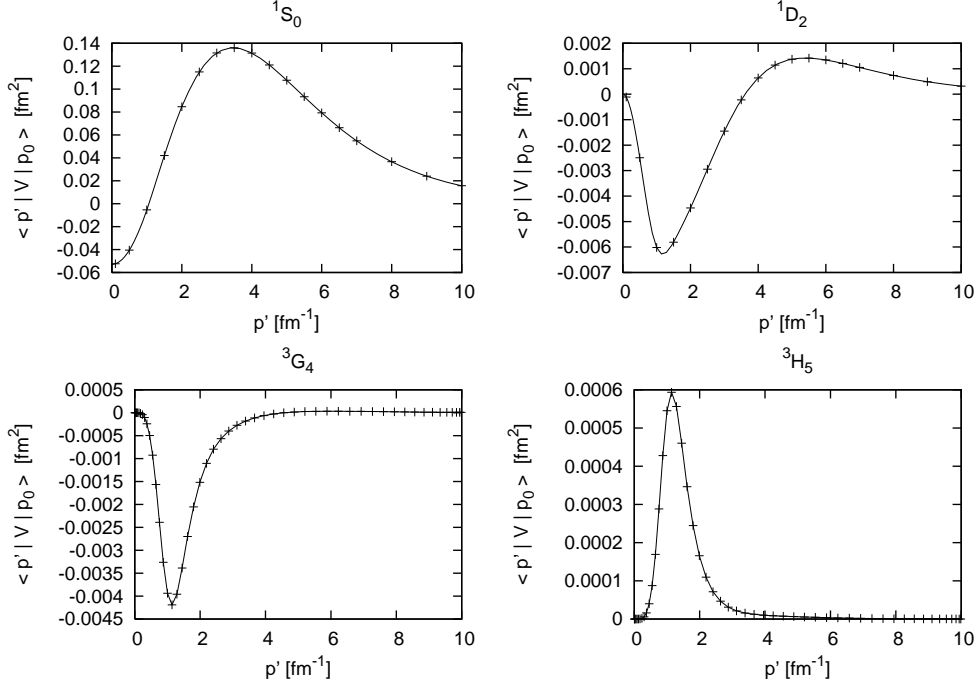


Fig. 1. Comparison of the traditional (crosses) and the new (solid line) method of PWD for the Bonn B potential. The matrix elements of selected uncoupled channels with $t = 1$ (1S_0 , 1D_2) and $t = 0$ (3G_4 , 3H_5) are shown for a fixed value of $p_0 = 1 \text{ fm}^{-1}$ as a function of the p' momentum.

$$V^{(1)} = F_1 \boldsymbol{\sigma}_2 \cdot \mathbf{q}_2 \boldsymbol{\sigma}_3 \cdot \mathbf{q}_3 \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 + F_2 \boldsymbol{\sigma}_1 \cdot (\mathbf{q}_2 \times \mathbf{q}_3) \boldsymbol{\sigma}_2 \cdot \mathbf{q}_2 \boldsymbol{\sigma}_3 \cdot \mathbf{q}_3 \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3), \quad (17)$$

where $\mathbf{q}_i \equiv \mathbf{p}'_i - \mathbf{p}_i$ and \mathbf{p}_i (\mathbf{p}'_i) is the initial (final) momentum of nucleon i . Further, g_A , m_π and F_π refer to the nucleon axial vector coupling constant, pion mass and decay constants, respectively, while c_i are low-energy constants from the subleading pion-nucleon Lagrangian. The scalar functions F_1 and F_2 are

$$F_1 = \left(\frac{g_A}{2F_\pi} \right)^2 \frac{1}{(\mathbf{q}_2^2 + m_\pi^2)(\mathbf{q}_3^2 + m_\pi^2)} \times \left(-\frac{4c_1 m_\pi^2}{F_\pi^2} + \frac{2c_3}{F_\pi^2} \mathbf{q}_2 \cdot \mathbf{q}_3 \right) \quad (18)$$

and

$$F_2 = \left(\frac{g_A}{2F_\pi} \right)^2 \frac{1}{(\mathbf{q}_2^2 + m_\pi^2)(\mathbf{q}_3^2 + m_\pi^2)} \frac{c_4}{F_\pi^2}. \quad (19)$$

