

Two-nucleon systems in three dimensions

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A recently developed formulation for treating two- and three-nucleon bound states in a three-dimensional formulation based on spin-momentum operators is extended to nucleon-nucleon scattering. Here the nucleon-nucleon T -matrix is represented by six spin-momentum operators accompanied by six scalar functions of momentum vectors. We present the formulation and provide numerical examples for the deuteron and nucleon-nucleon scattering observables. A comparison to results from a standard partial-wave decomposition establishes the reliability of this formulation.

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I. INTRODUCTION

A standard way to obtain scattering observables for nucleon-nucleon (NN) scattering is to solve the Schrödinger equation either in momentum or coordinate space by taking advantage of rotational invariance and introducing a partial-wave basis. This is a well-established procedure and has, at low energies (below the pion production threshold), a clear physical meaning. At higher energies the number of partial waves needed to obtain converged results increases and approaches based on a direct evaluation of the scattering equation in terms of vector variables become more appealing.

The experience in three- and four-nucleon calculations [1,2] in particular shows that the standard treatment based on a partial-wave projected momentum space basis is quite successful at lower energies, but becomes increasingly more tedious with increasing energy, since each building block requires extended algebra and intricate numerical realizations. On the other hand, for a system of three bosons interacting via scalar forces, it has been demonstrated to be relatively easy to calculate a three-body bound state [3] as well as three-body scattering [4] in the Faddeev scheme when avoiding an angular momentum decomposition altogether. Thus it is only natural to strive to solve the three nucleon (3N) Faddeev equations in a similar fashion.

Recently we proposed a three-dimensional (3D) formulation of the Faddeev equations for 3N bound states [5] and 3N scattering [6] in which the spin-momentum operators are evaluated analytically, leaving the Faddeev equations as a finite set of coupled equations for scalar functions depending only on vector momenta. One of the basic foundations of this formulation rests on the fact that the most general form of the NN interaction can only depend on six linearly independent spin-momentum operators, which in turn dictate the form of the NN bound and scattering state. Here we extend the formulation of the NN bound state given in [5] to NN scattering and provide a numerical realization.

There have been several approaches to formulating NN scattering without employing a partial-wave decomposition.

A helicity formulation related to the total NN spin was proposed in [7], which was extended to 3N bound-state calculations in [8]. The spectator equation for relativistic NN scattering has been successfully solved in [9] using a helicity formulation. Aside from NN scattering, 3D formulations for the scattering of pions off nucleons [10] and protons off light nuclei [11] have recently been successfully carried out.

In Sec. II we introduce the formal structure of our approach starting from the most general form of the NN potential. We derive the resulting Lippmann-Schwinger equation and show how to extract Wolfenstein parameters and NN scattering observables. Numerical realizations of our approach that employ a recent chiral next-to-next-leading order (NNLO) NN force [12–14] as well as the standard one-boson-exchange potential Bonn B [15] are presented in Sec. III. The scalar functions, which result from the evaluation of the spin-momentum operators and have to be calculated only once, are given in Appendices A and B. Finally, we conclude in Sec. IV. The more technical information necessary to perform calculations with the chiral potential is given in Appendix C. In Appendix D the Bonn B potential is presented in the form required by our formulation.

II. THE FORMAL STRUCTURE

We start by projecting the NN potential on the NN isospin states $|tm_t\rangle$, with $t = 0, m_t = 0$ being the singlet and $t = 1, m_t = -1, 0, 1$ the triplet. We assume that isospin is conserved, but allow for charge independence and charge symmetry breaking, and thus for a dependence on m_t :

$$\langle t'm'_t | V | tm_t \rangle = \delta_{tt'} \delta_{m_t m'_t} V^{tm_t}. \quad (2.1)$$

Furthermore, the most general rotational, parity and time reversal invariant form of the off-shell NN force can be expanded into six scalar spin-momentum operators [16], which we choose as

$$w_1(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) = 1,$$

$$w_2(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) = \sigma_1 \cdot \sigma_2,$$

$$\begin{aligned} w_3(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) &= i(\sigma_1 + \sigma_2) \cdot (\mathbf{p} \times \mathbf{p}'), \\ w_4(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) &= \sigma_1 \cdot (\mathbf{p} \times \mathbf{p}') \sigma_2 \cdot (\mathbf{p} \times \mathbf{p}'), \\ w_5(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) &= \sigma_1 \cdot (\mathbf{p}' + \mathbf{p}) \sigma_2 \cdot (\mathbf{p}' + \mathbf{p}), \\ w_6(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) &= \sigma_1 \cdot (\mathbf{p}' - \mathbf{p}) \sigma_2 \cdot (\mathbf{p}' - \mathbf{p}). \end{aligned} \quad (2.2)$$

Each of these operators is multiplied with scalar functions that depend only on the momenta \mathbf{p} and \mathbf{p}' , leading to the most general expansion for any NN potential:

$$V^{tm_t} \equiv \sum_{j=1}^6 v_j^{tm_t}(\mathbf{p}', \mathbf{p}) w_j(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}). \quad (2.3)$$

The property of Eq. (2.1) carries over to the NN t -operator, which fulfills the Lippmann-Schwinger (LS) equation

$$t^{tm_t} = V^{tm_t} + V^{tm_t} G_0 t^{tm_t}, \quad (2.4)$$

with $G_0(z) = (z - H_0)^{-1}$ being the free resolvent. The T -matrix element has an expansion analogous to the potential,

$$t^{tm_t} \equiv \sum_{j=1}^6 t_j^{tm_t}(\mathbf{p}', \mathbf{p}) w_j(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}). \quad (2.5)$$

Inserting Eqs. (2.3) and (2.5) into the LS equation (2.4), operating with $w_k(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})$ from the left and performing the trace in the NN spin space leads to

$$\begin{aligned} &\sum_j A_{kj}(\mathbf{p}', \mathbf{p}) t_j^{tm_t}(\mathbf{p}', \mathbf{p}) \\ &= \sum_j A_{kj}(\mathbf{p}', \mathbf{p}) v_j^{tm_t}(\mathbf{p}', \mathbf{p}) + \int d^3 p'' \sum_{jj'} v_j^{tm_t}(\mathbf{p}', \mathbf{p}'') \\ &\quad \times G_0(p'') t_{j'}^{tm_t}(\mathbf{p}'', \mathbf{p}) B_{kjj'}(\mathbf{p}', \mathbf{p}'', \mathbf{p}). \end{aligned} \quad (2.6)$$

The scalar coefficients A_{kj} and $B_{kjj'}$ are defined as

$$A_{kj}(\mathbf{p}', \mathbf{p}) \equiv \text{Tr}[w_k(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) w_j(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})], \quad (2.7)$$

$$B_{kjj'}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) \equiv \text{Tr}[w_k(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) w_j(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}'') \times w_{j'}(\sigma_1, \sigma_2, \mathbf{p}'', \mathbf{p})]. \quad (2.8)$$

Here all spin dependencies are analytically evaluated, and the coefficients only depend on the vectors \mathbf{p} , \mathbf{p}' , and \mathbf{p}'' . The explicit expressions for the coefficients are given in Appendix A.

Thus we end up with a set of six coupled equations for the scalar functions $t_j^{tm_t}(\mathbf{p}', \mathbf{p})$, which depend for fixed $|\mathbf{p}|$ on two other variables, $|\mathbf{p}'|$ and the cosine of the relative angle between the vectors \mathbf{p}' and \mathbf{p} , given by $\hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}$.

Since Eqs. (2.3) and (2.5) are completely general, any arbitrary NN force can be cast into this form and serve as input. Finalizing the formulation, we only need to antisymmetrize in the initial state by applying $(1 - P_{12})|\mathbf{p}\rangle|m_1 m_2\rangle|tm_t\rangle$, and consider the on-shell T -matrix element for the given tm_t :

$$\begin{aligned} M_{m'_1 m'_2, m_1 m_2}^{tm_t} &\equiv -\frac{m}{2}(2\pi)^2 t_{m'_1 m'_2, m_1 m_2}^{tm_t}(\mathbf{p}', \mathbf{p})|_{\text{on-shell}} \\ &= -\frac{m}{2}(2\pi)^2 \left\{ \langle m'_1 m'_2 | [t^{tm_t}(\mathbf{p}', \mathbf{p}) \right. \\ &\quad \left. + (-)^t t^{tm_t}(\mathbf{p}', -\mathbf{p}) P_{12}^s] | m_1 m_2 \rangle \right\}. \end{aligned} \quad (2.9)$$

Here P_{12}^s interchanges the spin magnetic quantum numbers for the initial particles, m represents the nucleon mass.

For the on-shell condition, characterized by $|\mathbf{p}'| = |\mathbf{p}|$, the vectors $\mathbf{p} - \mathbf{p}'$ and $\mathbf{p} + \mathbf{p}'$ are orthogonal. Under this condition,

the operator $\sigma_1 \cdot \sigma_2$ can be represented as a linear combination of the operators w_j , $j = 4-6$ [17]; that is

$$\begin{aligned} \sigma_1 \cdot \sigma_2 &= \frac{1}{(\mathbf{p} \times \mathbf{p}')^2} \sigma_1 \cdot (\mathbf{p} \times \mathbf{p}') \sigma_2 \cdot (\mathbf{p} \times \mathbf{p}') \\ &\quad + \frac{1}{(\mathbf{p} + \mathbf{p}')^2} \sigma_1 \cdot (\mathbf{p} + \mathbf{p}') \sigma_2 \cdot (\mathbf{p} + \mathbf{p}') \\ &\quad + \frac{1}{(\mathbf{p} - \mathbf{p}')^2} \sigma_1 \cdot (\mathbf{p} - \mathbf{p}') \sigma_2 \cdot (\mathbf{p} - \mathbf{p}'). \end{aligned} \quad (2.10)$$

We can use the relation of Eq. (2.10) for internal consistency checks of the calculations. However, in order to keep the most general off-shell structure of Eq. (2.5), we need to keep all six terms. We will come back to the numerical implications of this fact below.

From Eq. (2.9) we read off that the scattering matrix is given by

$$\begin{aligned} M_{m'_1 m'_2, m_1 m_2}^{tm_t} &= -\frac{m}{2}(2\pi)^2 \sum_{j=1}^6 [t_j^{tm_t}(\mathbf{p}', \mathbf{p}) \langle m'_1 m'_2 | w_j(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) | m_1 m_2 \rangle \\ &\quad + (-)^t t_j^{tm_t}(\mathbf{p}', -\mathbf{p}) \langle m'_1 m'_2 | w_j(\sigma_1, \sigma_2, \mathbf{p}', -\mathbf{p}) | m_2 m_1 \rangle]. \end{aligned} \quad (2.11)$$

On the other hand, the standard form of the on-shell T matrix for given quantum numbers tm_t [17] reads in the Wolfenstein representation

$$\begin{aligned} M_{m'_1 m'_2, m_1 m_2}^{tm_t} &= a^{tm_t} \langle m'_1 m'_2 | m_1 m_2 \rangle \\ &\quad - i \frac{c^{tm_t}}{|\mathbf{p} \times \mathbf{p}'|} \langle m'_1 m'_2 | w_3(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) | m_1 m_2 \rangle \\ &\quad + \frac{m^{tm_t}}{|\mathbf{p} \times \mathbf{p}'|^2} \langle m'_1 m'_2 | w_4(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) | m_1 m_2 \rangle \\ &\quad + \frac{(g+h)^{tm_t}}{(\mathbf{p} + \mathbf{p}')^2} \langle m'_1 m'_2 | w_5(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) | m_1 m_2 \rangle \\ &\quad + \frac{(g-h)^{tm_t}}{(\mathbf{p} - \mathbf{p}')^2} \langle m'_1 m'_2 | w_6(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p}) | m_1 m_2 \rangle. \end{aligned} \quad (2.12)$$

Due to the action of P_{12}^s in Eq. (2.9), which interchanges m_1 with m_2 , the two parts of Eq. (2.11) yield different results. Again, standard relations [17,18] must be applied to extract the Wolfenstein parameters:

$$\begin{aligned} a^{tm_t} &= \frac{1}{4} \text{Tr}(M), \\ c^{tm_t} &= -i \frac{1}{8} \text{Tr} \left[M \frac{w_3(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{|\mathbf{p} \times \mathbf{p}'|} \right], \\ m^{tm_t} &= \frac{1}{4} \text{Tr} \left[M \frac{w_4(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{|\mathbf{p} \times \mathbf{p}'|^2} \right], \\ (g+h)^{tm_t} &= \frac{1}{4} \text{Tr} \left[M \frac{w_5(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{(\mathbf{p} + \mathbf{p}')^2} \right], \\ (g-h)^{tm_t} &= \frac{1}{4} \text{Tr} \left[M \frac{w_6(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{(\mathbf{p} - \mathbf{p}')^2} \right]. \end{aligned} \quad (2.13)$$

It is straightforward to work out those relations starting from Eq. (2.11). In order to simplify the notation we write $t_j \equiv t_j^{tm_t}(\mathbf{p}', \mathbf{p})$, $\tilde{t}_j \equiv t_j^{tm_t}(\mathbf{p}', -\mathbf{p})$, and $x \equiv \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}$ and obtain

$$\begin{aligned} a^{tm_t} &= t_1 + (-)^t \left[\frac{1}{2} \tilde{t}_1 + \frac{3}{2} \tilde{t}_2 + \frac{1}{2} p^4 (1 - x^2) \tilde{t}_4 \right. \\ &\quad \left. + p^2 (1 - x) \tilde{t}_5 + p^2 (1 + x) \tilde{t}_6 \right], \\ c^{tm_t} &= i p^2 \sqrt{1 - x^2} [t_3 - (-)^t \tilde{t}_3], \\ m^{tm_t} &= t_2 + p^4 (1 - x^2) t_4 + (-)^t \left[\frac{1}{2} \tilde{t}_1 - \frac{1}{2} \tilde{t}_2 + \frac{1}{2} p^4 (1 - x^2) \tilde{t}_4 \right. \\ &\quad \left. - p^2 (1 - x) \tilde{t}_5 - p^2 (1 + x) \tilde{t}_6 \right], \\ g^{tm_t} &= t_2 + p^2 (1 + x) t_5 + p^2 (1 - x) t_6 + (-)^t \\ &\quad \times \left[\frac{1}{2} \tilde{t}_1 - \frac{1}{2} \tilde{t}_2 - \frac{1}{2} p^4 (1 - x^2) \tilde{t}_4 \right], \\ h^{tm_t} &= p^2 (1 + x) t_5 - p^2 (1 - x) t_6 \\ &\quad + (-)^t [-p^2 (1 - x) \tilde{t}_5 + p^2 (1 + x) \tilde{t}_6]. \end{aligned} \quad (2.14)$$

It remains to consider the particle representation. For the proton-proton or neutron-neutron system the isospin is $t = 1$. Thus, the above given Wolfenstein parameters are already the physical ones and enter the calculation of observables. In the case of the neutron-proton system both isospins contribute and the physical amplitudes are given by $\frac{1}{2}(a^{00} + a^{10})$, $\frac{1}{2}(c^{00} + c^{10})$, etc.

Once the Wolfenstein parameters are known, all NN observables can readily be calculated taking well-defined bilinear products thereof [17]. For example, the spin-averaged differential cross section I_0 is given as $\frac{1}{4}\text{Tr}(MM^\dagger)$.

For completeness, we also give the derivation of the deuteron which carries isospin $t = 0$ and total spin $s = 1$. We employ the operator form from Ref. [7],

$$\begin{aligned} \langle \mathbf{p} | \Psi_{m_d} \rangle &= \left[\phi_1(p) + \left(\boldsymbol{\sigma}_1 \cdot \mathbf{p} \boldsymbol{\sigma}_2 \cdot \mathbf{p} - \frac{1}{3} p^2 \right) \phi_2(p) \right] |1m_d\rangle \\ &\equiv \sum_{k=1}^2 \phi_k(p) b_k(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}) |1m_d\rangle, \end{aligned} \quad (2.15)$$

where $|1m_d\rangle$ describes the state in which the two spin- $\frac{1}{2}$ states are coupled to the total spin 1 and the magnetic quantum number m_d . The definition of the operators b_k can be easily read off the first line of Eq. (2.15). The two scalar functions $\phi_1(p)$ and $\phi_2(p)$ are related in a simple way to the standard s - and d -wave components of the deuteron wave function, $\psi_0(p)$ and $\psi_2(p)$ by [7]

$$\begin{aligned} \psi_0(p) &= \phi_1(p), \\ \psi_2(p) &= \frac{4p^2}{3\sqrt{2}} \phi_2(p). \end{aligned} \quad (2.16)$$

Next we use the Schrödinger equation in integral form projected on isospin states,

$$\Psi_{m_d} = G_0 V^{00} \Psi_{m_d}. \quad (2.17)$$

Inserting the explicit expression of Eq. (2.15) we obtain

$$\begin{aligned} &\left[\phi_1(p) + \left(\boldsymbol{\sigma}_1 \cdot \mathbf{p} \boldsymbol{\sigma}_2 \cdot \mathbf{p} - \frac{1}{3} p^2 \right) \phi_2(p) \right] |1m_d\rangle \\ &= \frac{1}{E_d - \frac{p^2}{m}} \int d^3 p' \sum_{j=1}^6 v_j^{00}(\mathbf{p}, \mathbf{p}') w_j(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}, \mathbf{p}') \\ &\quad \times \left[\phi_1(p') + \left(\boldsymbol{\sigma}_1 \cdot \mathbf{p}' \boldsymbol{\sigma}_2 \cdot \mathbf{p}' - \frac{1}{3} p'^2 \right) \phi_2(p') \right] |1m_d\rangle, \end{aligned} \quad (2.18)$$

where E_d is the deuteron binding energy. We remove the spin dependence by projecting from the left with $\langle 1m_d | b_k(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p})$ and summing over m_d . This leads to

$$\begin{aligned} &\sum_{m_d=-1}^1 \langle 1m_d | b_k(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}) \sum_{k'=1}^2 \phi_{k'}(p) b_{k'}(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}) | 1m_d \rangle \\ &= \frac{1}{E_d - \frac{p^2}{m}} \sum_{m_d=-1}^1 \int d^3 p' \sum_{j=1}^6 v_j^{00}(\mathbf{p}, \mathbf{p}') w_j(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}, \mathbf{p}') \\ &\quad \times \sum_{k''=1}^2 \phi_{k''}(p') b_{k''}(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}') | 1m_d \rangle. \end{aligned} \quad (2.19)$$

Defining the scalar functions

$$A_{kk'}^d(p) \equiv \sum_{m_d=-1}^1 \langle 1m_d | b_k(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}) b_{k'}(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}) | 1m_d \rangle \quad (2.20)$$

and

$$\begin{aligned} B_{kj k''}^d(\mathbf{p}, \mathbf{p}') &\equiv \sum_{m_d=-1}^1 \langle 1m_d | b_k(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}) w_j(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}, \mathbf{p}') \\ &\quad \times b_{k''}(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \mathbf{p}') | 1m_d \rangle, \end{aligned} \quad (2.21)$$

we obtain for Eq. (2.19)

$$\begin{aligned} \sum_{k'=1}^2 A_{kk'}^d(p) \phi_{k'}(p) &= \frac{1}{E_d - \frac{p^2}{m}} \int d^3 p' \sum_{j=1}^6 v_j^{00}(\mathbf{p}, \mathbf{p}') \\ &\quad \times \sum_{k''=1}^2 B_{kj k''}^d(\mathbf{p}, \mathbf{p}') \phi_{k''}(p'). \end{aligned} \quad (2.22)$$

Note that $A_{kk'}^d$ and $B_{kj k''}^d$ are both independent of the interaction. Therefore, these coefficients can be prepared beforehand for all calculations of the deuteron bound state, which consists of two coupled equations for the functions $\phi_1(p)$ and $\phi_2(p)$. The summation over m_d guarantees the scalar nature of the functions $A_{kk'}^d(p)$ and $B_{kj k''}^d(\mathbf{p}, \mathbf{p}')$, which are given in Appendix B. The azimuthal angle can be trivially integrated out, leading to the final form of the deuteron

equation

$$\sum_{k'=1}^2 A_{kk'}^d(p) \phi_{k'}(p) = \frac{2\pi}{E_d - \frac{p^2}{m}} \sum_{k''=1}^2 \int_0^\infty dp' p'^2 \phi_{k''}(p') \times \int_{-1}^1 dx \sum_{j=1}^6 v_j^{00}(p, p', x) B_{kj}^d(p, p', x), \quad (2.23)$$