We consider first the two isospin matrix elements

$$\hat{I}_1(t', T', m_{T'}, t, T, m_T) \equiv \langle (t' \frac{1}{2}) T' m_{T'} | \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3 | (t \frac{1}{2}) T m_T \rangle \quad (20)$$

and

$$\hat{I}_2(t', T', m_{T'}, t, T, m_T) \equiv \langle (t' \frac{1}{2}) T' m_{T'} | \boldsymbol{\tau}_1 \cdot (\boldsymbol{\tau}_2 \times \boldsymbol{\tau}_3) | (t \frac{1}{2}) T m_T \rangle. \quad (21)$$

The matrix elements $\hat{I}_1(t', T', m_{T'}, t, T, m_T)$ are particularly simple and are given as

$$\hat{I}_1(t', T', m_{T'}, t, T, m_T) = (2t(t+1) - 3) \delta_{t,t'} \delta_{T,T'} \delta_{m_T, m_{T'}}. \quad (22)$$

The (purely imaginary) matrix elements $\hat{I}_2(t', T', m_{T'}, t, T, m_T)$ can be written as

$$\hat{I}_2(t', T', m_{T'}, t, T, m_T) = i\sqrt{3}(-1)^{t+1} \delta_{t+t', 1} \delta_{T, \frac{1}{2}} \delta_{T', \frac{1}{2}} \delta_{m_T, m_{T'}}. \quad (23)$$

From Eqs. (22) and (23) we infer immediately that the two parts of the considered 3N force (17) will not contribute simultaneously to the same matrix element $G(l', \lambda', L', s', S', l, \lambda, L, s, S, J)$.

For this first simple study we construct 16 $|\beta\rangle$ states for $J = \frac{1}{2}$ and positive parity $\pi = (-1)^{l+\lambda}$ satisfying the additional condition $l \leq 2$ and $\lambda \leq 2$. Their quantum numbers are given in Table 1.

Next we perform the steps described in Sec. 4 and obtain 256 integrands $\tilde{G}(l', \lambda', L', s', S', l, \lambda, L, s, S, J) \equiv \tilde{G}(\beta', \beta)$ such that

$$G(\beta', \beta) \equiv \langle (t' \frac{1}{2}) T' m_{T'} | \langle p' q' \beta' | V^{3N} | p q \beta \rangle | (t \frac{1}{2}) T m_T \rangle \equiv \int d\hat{p}' \int d\hat{q}' \int d\hat{p} \int d\hat{q} \tilde{G}(\beta', \beta). \quad (24)$$

Here we show just few (relatively simple) examples. (Note that in the first two cases the scalar nature of the

Table 1. List of $|\beta\rangle$ states for $J^\pi = \frac{1}{2}^+$, $l \leq 2$ and $\lambda \leq 2$.

β	l	s	λ	L	S	t
1	0	0	0	0	1	1
2	0	1	0	0	1	0
3	0	1	2	2	1	0
4	1	0	1	0	1	0
5	1	0	1	1	1	0
6	1	1	1	0	1	1
7	1	1	1	1	1	1
8	1	1	1	1	1	1
9	1	1	1	2	1	1
10	2	1	0	2	1	0
11	2	0	2	0	1	1
12	2	0	2	1	1	1
13	2	1	2	0	1	0
14	2	1	2	1	1	0
15	2	1	2	1	1	0
16	2	1	2	2	1	0

Table 2. Stability of the selected five fold integrals with respect to the number of Gaussian points N (see text). In the last row the values obtained with standard PWD [14,15] are given. All matrix elements are in fm⁵.

N	$G(1,1)$	$G(2,1)$	$G(6,12)$	$G(5,11)$
12	443.565	1200.160	-5.52616	-5.24720
24	443.618	1200.223	-5.49311	-5.48527
36	443.618	1200.219	-5.49290	-5.48630
48	443.618	1200.219	-5.49290	-5.48626
standard PWD	443.618	1200.219	-5.49274	-5.48597

Table 3. Stability of the selected six fold integrals with respect to the number of Gaussian points N (see text). All matrix elements are in fm⁵.