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

III. NUMERICAL REALIZATION

A. The deuteron

For a numerical treatment of Eq. (2.23), it is convenient to first define

$$Z_{k,k'}(p, p') \equiv \int_{-1}^1 dx \sum_{j=1}^6 v_j^{00}(p, p', x) B_{kj}^d(p, p', x), \quad (3.1)$$

and then assume that the integral over p' will be carried out with some choice of Gaussian points and weights (p_j, g_j) with $j = 1, 2, \dots, N$. This leads to

$$\begin{aligned} & \sum_{k'=1}^2 \sum_{j=1}^N \left[g_j p_j^2 Z_{kk'}(p_i, p_j) + \delta_{ij} \frac{p_j^2}{2m\pi} A_{kk'}^d(p_i) \right] \phi_{k'}(p_j) \\ &= E_d \sum_{k'=1}^2 \frac{1}{2\pi} A_{kk'}^d(p_i) \phi_{k'}(p_i). \end{aligned} \quad (3.2)$$

Eq. (3.2) can be written as a so-called generalized eigenvalue problem

$$R\xi = E_d Y\xi, \quad (3.3)$$

or

$$\sum_{l'=1}^{2N} R_{ll'} \xi_{l'} = E_d \sum_{l'=1}^{2N} Y_{ll'} \xi_{l'}, \quad (3.4)$$

where

$$\begin{aligned} l &= i + (k-1)N, \\ \xi_{l'} &= \phi_{k'}(p_j), \quad l' = j + (k'-1)N, \\ R_{ll'} &= g_j p_j^2 Z_{kk'}(p_i, p_j) + \delta_{ij} \frac{p_j^2}{2m\pi} A_{kk'}^d(p_i), \\ Y_{ll'} &= \delta_{ij} \frac{1}{2\pi} A_{kk'}^d(p_i). \end{aligned} \quad (3.5)$$

TABLE I. The parameters of the chiral potential of Ref. [13] in order NNLO. The LECs are given for the cutoff combination $\Lambda = 600$ MeV and $\tilde{\Lambda} = 700$ MeV. The pion decay constant F_π and masses are given in MeV. The constants c_i are given in GeV^{-1} , C_s and C_T in GeV^{-2} , and the other C_i in GeV^{-4} .

g_A	F_π	m_{π^0}	m_{π^\pm}	m	c_1	c_3	c_4	
1.29	92.4	134.977	139.570	938.919	-0.81	-3.40	3.40	
C_s -112.932	C_T 2.60161	C_1 385.633	C_2 1343.49	C_3 -121.543	C_4 -614.322	C_5 1269.04	C_6 -26.4880	C_7 -1385.12

Since $A_{11}^d \neq 0$, $A_{12}^d = A_{21}^d = 0$ and $A_{22}^d \neq 0$, the matrix Y is diagonal and can be easily inverted, and we encounter an eigenvalue problem

$$(Y^{-1} R)\xi = E_d \xi, \quad (3.6)$$

which is of the same type and dimension as is being solved for the deuteron wave function in a standard partial-wave representation, where one calculates the s - and d -wave components, $\psi_0(p)$ and $\psi_2(p)$. The connection between the two solutions, $[\phi_1(p), \phi_2(p)]$ and $[\psi_0(p), \psi_2(p)]$, given by Eqs. (2.16) provides a direct check of the numerical accuracy.

As a first example we use a chiral NNLO potential [13], which for the convenience of the reader is briefly described in Appendix C. For the specific calculation performed here we take the neutron-proton version of this potential and employ the parameters listed in Table I.

We consistently use these potential parameters in the 3D and the PW calculations. In the first case, we solve Eq. (3.6) for $\phi_1(p)$ and $\phi_2(p)$ and then use Eqs. (2.16) to obtain $\psi_0(p)$ and $\psi_2(p)$. In the second case, we employ the standard partial-wave representation of the potential and solve the Schrödinger equation directly for $\psi_0(p)$ and $\psi_2(p)$. Both methods give the same value for the deuteron binding energy, namely $E_d = -2.19993$ MeV and s -state probability $P_s = 95.291\%$. The wave functions are identical as can be seen in Fig. 1.

For the second NN force we choose the Bonn B potential [15], which has a more intricate structure due to the different meson-exchanges and the Dirac spinors. The operator form of this potential, corresponding to the basis of Eq. (2.2), is derived in Appendix D and the parameters are given in Table II. In this case, the nucleon mass is set to $m = 939.039$ MeV. Again, we have excellent agreement between the 3D and the partial-wave-based calculation for the deuteron binding energy, $E_d = -2.2242$ MeV, the s -state probability ($P_s = 95.014\%$), and the wave functions, which are displayed in Fig. 2.

In summary, we confirm that the 3D approach gives numerically stable results, which are in perfect agreement with the calculations based on standard partial-wave methods.

B. NN scattering observables

The inhomogeneous LS equation (2.6) for the six components $t_j^{lm_l}$ can be solved for a fixed value of p . For the vectors $\hat{\mathbf{p}}$ and $\hat{\mathbf{p}}'$ we choose the explicit representation

$$\begin{aligned} \hat{\mathbf{p}} &= (0, 0, 1), \\ \hat{\mathbf{p}}' &= (\sqrt{1-x'^2}, 0, x'), \\ \hat{\mathbf{p}}'' &= (\sqrt{1-x''^2} \cos \varphi'', \sqrt{1-x''^2} \sin \varphi'', x''), \end{aligned} \quad (3.7)$$

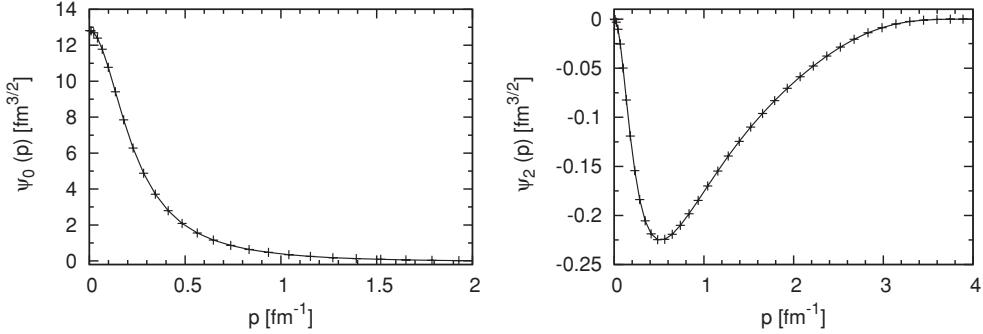


FIG. 1. The *s*-wave (left) and *d*-wave (right) component of the deuteron wave function as a function of the relative momentum p for the chiral NNLO potential specified in the text. Crosses represent results obtained with the operator approach and solid lines are from the standard partial-wave decomposition.

so that the scalar products become

$$\begin{aligned} \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}} &= x', \\ \hat{\mathbf{p}}'' \cdot \hat{\mathbf{p}} &= x'', \\ \hat{\mathbf{p}}' \cdot \hat{\mathbf{p}}'' &= x'x'' + \sqrt{1-x'^2}\sqrt{1-x''^2} \cos\varphi'' \equiv y. \end{aligned} \quad (3.8)$$

Let us now calculate the integral term on the right-hand-side of Eq. (2.6) for a positive energy of the NN system, $E_{\text{c.m.}} \equiv \frac{p_0^2}{m}$:

$$S_k(p', p, x') \equiv \int_0^{\bar{p}} dp'' p''^2 \frac{1}{p_0^2 - p''^2 + i\epsilon} f_k(p''; p', p, x'), \quad (3.9)$$

where

$$\begin{aligned} f_k(p''; p', p, x') &\equiv f_k(p'') \\ &\equiv m \sum_{j,j'=1}^6 \int_{-1}^1 dx'' \int_0^{2\pi} d\varphi'' B_{kj'j}(p', p'', p, x', x'', \varphi'') \\ &\quad \times v_j(p', p'', y) t_{j'}(p'', p, x''). \end{aligned} \quad (3.10)$$

Here the index tm_t for the T -matrix element is omitted for simplicity. For the momentum integration in Eq. (3.9) an upper bound \bar{p} is introduced since the contributions to the integral for larger momenta are insignificant, so the potential and the

TABLE II. Meson parameters for the Bonn B potential [15]. The σ parameters shown in the table are for NN total isospin 0. For NN total isospin 1 they should be replaced by $m_\sigma = 550$ MeV, $\frac{g_\sigma^2}{4\pi} = 8.9437$, $\Lambda_\alpha = 1.9$ GeV and $n = 1$.

meson	m_α [MeV]	$\frac{g_\alpha^2}{4\pi}$	$\frac{f_\alpha}{g_\alpha}$	Λ_α [GeV]	n
π	138.03	14.4		1.7	1
η	548.8	3		1.5	1
δ	983	2.488		2	1
σ	720	18.3773		2	1
ρ	769	0.9	6.1	1.85	2
ω	782.6	24.5	0	1.85	2

t -matrix are essentially zero. The integral of Eq. (3.9) can then be treated in a standard fashion and one obtains

$$\begin{aligned} S_k(p', p, x') &= \int_0^{\bar{p}} dp'' \frac{p''^2 f_k(p'') - p_0^2 f_k(p_0)}{p_0^2 - p''^2} \\ &\quad + \frac{1}{2} p_0 f_k(p_0) \left(\ln \frac{\bar{p} + p_0}{\bar{p} - p_0} - i\pi \right). \end{aligned} \quad (3.11)$$

It is tempting to solve Eq. (2.6) by iteration and then sum the resulting Neumann series with a Padé scheme. The determinant of the 6×6 matrix $A(p', p, x')$, which appears on both sides of (2.6), can be easily calculated with the result

$$\det(A) = -65536 p^8 p'^8 (p^2 - p'^2)^2 (1 - x'^2)^4. \quad (3.12)$$

In particular, this determinant is zero for $p' = p$ and $x' = \pm 1$. However, by a careful choice of the p , p' and x' points, it is possible to work with nonzero values of $\det(A)$, so that the matrix A can be inverted. In this case, Eq. (2.6) can be written as

$$t(p', p, x') = v(p', p, x') + A^{-1}(p', p, x') S(p', p, x'), \quad (3.13)$$

where $t(p', p, x')$, $v(p', p, x')$, and $S(p', p, x')$ denote now six-dimensional vectors with components t_j , v_j , and S_j . Note that $S(p', p, x')$ contains the unknown vector $t(p', p, x')$. We arrive at the following iteration scheme:

$$\begin{aligned} t^{(1)}(p', p, x') &= v(p', p, x'), \\ t^{(n)}(p', p, x') &= v(p', p, x') + A^{-1}(p', p, x') S^{(n-1)}(p', p, x') \\ &\quad \text{for } n > 1, \end{aligned} \quad (3.14)$$

where $S^{(n-1)}(p', p, x')$ is calculated using the vector $t(p', p, x')$ from the previous iteration; namely, $t^{(n-1)}(p', p, x')$. However, our experience with this iteration scheme is discouraging. Numerically, $\det(A)$ can be very close to zero, and in such cases the rank of matrix A can vary from 2 to 5. As a consequence, it is very difficult to maintain numerical stability for this iterative method. Another drawback

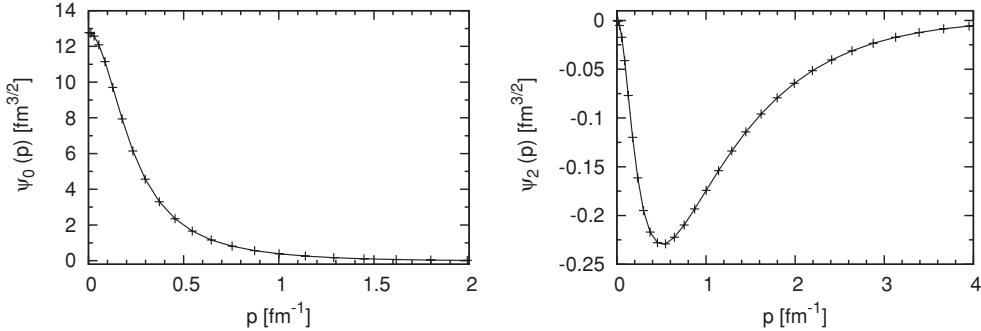


FIG. 2. The same as in Fig. 1, but for the Bonn B potential [15].

of using the inverse of A is that it is impossible to obtain the on-shell matrix element $t(p_0, p_0, x')$ directly. One would have to rely on numerical interpolations for calculating on-shell matrix elements.

For this reason, we decided to solve Eq. (2.6) directly as a system of inhomogeneous coupled algebraic equations. To this aim we first perform a discretization with respect to the different variables in the problem. As typical grid sizes we take $n_x = 36$ Gaussian points for the x'' integration, and use the same grid for the x' points. Furthermore, we use $n_p = 36$ Gaussian points for the p' and p'' grids, which are defined in the interval $(0, \bar{p} = 40 \text{ fm}^{-1})$. These points are distributed in such a way that p_0 is avoided and the same number of points is put symmetrically into two narrow intervals on each side of p_0 [19]. Such a choice proved advantageous in the treatment of the 1S_0 channel for the PWD calculations and is kept here. In addition, p_0 is added to the set of p' points. Finally, we choose $n_{\varphi''} = 60$ Gaussian points for the φ'' integration. Thus, we arrive at a system of $6 \times (n_p + 1) \times n_x$ linear equations of the form

$$H\xi = b, \quad (3.15)$$

where the vector ξ represents all unknown values of $t_j(p', p, x')$ for fixed p . If we choose from the very beginning $p = p_0$, then the solution of Eq. (3.15) contains the on-shell T matrix in the operator form; namely $t_j(p_0, p_0, x')$.

It is clear that for the on-shell t -matrix the solution cannot be unique, since the six operators become linearly dependent on each other [see Eq. (2.10)]. In principle, one therefore expects that Eq. (3.15) is noninvertible and that tools like a singular value decomposition are required for the solution. However, we found that this is not required since the standard LU decomposition of Numerical Recipes [20] worked safely for both interactions, all the considered laboratory energies, and different choices of the mesh points. Interestingly, the actual solution for the on-shell T -matrix is not unique as expected and depends even on the optimization level of the compiler. However, the observables turn out to be stable and unique.

Of course, setting $p = p_0$ is not necessary. For $p \neq p_0$ the system of equations (3.15) has a unique and smooth solution and afterwards the interpolation to the on-shell case can be safely performed.

The path to NN observables is straightforward. From Eq. (2.11) we evaluate first the scattering matrix M for all possible spin projections m'_1, m'_2, m_1 , and m_2 , noting that on-shell

$$t_j^{tm_l}(\mathbf{p}', \mathbf{p}) = t_j^{tm_l}(p_0, p_0, x') \quad (3.16)$$

and

$$t_j^{tm_l}(\mathbf{p}', -\mathbf{p}) = t_j^{tm_l}(p_0, p_0, -x'). \quad (3.17)$$

Since we use a set of x' points which is symmetric with respect to $x' = 0$, no interpolation is required and M is easily obtained. Before we can make use of Eq. (2.13), we calculate matrix elements of the modified operators w_j appearing in (2.13), in the same representation as for the matrix M :

$$\begin{aligned} \langle m'_1 m'_2 | & \frac{w_3(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{|\mathbf{p} \times \mathbf{p}'|} | m_1 m_2 \rangle \\ \langle m'_1 m'_2 | & \frac{w_4(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{|\mathbf{p} \times \mathbf{p}'|^2} | m_1 m_2 \rangle \\ \langle m'_1 m'_2 | & \frac{w_5(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{(\mathbf{p} + \mathbf{p}')^2} | m_1 m_2 \rangle \\ \langle m'_1 m'_2 | & \frac{w_6(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{(\mathbf{p} - \mathbf{p}')^2} | m_1 m_2 \rangle. \end{aligned} \quad (3.18)$$

For this calculation symbolic software like Mathematica[©] [21] proves very useful. In the next step, the Wolfenstein parameters are calculated as sums over m'_1, m'_2, m_1 and m_2 . For example,

$$\begin{aligned} a^{tm_l} &= \frac{1}{4} \sum_{m'_1, m'_2} \sum_{m_1, m_2} m'_1 m'_2, m_1 m_2 \delta_{m'_1 m_1} \delta_{m'_2 m_2}, \\ c^{tm_l} &= -i \frac{1}{8} \sum_{m'_1, m'_2} \sum_{m_1, m_2} m'_1 m'_2, m_1 m_2 \\ &\quad \times \langle m_1 m_2 | \frac{w_3(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})}{|\mathbf{p} \times \mathbf{p}'|} | m'_1 m'_2 \rangle. \end{aligned} \quad (3.19)$$

Finally, the NN observables result from the Wolfenstein parameters as simple bilinear expressions [17].

In Figs. 3–6 we compare a selected set of observables calculated with the new 3D method to results obtained by

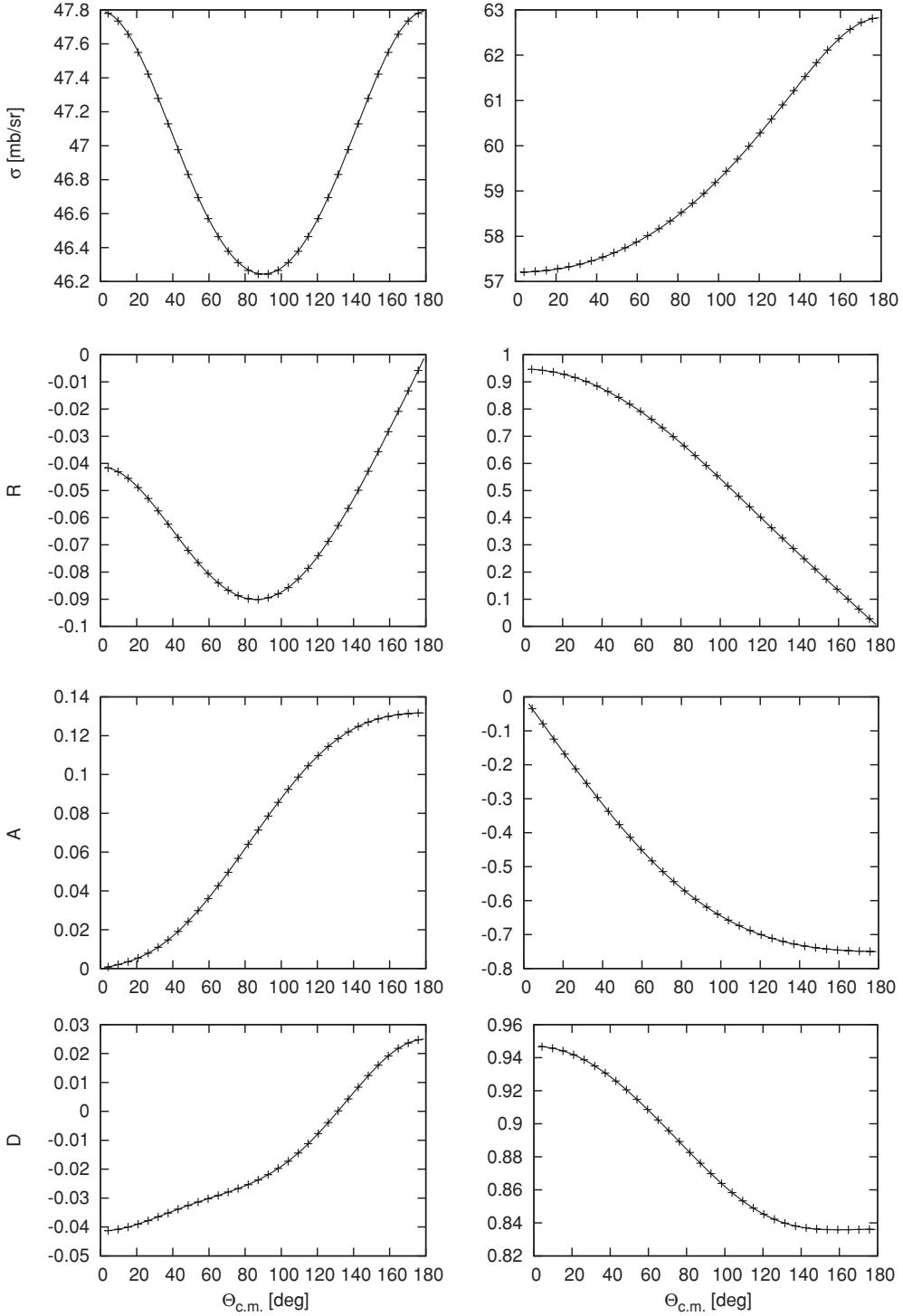


FIG. 3. Selected observables for the neutron-neutron (left panel) and neutron-proton (right panel) system at the projectile laboratory kinetic energy of 13 MeV as a function of the center-of-mass angle θ for the chiral NNLO potential [13]. Crosses represent results obtained with the operator approach and solid lines represent fully converged results from the standard PWD. For the definition of the R , A and D observables see, for example, Ref. [17].

using a standard partial-wave decomposition, employing the same potentials we used for the deuteron calculations. For the chiral potential, we chose two laboratory kinetic energies 13 and 150 MeV, whereas for the Bonn B potential the higher energy is chosen to be 300 MeV. We made sure that in

all cases a sufficient number of partial waves is included to obtain converged results in the standard PWD approach. For all the energies considered, our converged PWD results agree perfectly with predictions obtained from the new 3D approach.