N	$G(1,1)$	$G(2,1)$	$G(6,12)$	$G(5,11)$
12	443.510	1200.365	-5.55695	-5.14678
24	443.619	1200.218	-5.49277	-5.48785
36	443.618	1200.219	-5.49290	-5.48626
48	443.618	1200.219	-5.49290	-5.48626

$\tilde{G}(\beta', \beta)$ functions is clearly visible.)

$$\begin{aligned}
\tilde{G}(1,1) &= -\frac{1}{16\pi^2} F_1 \hat{I}_1(1, T', m_{T'}, 1, T, m_T) \mathbf{q}_2 \cdot \mathbf{q}_3, \\
\tilde{G}(2,1) &= -\frac{i}{16\pi^2 \sqrt{3}} F_2 \hat{I}_2(0, T', m_{T'}, 1, T, m_T) \\
&\quad \times \left((\mathbf{q}_2 \cdot \mathbf{q}_3)^2 - \mathbf{q}_2^2 \mathbf{q}_3^2 \right), \\
\tilde{G}(5,11) &= \frac{1}{2\sqrt{3}} F_2 \hat{I}_2(0, T', m_{T'}, 1, T, m_T) (\mathbf{q}_2 \cdot \mathbf{q}_3) \\
&\quad \times \mathcal{Y}_{2,2}^{0,0}(\hat{p}, \hat{q}) \left(\sqrt{2} (q_{4x} - iq_{4y}) \mathcal{Y}_{1,1}^{*1,-1}(\hat{p}', \hat{q}') \right. \\
&\quad \left. + 2q_{4z} \mathcal{Y}_{1,1}^{*1,0}(\hat{p}', \hat{q}') \right. \\
&\quad \left. - \sqrt{2} (q_{4x} + iq_{4y}) \mathcal{Y}_{1,1}^{*1,1}(\hat{p}', \hat{q}') \right), \\
\tilde{G}(6,12) &= \frac{1}{6} F_1 \hat{I}_1(1, T', m_{T'}, 1, T, m_T) \mathcal{Y}_{1,1}^{*0,0}(\hat{p}', \hat{q}') \\
&\quad \left(\sqrt{2} (q_{2z} (q_{3x} + iq_{3y}) \right. \\
&\quad \left. - (q_{2x} + iq_{2y}) q_{3z} \right) \mathcal{Y}_{2,2}^{1,-1}(\hat{p}, \hat{q}) \\
&\quad + 2i (q_{2y} q_{3x} - q_{2x} q_{3y}) \mathcal{Y}_{2,2}^{1,0}(\hat{p}, \hat{q}) \\
&\quad + \sqrt{2} (q_{2z} (q_{3x} - iq_{3y}) \\
&\quad \left. - (q_{2x} - iq_{2y}) q_{3z} \right) \mathcal{Y}_{2,2}^{1,1}(\hat{p}, \hat{q}), \quad (25)
\end{aligned}$$

where $\mathbf{q}_4 \equiv \mathbf{q}_2 \times \mathbf{q}_3$ and the Cartesian components of the \mathbf{q}_i vectors are denoted as q_{ix} , q_{iy} and q_{iz} . Of course, vectors \mathbf{q}_i are now expressed in terms of the initial and final Jacobi momenta in the following way

$$\begin{aligned}
\mathbf{q}_1 &= \mathbf{q}' - \mathbf{q} \\
\mathbf{q}_2 &= \mathbf{p}' - \frac{1}{2} \mathbf{q}' - \left(\mathbf{p} - \frac{1}{2} \mathbf{q} \right) \\
\mathbf{q}_3 &= -\mathbf{p}' - \frac{1}{2} \mathbf{q}' - \left(-\mathbf{p} - \frac{1}{2} \mathbf{q} \right). \quad (26)
\end{aligned}$$

Many of the $\tilde{G}(\beta', \beta)$ functions are very lengthy. Using symbolic manipulations software like *Mathematica* © [11]

one can write down these expressions directly as a part of a Fortran or a C code. The expressions given above have to be integrated over five angles. With the choice of variables discussed in Sec. 4. we calculated the five fold integrals for fixed magnitudes of the momenta p , q , p' and q' . They were chosen quite arbitrarily: $p = 1 \text{ fm}^{-1}$, $q = 2 \text{ fm}^{-1}$, $p' = 3 \text{ fm}^{-1}$, $q' = 4 \text{ fm}^{-1}$. For the isospin quantum numbers we assumed that $T = T' = m_T = m_{T'} = \frac{1}{2}$. The 3N force parameters were taken as $g_A = 1.29$, $F_\pi = 92.4 \text{ MeV}$, $m_\pi = 138.0 \text{ MeV}/c^2$, $c_1 = -0.81 \text{ GeV}^{-1}$, $c_3 = -3.4 \text{ GeV}^{-1}$, $c_4 = 3.4 \text{ GeV}^{-1}$. Such single five fold integrals can be easily calculated on a PC. For a simple test we chose the same number of Gaussian integral points N in each of the five dimensions and checked the stability of the integrals with respect to N . Even in this most simple way, we found a good convergence, which is shown in Table 2. To check numerically the scalar nature of our integrands we calculated also the corresponding six fold integrals, where ϕ_q was an additional integration variable and checked their stability (see Table 3). We see from Tables 2 and 3 that the results from the five and six fold integrations agree very well with each other. We calculated the same matrix elements using standard PWD [14,15]. The results are shown in the last row of Table 2. They agree very well with the numbers obtained using the new method. Thus we conclude that the presented procedure might be used to efficiently automate the very cumbersome standard PWD of the 3N force. Calculation of all matrix elements for the whole grids of p , q , p' and q' points, especially for bigger values of J , will require an implementation of the algorithm on parallel architectures. Implementing such a code is much simpler than implementing a code based on the traditional PWD.

6 Summary and Outlook

We propose a new general method of calculating the PWD of any NN potential which is given in momentum space in terms of operators acting in the 2N spin and isospin spaces. Once the expansion coefficients in the operator basis are determined, the matrix elements of interest are obtained as simple one dimensional integrals, independent from the particular form of the NN potential. We demonstrate this method with two examples, the one-boson-exchange BonnB potential and a recently derived chiral NNLO potential. In both cases the agreement between our new method and traditionally employed one to obtaining partial wave projected matrix elements is perfect.

This method can be extended to treat three-nucleon forces, for which a traditional PWD is a formidable task. In order to show the power of our new method, we performed a simple feasibility study for the TPE chiral 3N force. A very good agreement between the new method and standard PWD shows that the very complex traditional approach can be replaced by this straightforward and efficient algebraic method. An ‘automated’ PWD for the 3NF is of great importance in view of awaiting applications in the 3N systems. The numerous contributions to the chiral N3LO 3N force [16,17] can be handled only with such an efficient and simple procedure.

Acknowledgments

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A Integrals for the 2N potential

This appendix collects the expressions for the partial wave decomposition of the NN potential for the partial waves with total 2N angular momentum $j \leq 2$. The expressions for higher j can be obtained on request from one of the authors (JG) either in analytical form or as Fortran or C code.

The second function for $j = 0$ is ($H(0, 0, 0, 0)$ was given in Sec. 2):

$$H(1, 1, 1, 0) = 2\pi \int_{-1}^1 dx \left\{ [f(1) + f(2)] x + 2f(3) pp'(x^2 - 1) + f(4) p^2 p'^2 x(1 - x^2) - f(5) [2p'p + x(p'^2 + p^2)] + f(6) [2p'p - x(p'^2 + p^2)] \right\}. \quad (27)$$

The functions for $j = 1$ are given by

$$H(1, 1, 0, 1) = 2\pi \int_{-1}^1 dx \left\{ [f(1) + 3f(2)] x + f(4) p^2 p'^2 x(x^2 - 1) - f(5) x [2p'px + (p'^2 + p^2)] + f(6) x [2p'px - (p'^2 + p^2)] \right\}, \quad (28)$$

$$H(1, 1, 1, 1) = 2\pi \int_{-1}^1 dx \left\{ [f(1) + f(2)] x + f(3) p'p(x^2 - 1) + f(5) [x(p'^2 + p^2) + p'p(x^2 + 1)] + f(6) [x(p'^2 + p^2) - p'p(x^2 + 1)] \right\}, \quad (29)$$