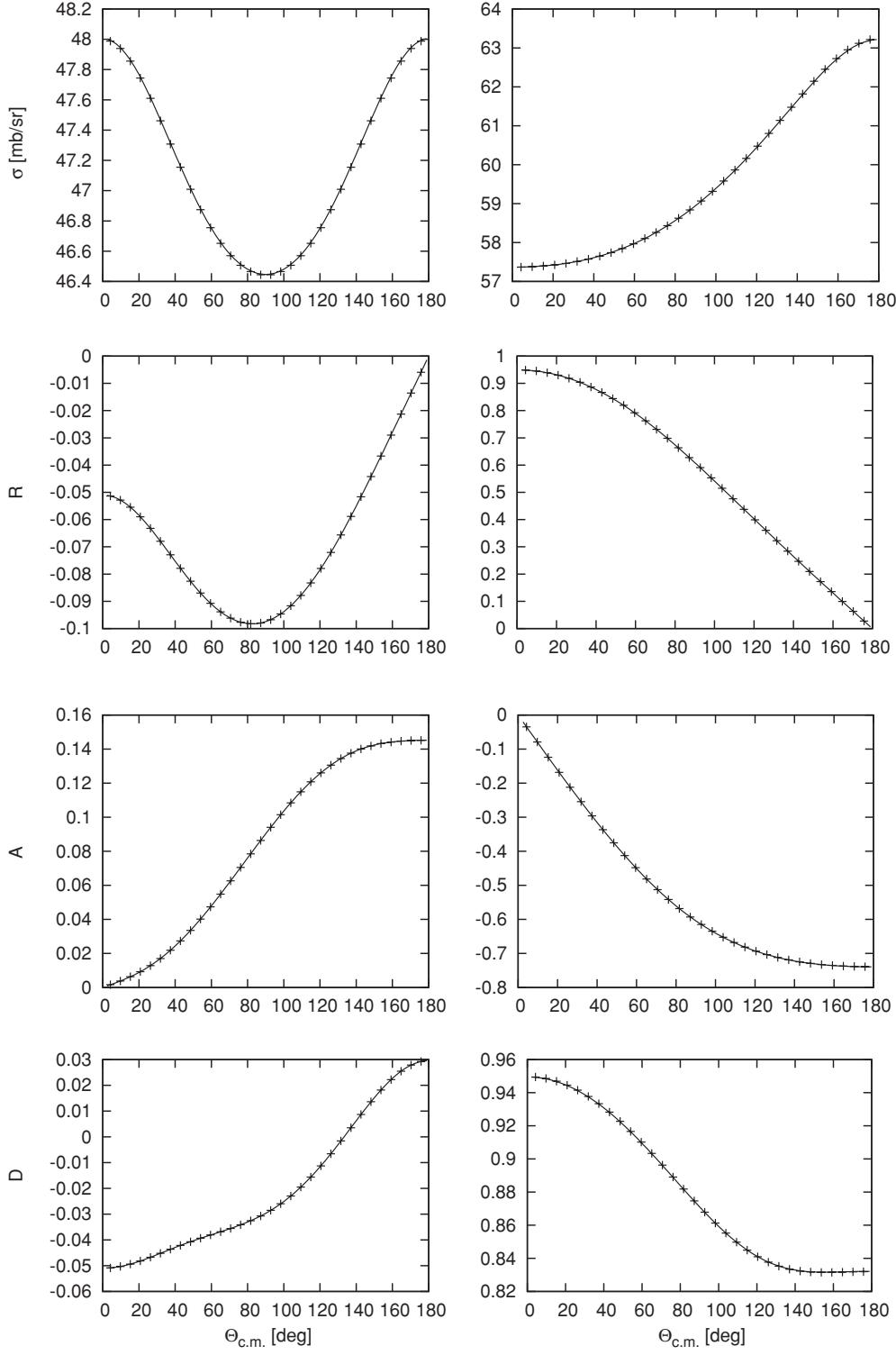


FIG. 4. The same as in Fig. 3, but for the Bonn B potential [15].

In Figs. 7 and 8 we demonstrate the convergence with respect to different maximum total angular momenta j_{\max} toward the results calculated using our new 3D method for the differential cross section and the asymmetry A . Here we employ the Bonn B potential and show the calculations for the neutron-neutron and neutron-proton cases separately. As one

can see, quite a sizable number of partial waves is required for a converged calculation at 300 MeV. Finally, in Fig. 9 we display the Wolfenstein amplitudes for neutron-proton scattering at 300 MeV laboratory kinetic energy. Again, we compare partial-wave-based calculations for different maximum total angular momenta j_{\max} to the 3D calculation. We observe that

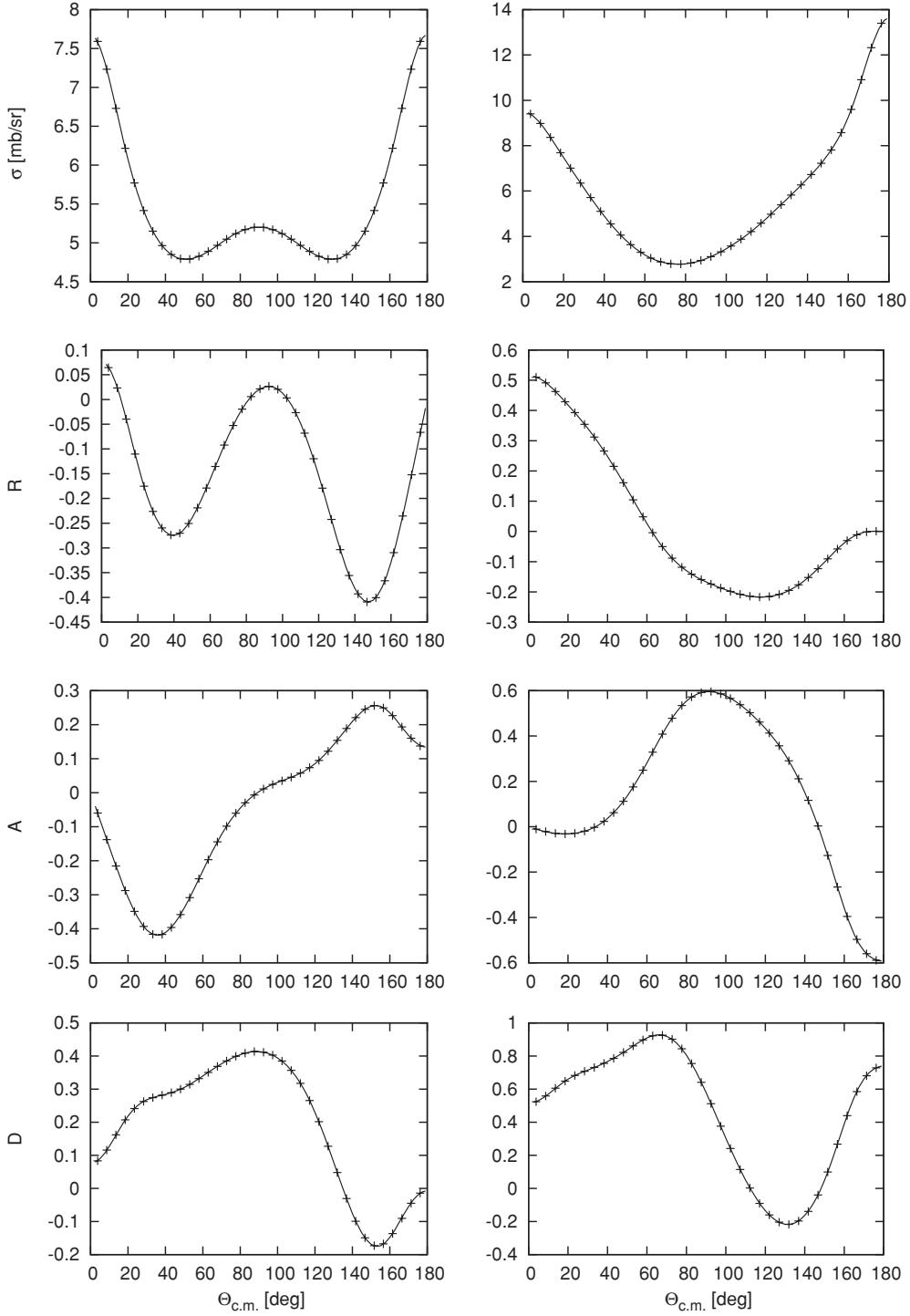


FIG. 5. The same as in Fig. 3, but for the projectile laboratory kinetic energy of 150 MeV.

the maximum number of partial waves needed for obtaining a converged result is quite different for the different amplitudes.

IV. SUMMARY AND CONCLUSIONS

Two-nucleon scattering at intermediate energies of a few hundred MeV requires quite a few angular momentum states

in order to achieve convergence of, for example, scattering observables. We formulated and numerically illustrated an approach to treating the NN system working directly with momentum vectors and using spin-momentum operators multiplied by scalar functions, which only depend on the momentum vectors. This approach is quite natural, since any general NN force being invariant under time-reversal, parity, and Galilei (or Lorentz) transformations can only