$$H(0, 0, 1, 1) = \frac{2\pi}{3} \int_{-1}^1 dx \left\{ 3[f(1) + f(2)] + f(4) p^2 p'^2 (1 - x^2) + f(5) [p'^2 + p^2 + 2p'px] + f(6) [p'^2 + p^2 - 2p'px] \right\}, \quad (30)$$

$$H(0, 2, 1, 1) = 2\pi \frac{\sqrt{2}}{3} \int_{-1}^1 dx \left\{ f(4) p'^2 p^2 (x^2 - 1) + f(5) [(3x^2 - 1)p'^2 + 2p^2 + 4p'px] + f(6) [(3x^2 - 1)p'^2 + 2p^2 - 4p'px] \right\}, \quad (31)$$

$$H(2, 0, 1, 1) = 2\pi \frac{\sqrt{2}}{3} \int_{-1}^1 dx \left\{ f(4) p'^2 p^2 (x^2 - 1) + f(5) [2p'^2 + (x^2 - 1)p^2 + 4p'px] + f(6) [2p'^2 + (x^2 - 1)p^2 - 4p'px] \right\}, \quad (32)$$

and

$$\begin{aligned}
H(2, 2, 1, 1) = & \frac{\pi}{3} \int_{-1}^1 dx \left\{ 3[f(1) + f(2)](3x^2 - 1) \right. \\
& + 18f(3) p' p x (x^2 - 1) \\
& + f(4) p'^2 p^2 (14x^2 - 5 - 9x^4) \\
& + f(5) [(1 - 3x^2)(p'^2 + p^2) - 4p' p x] \\
& \left. + f(6) [(1 - 3x^2)(p'^2 + p^2) + 4p' p x] \right\}. \quad (33)
\end{aligned}$$

The functions for $j = 2$ are given by

$$\begin{aligned}
H(2, 2, 0, 2) = & \pi \int_{-1}^1 dx (1 - 3x^2) \left\{ [-f(1) + 3f(2)] \right. \\
& - f(4) p'^2 p^2 (x^2 - 1) \\
& + f(5) [(p'^2 + p^2) + 2p' p x] \\
& \left. + f(6) [(p'^2 + p^2) - 2p' p x] \right\}, \quad (34)
\end{aligned}$$

$$\begin{aligned}
H(2, 2, 1, 2) = & \pi \int_{-1}^1 dx \left\{ [f(1) + f(2)](3x^2 - 1) \right. \\
& + 2f(3) p' p x (x^2 - 1) \\
& + f(4) p'^2 p^2 [x^4 - 2x^2 + 1] \\
& + f(5) [(3x^2 - 1)(p'^2 + p^2) + 4p' p x^3] \\
& \left. + f(6) [x(3x^2 - 1)(p'^2 + p^2) - 4p' p x^3] \right\}, \quad (35)
\end{aligned}$$

$$\begin{aligned}
H(1, 1, 1, 2) = & \frac{2\pi}{5} \int_{-1}^1 dx \left\{ 5x[f(1) + f(2)] \right. \\
& + 5f(3) p' p (1 - x^2) \\
& + 2f(4) p'^2 p^2 x (1 - x^2) \\
& + f(5) [x(p'^2 + p^2) + p' p (3x^2 - 1)] \\
& \left. + f(6) [x(p'^2 + p^2) - p' p (3x^2 - 1)] \right\}, \quad (36)
\end{aligned}$$

$$\begin{aligned}
H(1, 3, 1, 2) = & 2\pi \frac{\sqrt{6}}{5} \int_{-1}^1 dx \left\{ f(4) p'^2 p^2 x (x^2 - 1) \right. \\
& + f(5) [p'^2 x (5x^2 - 3) + 2p^2 x + 2p' p (3x^2 - 1)] \\
& \left. + f(6) [p'^2 x (5x^2 - 3) + 2p^2 x - 2p' p (3x^2 - 1)] \right\}, \quad (37)
\end{aligned}$$