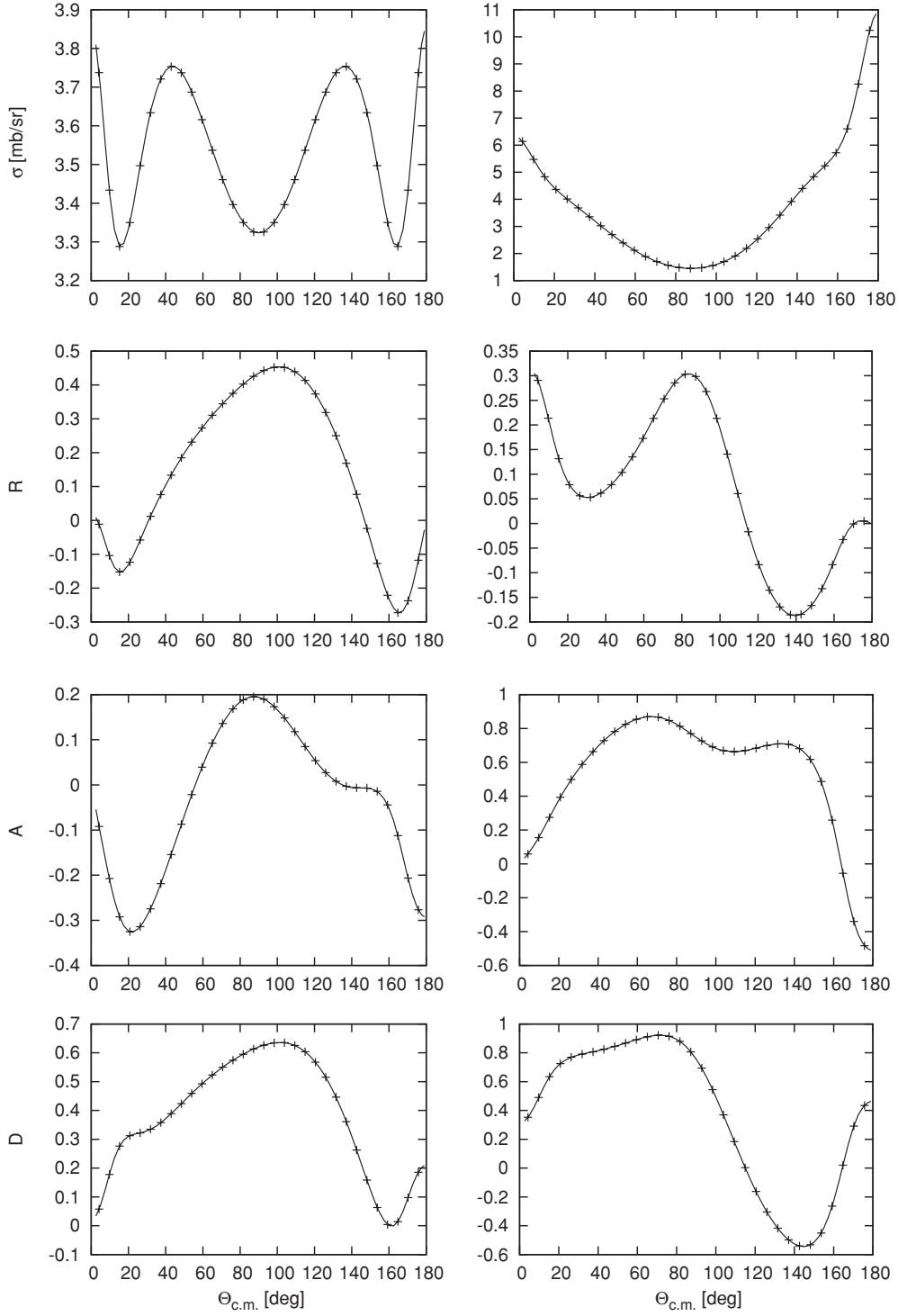


FIG. 6. The same as in Fig. 4, but for the projectile laboratory kinetic energy of 300 MeV.

depend on six linear independent spin-momentum operators. The representation of the NN potential using spin-momentum operators leads to a system of six coupled equations of scalar functions (depending on momentum vectors) for the NN T -matrix, once the spin-momentum operators are analytically calculated by performing suitable trace operations.

We calculated deuteron properties and NN scattering observables using two different NN potentials, one derived from

chiral effective field theory and one from meson exchange. For all cases we found perfect agreement between the calculations based on our new method and conventional calculations using a partial-wave basis.

This work is intended to serve as starting point toward treating three-nucleon systems without partial waves. The theoretical formulation has already been given for the 3N bound state (including 3N forces) in Ref. [5] and for 3N

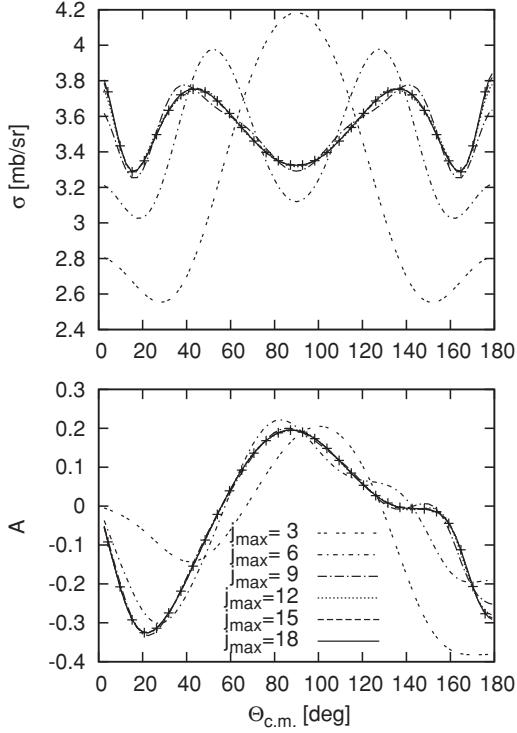


FIG. 7. The convergence of the PWD results for the differential cross section and the depolarization coefficient A [17] for neutron-neutron scattering based on different numbers of partial waves determined by the maximal total angular momentum j_{\max} of the NN system (lines) with respect to the result of the three-dimensional calculation (crosses) for the projectile laboratory kinetic energy of 300 MeV and the Bonn B potential [15].

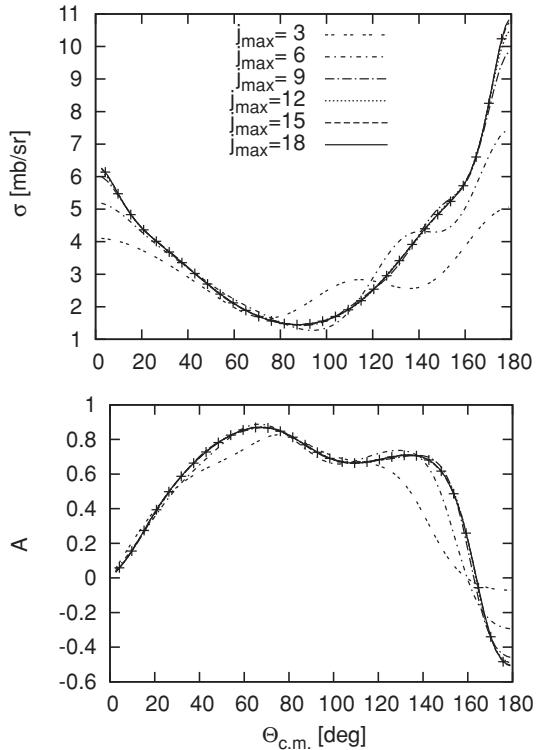


FIG. 8. The same as in Fig. 7, but for neutron-proton scattering.

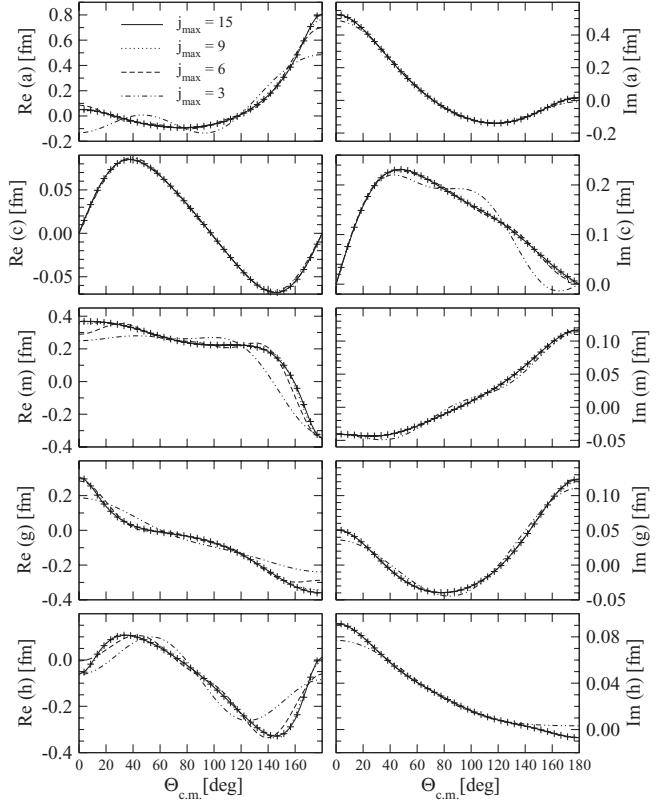


FIG. 9. The Wolfenstein parameters for neutron-proton scattering for the projectile laboratory kinetic energy of 300 MeV calculated with the Bonn B potential [15]. Results of the 3D calculation are given by the crosses. The convergence of the PWD results for increasing values of maximum angular momentum j_{\max} is shown by the different curves labeled in the figure. The left panels show the real parts of the amplitudes, whereas the imaginary parts are displayed in the right panels.

scattering in Ref. [6]. For a much simpler case, when spin- and isospin-degrees are neglected, the feasibility of three-body scattering calculations in the GeV regime has already been demonstrated [4], even including Poincaré symmetry [22]. Since our approach leads to coupled equations of scalar functions of momentum vectors, the generalization to include spin degrees of freedom appears feasible. In the 3N system not only the number of partial waves increases rapidly, but also 3N forces appear as new dynamical input. In particular in the chiral approach, the number of 3NF contributions proliferates with the order of expansion of the theory. In higher orders many complicated terms contribute to the 3N force [13]. In this case, a traditional partial-wave decomposition of the 3NF poses a serious problem which has a chance to be alleviated by a direct three-dimensional treatment.

ACKNOWLEDGMENTS

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APPENDIX A: COEFFICIENTS FOR NN SCATTERING

In this appendix we present the expressions A and B given in Eqs. (2.7) and (2.8) for NN scattering. The coefficients $A_{ij}(\mathbf{p}', \mathbf{p})$ can be obtained in terms of the following four functions FA :

$$FA_3(\mathbf{p}', \mathbf{p}) = 4(\mathbf{p} \times \mathbf{p}')^2, \quad (A1)$$

$$FA_4(\mathbf{p}', \mathbf{p}) = 4(\mathbf{p}' + \mathbf{p})^2, \quad (A2)$$

$$FA_5(\mathbf{p}', \mathbf{p}) = 4(\mathbf{p}' - \mathbf{p})^2, \quad (A3)$$

$$FA_6(\mathbf{p}', \mathbf{p}) = 4(p'^2 - p^2)^2. \quad (A4)$$

The nonzero coefficients $A_{ij}(\mathbf{p}', \mathbf{p})$ are

$$A_{11}(\mathbf{p}', \mathbf{p}) = 4, \quad (A5)$$

$$A_{22}(\mathbf{p}', \mathbf{p}) = 12, \quad (A6)$$

$$A_{24}(\mathbf{p}', \mathbf{p}) = A_{42}(\mathbf{p}', \mathbf{p}) = FA_3(\mathbf{p}', \mathbf{p}), \quad (A7)$$

$$A_{25}(\mathbf{p}', \mathbf{p}) = A_{52}(\mathbf{p}', \mathbf{p}) = FA_4(\mathbf{p}', \mathbf{p}), \quad (A8)$$

$$A_{26}(\mathbf{p}', \mathbf{p}) = A_{62}(\mathbf{p}', \mathbf{p}) = FA_5(\mathbf{p}', \mathbf{p}), \quad (A9)$$

$$A_{33}(\mathbf{p}', \mathbf{p}) = -2FA_3(\mathbf{p}', \mathbf{p}), \quad (A10)$$

$$A_{44}(\mathbf{p}', \mathbf{p}) = \frac{1}{4}A_{24}^2(\mathbf{p}', \mathbf{p}), \quad (A11)$$

$$A_{55}(\mathbf{p}', \mathbf{p}) = \frac{1}{4}A_{25}^2(\mathbf{p}', \mathbf{p}), \quad (A12)$$

$$A_{56}(\mathbf{p}', \mathbf{p}) = A_{65}(\mathbf{p}', \mathbf{p}) = FA_6(\mathbf{p}', \mathbf{p}), \quad (A13)$$

$$A_{66}(\mathbf{p}', \mathbf{p}) = \frac{1}{4}A_{26}^2(\mathbf{p}', \mathbf{p}). \quad (A14)$$

All other $A_{ij}(\mathbf{p}', \mathbf{p}) = 0$.