$$\begin{aligned}
H(3, 1, 1, 2) = & 2\pi \frac{\sqrt{6}}{5} \int_{-1}^1 dx \left\{ f(4) p'^2 p^2 x (x^2 - 1) \right. \\
& + f(5) [2p'^2 + p^2 x (5x^2 - 3) + 2p' p (3x^2 - 1)] \\
& \left. + f(6) [2p'^2 + p^2 x (5x^2 - 3) - 2p' p (3x^2 - 1)] \right\}, \quad (38)
\end{aligned}$$

$$\begin{aligned}
H(3, 3, 1, 2) = & \frac{\pi}{5} \int_{-1}^1 dx \left\{ 5x(5x^2 - 3) [f(1) + f(2)] \right. \\
& + 10f(3) p' p (1 + 5x^4 6x^2) \\
& + f(4) p'^2 p^2 x (44x^2 - 25x^4 - 19) \\
& + f(5) [(p'^2 + p^2)x(3 - 5x^2) + 2p' p (1 - 3x^2)] \\
& \left. + f(6) [(p'^2 + p^2)x(3 - 5x^2) - 2p' p (1 - 3x^2)] \right\}. \quad (39)
\end{aligned}$$

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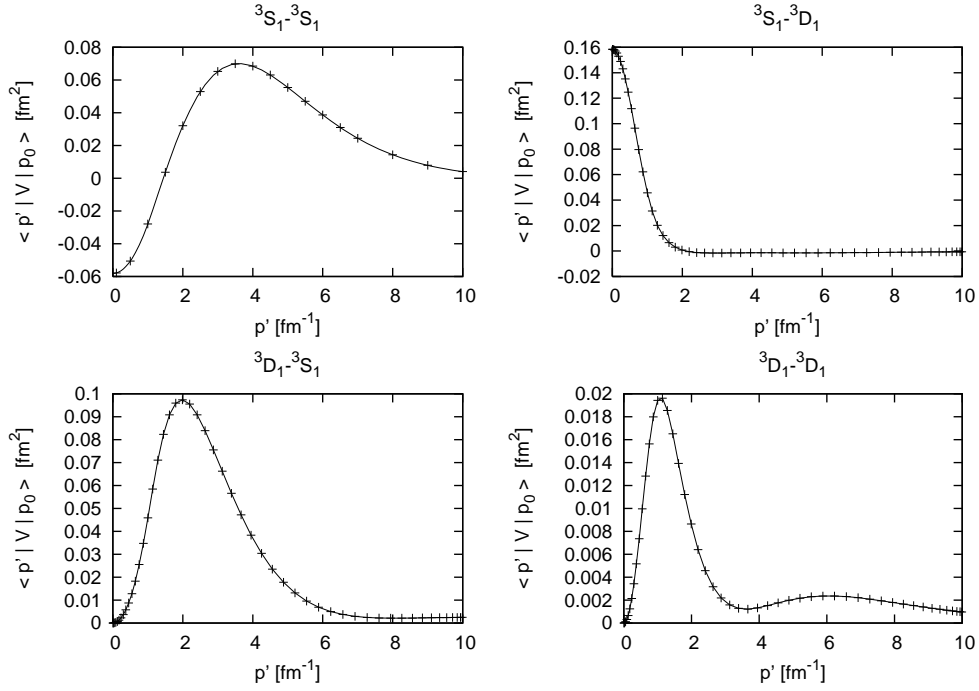


Fig. 2. The same as in Fig. 1 for one selected coupled channel case with $t = 0$.