The nonvanishing coefficients $B_{ijk}(\mathbf{p}', \mathbf{p}'', \mathbf{p})$ can be expressed by means of the following 25 functions FB :

$$FB_{3a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p} \times \mathbf{p}'')^2, \quad (A15)$$

$$FB_{3b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p}'' \times \mathbf{p}')^2, \quad (A16)$$

$$FB_{3c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p} \times \mathbf{p}')^2, \quad (A17)$$

$$FB_{4a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p}'' + \mathbf{p})^2, \quad (A18)$$

$$FB_{4b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p}' + \mathbf{p}'')^2, \quad (A19)$$

$$FB_{4c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p}' + \mathbf{p})^2, \quad (A20)$$

$$FB_{5a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p}'' - \mathbf{p})^2, \quad (A21)$$

$$FB_{5b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p}' - \mathbf{p}'')^2, \quad (A22)$$

$$FB_{5c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4(\mathbf{p}' - \mathbf{p})^2, \quad (A23)$$

$$FB_{6a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = -8(\mathbf{p}'' \times \mathbf{p}') \cdot (\mathbf{p} \times \mathbf{p}''), \quad (A24)$$

$$FB_{6b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = -8(\mathbf{p} \times \mathbf{p}') \cdot (\mathbf{p}'' \times \mathbf{p}'), \quad (A25)$$

$$FB_{6c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = -8(\mathbf{p} \times \mathbf{p}') \cdot (\mathbf{p} \times \mathbf{p}''), \quad (A26)$$

$$FB_7(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 4[(\mathbf{p} \times \mathbf{p}') \cdot (\mathbf{p}'' \times \mathbf{p}')]^2, \quad (A27)$$

$$FB_{8a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' + \mathbf{p}'') \cdot (\mathbf{p}'' + \mathbf{p})], \quad (A28)$$

$$FB_{8b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' + \mathbf{p}) \cdot (\mathbf{p}' + \mathbf{p}'')], \quad (A29)$$

$$FB_{8c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' + \mathbf{p}) \cdot (\mathbf{p}'' + \mathbf{p})], \quad (A30)$$

$$FB_{9a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' - \mathbf{p}'') \cdot (\mathbf{p}'' - \mathbf{p})], \quad (A31)$$

$$FB_{9b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' - \mathbf{p}) \cdot (\mathbf{p}' - \mathbf{p}'')], \quad (A32)$$

$$FB_{9c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' - \mathbf{p}) \cdot (\mathbf{p}'' - \mathbf{p})], \quad (A33)$$

$$FB_{10a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' + \mathbf{p}'') \cdot (\mathbf{p}'' - \mathbf{p})], \quad (A34)$$

$$FB_{10b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' + \mathbf{p}) \cdot (\mathbf{p}' - \mathbf{p}'')], \quad (A35)$$

$$FB_{10c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' - \mathbf{p}) \cdot (\mathbf{p}'' + \mathbf{p})], \quad (A36)$$

$$FB_{11a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' - \mathbf{p}'') \cdot (\mathbf{p}'' + \mathbf{p})], \quad (A37)$$

$$FB_{11b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' - \mathbf{p}) \cdot (\mathbf{p}' + \mathbf{p}'')], \quad (A38)$$

$$FB_{11c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 2[(\mathbf{p}' + \mathbf{p}) \cdot (\mathbf{p}'' - \mathbf{p})]. \quad (A39)$$

The nonzero $B_{ijk}(\mathbf{p}', \mathbf{p}'', \mathbf{p})$:

$$B_{122}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{212}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{221}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = 12, \quad (A40)$$

$$B_{124}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{214}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{3a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A41)$$

$$B_{125}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{215}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{4a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A42)$$

$$B_{126}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{216}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{5a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A43)$$

$$B_{133}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{233}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{6a}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A44)$$

$$B_{142}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{241}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{3b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A45)$$

$$B_{144}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = \frac{1}{16}FB_{6a}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A46)$$

$$\begin{aligned} B_{145}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) &= B_{146}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{154}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) \\ &= B_{164}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \\ &= B_{415}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{416}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) \\ &= B_{514}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \\ &= B_{614}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{451}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) \\ &= B_{461}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \\ &= B_{541}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{641}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) \\ &= FB_7(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \end{aligned} \quad (A47)$$

$$B_{152}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{251}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{4b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A48)$$

$$B_{155}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{8a}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A49)$$

$$B_{156}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{10a}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A50)$$

$$B_{162}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{261}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{5b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A51)$$

$$B_{165}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{11a}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A52)$$

$$B_{166}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{9a}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A53)$$

$$B_{313}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{323}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{6c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A54)$$

$$B_{412}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{421}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{3c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A55)$$

$$B_{414}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = \frac{1}{16}FB_{6c}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A56)$$

$$B_{512}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{521}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{4c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A57)$$

$$B_{515}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{8c}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A58)$$

$$B_{516}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{11c}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A59)$$

$$B_{612}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{621}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{5c}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A60)$$

$$B_{615}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{10c}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A61)$$

$$B_{616}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{9c}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A62)$$

$$B_{331}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = B_{332}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = FB_{6b}(\mathbf{p}', \mathbf{p}'', \mathbf{p}), \quad (A63)$$

$$B_{441}(\mathbf{p}', \mathbf{p}'', \mathbf{p}) = \frac{1}{16}FB_{6b}(\mathbf{p}', \mathbf{p}'', \mathbf{p})^2, \quad (A64)$$

$$\begin{aligned} B_{232}^d(\mathbf{p}, \mathbf{p}') &= -8\mathbf{p} \cdot \mathbf{p}'(\mathbf{p} \times \mathbf{p}')^2, \\ B_{242}^d(\mathbf{p}, \mathbf{p}') &= -\frac{20}{9}p^4p'^4 - 4(\mathbf{p} \cdot \mathbf{p}')^4 + \frac{56}{9}p^2p'^2(\mathbf{p} \cdot \mathbf{p}')^2, \\ B_{252}^d(\mathbf{p}, \mathbf{p}') &= \frac{4}{9}p^2p'^2(p^2 + p'^2) - \frac{16}{9}p^2p'^2(\mathbf{p} \cdot \mathbf{p}')^2 \\ &\quad - \frac{4}{3}(p^2 + p'^2)(\mathbf{p} \cdot \mathbf{p}')^2, \\ B_{262}^d(\mathbf{p}, \mathbf{p}') &= \frac{4}{9}p^2p'^2(p^2 + p'^2) + \frac{16}{9}p^2p'^2(\mathbf{p} \cdot \mathbf{p}') \\ &\quad - \frac{4}{3}(p^2 + p'^2)(\mathbf{p} \cdot \mathbf{p}')^2, \end{aligned} \quad (\text{B3})$$

$$\begin{aligned} B_{211}^d(\mathbf{p}, \mathbf{p}') &= B_{221}^d(\mathbf{p}, \mathbf{p}') = B_{231}^d(\mathbf{p}, \mathbf{p}') = 0, \\ B_{241}^d(\mathbf{p}, \mathbf{p}') &= -\frac{4}{3}p^2(\mathbf{p}' \times \mathbf{p})^2, \\ B_{251}^d(\mathbf{p}, \mathbf{p}') &= \frac{8}{3}p^4 + \frac{16}{3}p^2(\mathbf{p} \cdot \mathbf{p}') + 4(\mathbf{p} \cdot \mathbf{p}')^2 - \frac{4}{3}p^2p'^2, \\ B_{261}^d(\mathbf{p}, \mathbf{p}') &= \frac{8}{3}p^4 - \frac{16}{3}p^2(\mathbf{p} \cdot \mathbf{p}') + 4(\mathbf{p} \cdot \mathbf{p}')^2 - \frac{4}{3}p^2p'^2. \end{aligned} \quad (\text{B4})$$

The expressions for the functions B_{1k2}^d , $k = 1, \dots, 6$, can be obtained from the functions B_{2k1}^d by replacing $\mathbf{p} \leftrightarrow \mathbf{p}'$.

APPENDIX C: EXAMPLE OF A CHIRAL POTENTIAL

For this particular example we will use the next-to-next-to-leading order (NNLO) chiral potential from Ref. [12].