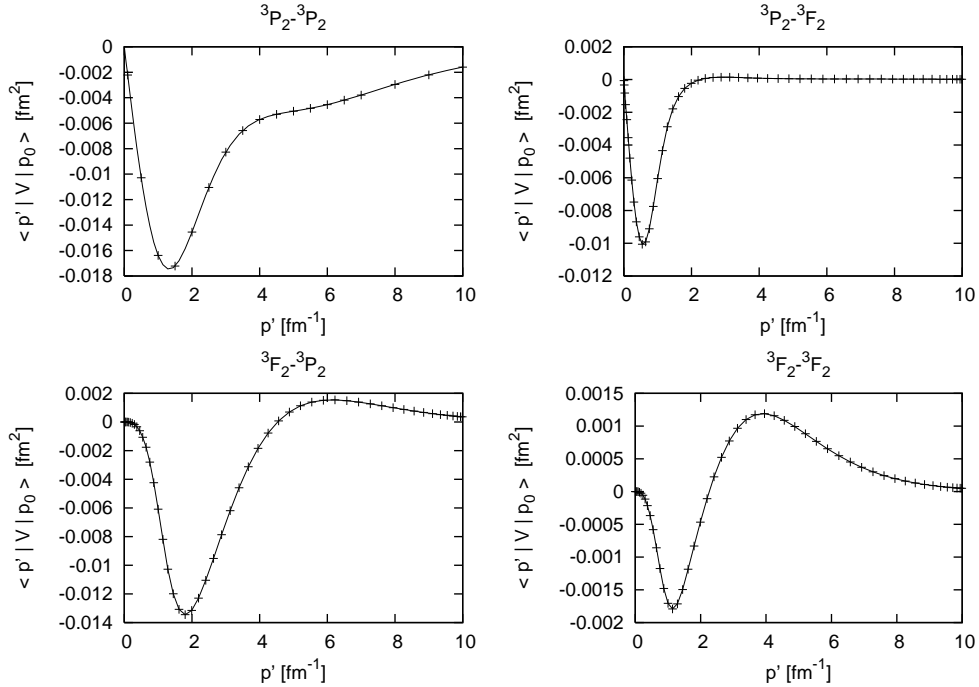


Fig. 3. The same as in Fig. 2 for one selected coupled channel case with $t = 1$.

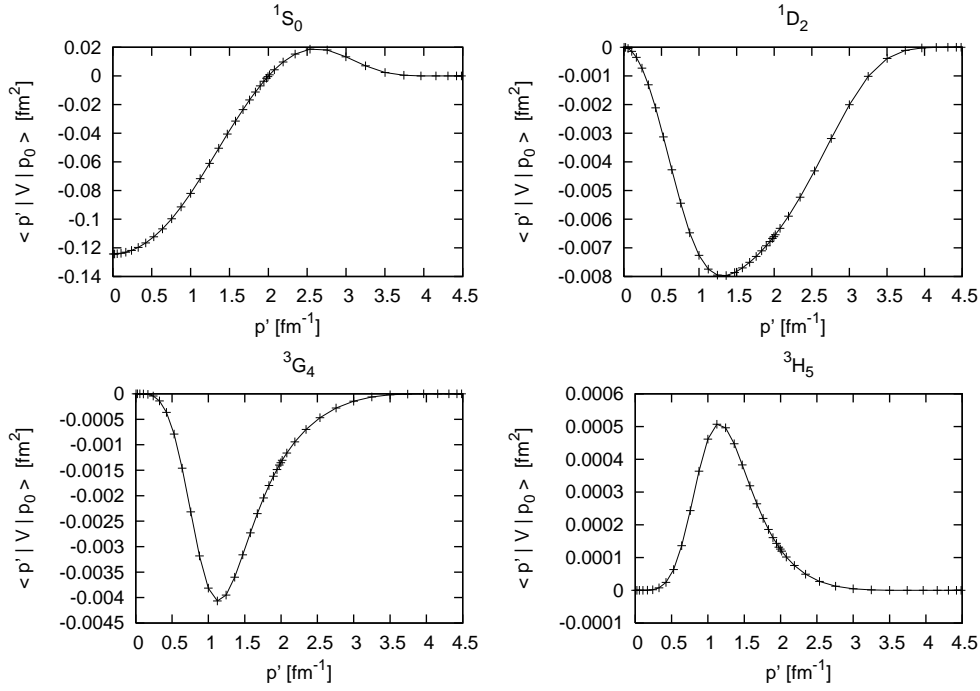


Fig. 4. The same as in Fig. 1 for the example of a chiral NNLO potential (see text for details).

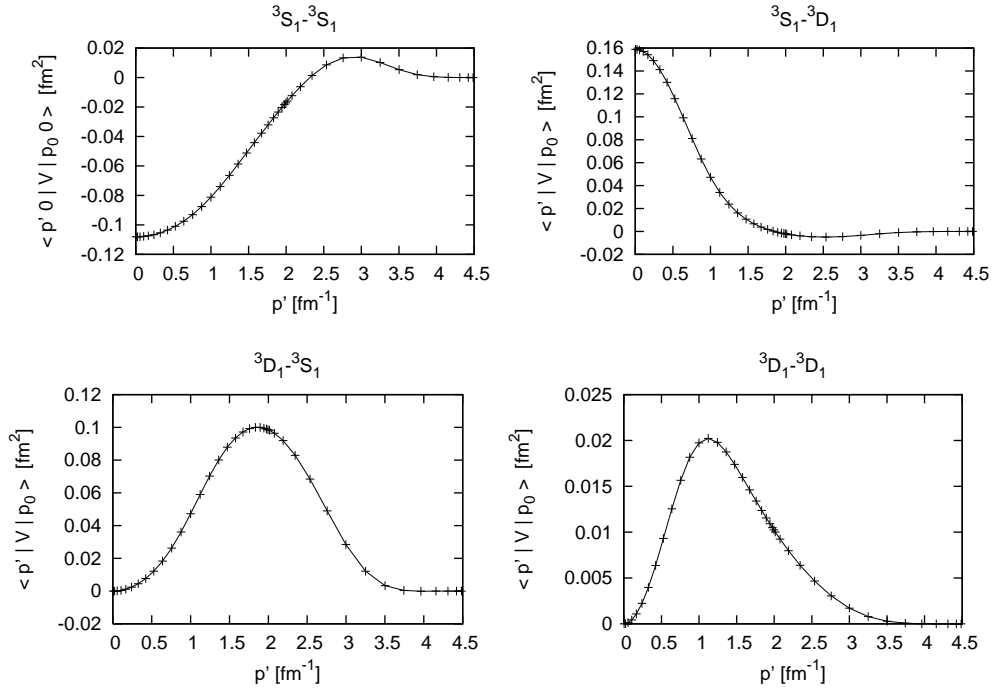


Fig. 5. The same as in Fig. 2 for the selected chiral NNLO potential.

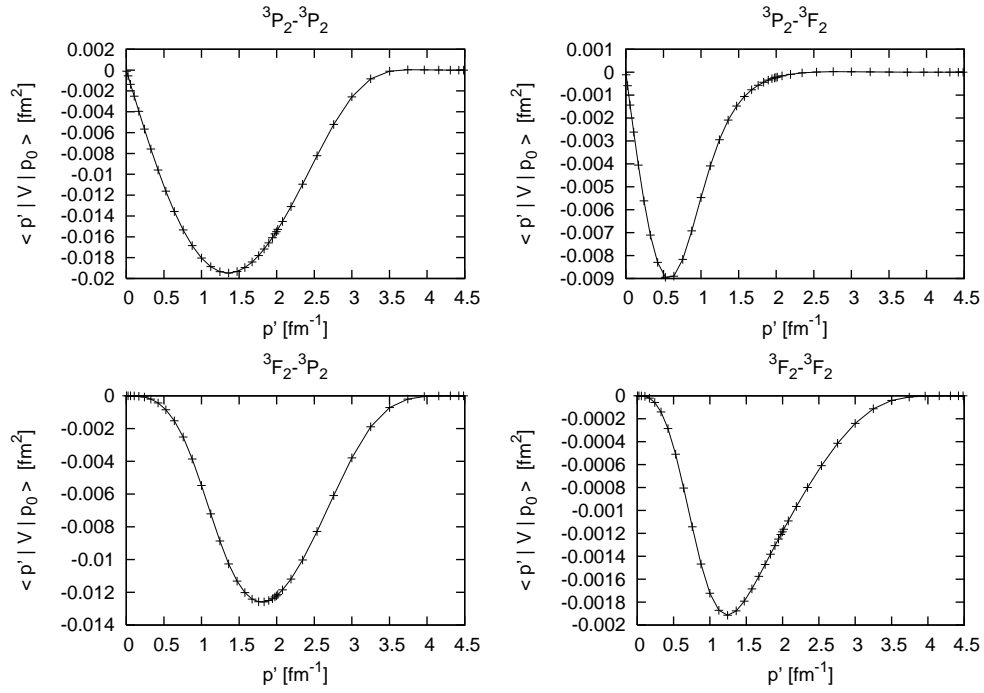


Fig. 6. The same as in Fig. 3 for the selected chiral NNLO potential.