The leading-order (LO) NN potential in the two-nucleon center-of-mass system (CMS) reads [13]

$$\begin{aligned} V_{\text{LO}} &= -\frac{1}{(2\pi)^3} \frac{g_A^2}{4F_\pi^2} \frac{\sigma_1 \cdot \mathbf{q} \sigma_2 \cdot \mathbf{q}}{\mathbf{q}^2 + M_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ &\quad + \frac{C_S}{(2\pi)^3} + \frac{C_T}{(2\pi)^3} \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2, \end{aligned} \quad (\text{C1})$$

where $\mathbf{q} = \mathbf{p}' - \mathbf{p}$, and m_π , F_π , and g_A denote the pion mass, the pion decay constant, and the nucleon axial coupling constants. At next-to-leading order (NLO), a renormalization of the low-energy constants (LECs) is required, and the contribution from the Goldberger-Treiman discrepancy leads to a modified value of g_A . The remaining contributions to the NN potential at this order are

$$\begin{aligned} V_{\text{NLO}} &= -\frac{1}{(2\pi)^3} \frac{\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2}{384\pi^2 F_\pi^4} L^{\tilde{\Lambda}}(q) \left[4m_\pi^2(5g_A^4 - 4g_A^2 - 1) \right. \\ &\quad \left. + \mathbf{q}^2(23g_A^4 - 10g_A^2 - 1) + \frac{48g_A^4 m_\pi^4}{4m_\pi^2 + \mathbf{q}^2} \right] \\ &\quad - \frac{1}{(2\pi)^3} \frac{3g_A^4}{64\pi^2 F_\pi^4} L^{\tilde{\Lambda}}(q) (\boldsymbol{\sigma}_1 \cdot \mathbf{q} \boldsymbol{\sigma}_2 \cdot \mathbf{q} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \mathbf{q}^2) \\ &\quad + \frac{C_1}{(2\pi)^3} \mathbf{q}^2 + \frac{C_2}{(2\pi)^3} \mathbf{k}^2 + \left[\frac{C_3}{(2\pi)^3} \mathbf{q}^2 + \frac{C_4}{(2\pi)^3} \mathbf{k}^2 \right] \\ &\quad \times \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + \frac{C_5}{(2\pi)^3} \frac{i}{2} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{q} \times \mathbf{k} \\ &\quad + \frac{C_6}{(2\pi)^3} \mathbf{q} \cdot \boldsymbol{\sigma}_1 \mathbf{q} \cdot \boldsymbol{\sigma}_2 + \frac{C_7}{(2\pi)^3} \mathbf{k} \cdot \boldsymbol{\sigma}_1 \mathbf{k} \cdot \boldsymbol{\sigma}_2, \end{aligned} \quad (\text{C2})$$

where $q \equiv |\mathbf{q}|$ and $\mathbf{k} = \frac{1}{2}(\mathbf{p}' + \mathbf{p})$. The loop function $L^{\tilde{\Lambda}}(q)$ is defined in the spectral function regularization (SFR) as [12]

$$L^{\tilde{\Lambda}}(q) = \theta(\tilde{\Lambda} - 2m_\pi) \frac{\omega}{2q} \ln \left[\frac{\tilde{\Lambda}^2 \omega^2 + q^2 s^2 + 2\tilde{\Lambda} q \omega s}{4m_\pi^2(\tilde{\Lambda}^2 + q^2)} \right], \quad (\text{C3})$$

with the abbreviations $\omega = (4m_\pi^2 + \mathbf{q}^2)^{1/2}$ and $s = (\tilde{\Lambda}^2 - 4m_\pi^2)^{1/2}$. Here, $\tilde{\Lambda}$ denotes the ultraviolet cutoff in the mass spectrum of the two-pion-exchange potential.

The contributions at NNLO again lead to the renormalization and redefinition of the LECs C_S , C_T , C_1, \dots, C_7 . The only new momentum dependence is due to the following terms:

$$\begin{aligned} V_{\text{NNLO}} &= -\frac{1}{(2\pi)^3} \frac{3g_A^2}{16\pi F_\pi^4} [2m_\pi^2(2c_1 - c_3) - c_3 \mathbf{q}^2] \\ &\quad \times (2m_\pi^2 + \mathbf{q}^2) A^{\tilde{\Lambda}}(q) - \frac{1}{(2\pi)^3} \frac{g_A^2 c_4}{32\pi F_\pi^4} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\ &\quad \times (4m_\pi^2 + q^2) A^{\tilde{\Lambda}}(q) (\boldsymbol{\sigma}_1 \cdot \mathbf{q} \boldsymbol{\sigma}_2 \cdot \mathbf{q} - \mathbf{q}^2 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2), \end{aligned} \quad (\text{C4})$$

where c_1 , c_3 , and c_4 are new πN LECs and the loop function $A^{\tilde{\Lambda}}(q)$ is given by

$$A^{\tilde{\Lambda}}(q) = \theta(\tilde{\Lambda} - 2m_\pi) \frac{1}{2q} \arctan \left[\frac{q(\tilde{\Lambda} - 2m_\pi)}{q^2 + 2\tilde{\Lambda} m_\pi} \right]. \quad (\text{C5})$$

The expressions of the potential given in Eqs. (C1), (C2), and (C4) show that this potential can be readily expressed in the operators w_j , $j = 1, \dots, 6$ of Eq. (2.2).

The chiral potential we consider in this example is the sum of

$$V \equiv V_{\text{LO}} + V_{\text{NLO}} + V_{\text{NNLO}}. \quad (\text{C6})$$

It requires regularization when inserted into the Lippmann-Schwinger equation, which is achieved by introducing a regulated potential of the form

$$V_{\text{reg}}(\mathbf{p}', \mathbf{p}) \equiv e^{-(p'/\Lambda^4)} V(\mathbf{p}', \mathbf{p}) e^{-(p^4/\Lambda^4)}, \quad (\text{C7})$$

with the cutoff parameter Λ .

APPENDIX D: SCALAR FUNCTIONS FOR THE BONN B POTENTIAL

For the convenience of the reader we give the expressions for the Bonn B potential from Ref. [15] in a form that is more suited for our 3D calculations. The expressions for the exchange of pseudo-scalar (ps), scalar (s), and vector (v) mesons are given by

$$\begin{aligned} V_{ps}(\mathbf{p}', \mathbf{p}) &= \frac{g_{ps}^2}{(2\pi)^3 4m^2} \sqrt{\frac{m}{E'}} \sqrt{\frac{m}{E}} \frac{F_{ps}^2[(\mathbf{p}' - \mathbf{p})^2]}{(\mathbf{p}' - \mathbf{p})^2 + m_{ps}^2} \frac{O_{ps}}{W' W}, \\ V_s(\mathbf{p}', \mathbf{p}) &= \frac{g_s^2}{(2\pi)^3 4m^2} \sqrt{\frac{m}{E'}} \sqrt{\frac{m}{E}} \frac{F_s^2[(\mathbf{p}' - \mathbf{p})^2]}{(\mathbf{p}' - \mathbf{p})^2 + m_s^2} \frac{O_s}{W' W}, \\ V_v(\mathbf{p}', \mathbf{p}) &= \frac{1}{(2\pi)^3 4m^2} \sqrt{\frac{m}{E'}} \sqrt{\frac{m}{E}} \frac{F_v^2[(\mathbf{p}' - \mathbf{p})^2]}{(\mathbf{p}' - \mathbf{p})^2 + m_v^2} \\ &\quad \times \frac{(g_v^2 O_{vv} + 2g_v f_v O_{vt} + f_v^2 O_{tt})}{W' W}, \end{aligned} \quad (\text{D1})$$

where m_α are the masses of the exchanged mesons, m the nucleon mass, $E = \sqrt{m^2 + \mathbf{p}^2}$ and $W = m + E$. The crucial quantities are the operators O_{ps} , O_s , O_{vv} , O_{vt} , and O_{tt} , which

are given in terms of the Dirac spinors as

$$O_{ps} = 4m^2 W' W \bar{u}(\mathbf{p}') \gamma^5 u(\mathbf{p}) \bar{u}(-\mathbf{p}') \gamma^5 u(-\mathbf{p}), \quad (\text{D2})$$

$$O_s = -4m^2 W' W \bar{u}(\mathbf{p}') u(\mathbf{p}) \bar{u}(-\mathbf{p}') u(-\mathbf{p}), \quad (\text{D3})$$

$$O_{vv} = 4m^2 W' W \bar{u}(\mathbf{p}') \gamma^\mu u(\mathbf{p}) \bar{u}(-\mathbf{p}') \gamma_\mu u(-\mathbf{p}), \quad (\text{D4})$$

$$\begin{aligned} O_{vt} = m W' W \{ & 4m \bar{u}(\mathbf{p}') \gamma^\mu u(\mathbf{p}) \bar{u}(-\mathbf{p}') \gamma_\mu u(-\mathbf{p}) - \bar{u}(\mathbf{p}') \gamma^\mu \\ & \times u(\mathbf{p}) \bar{u}(-\mathbf{p}') [(E' - E)(g_\mu^0 - \gamma_\mu \gamma^0) + (p_2 + p'_2)_\mu] \\ & \times u(-\mathbf{p}) - \bar{u}(\mathbf{p}') [(E' - E)(g^{0\mu} - \gamma^\mu \gamma^0) \\ & + (p_1 + p'_1)_\mu] u(\mathbf{p}) \bar{u}(-\mathbf{p}') \gamma_\mu u(-\mathbf{p}) \}, \end{aligned} \quad (\text{D5})$$

$$\begin{aligned} O_{tt} = W' W \{ & 4m^2 \bar{u}(\mathbf{p}') \gamma^\mu u(\mathbf{p}) \bar{u}(-\mathbf{p}') \gamma_\mu u(-\mathbf{p}) - 2m \bar{u}(\mathbf{p}') \gamma^\mu \\ & \times u(\mathbf{p}) \bar{u}(-\mathbf{p}') [(E' - E)(g_\mu^0 - \gamma_\mu \gamma^0) + (p_2 + p'_2)_\mu] \\ & \times u(-\mathbf{p}) - 2m \bar{u}(\mathbf{p}') [(E' - E)(g^{0\mu} - \gamma^\mu \gamma^0) \\ & + (p_1 + p'_1)_\mu] u(\mathbf{p}) \bar{u}(-\mathbf{p}') \gamma_\mu u(-\mathbf{p}) + \bar{u}(\mathbf{p}') [(E' - E) \\ & \times (g^{0\mu} - \gamma^\mu \gamma^0) + (p_1 + p'_1)_\mu] u(\mathbf{p}) \bar{u}(-\mathbf{p}') [(E' - E) \\ & \times (g_\mu^0 - \gamma_\mu \gamma^0) + (p_2 + p'_2)_\mu] u(-\mathbf{p}) \}, \end{aligned} \quad (\text{D6})$$

with $(p_1 + p'_1)_\mu = (E + E', \mathbf{p} + \mathbf{p}')$ and $(p_2 + p'_2)_\mu = (E + E', -\mathbf{p} - \mathbf{p}')$.

These operators act in the spin spaces of nucleons 1 and 2. The bilinear forms built with $\bar{u}(\mathbf{p}') \cdots u(\mathbf{p})$ contain σ_1 as acting in the spin space of nucleon 1 and the bilinear forms with $\bar{u}(-\mathbf{p}') \cdots u(-\mathbf{p})$ contain σ_2 and act in the spin space of nucleon 2. The spinors $u(\mathbf{q})$ are normalized according to the definitions given in Ref. [23] and are explicitly given as

$$u(\mathbf{q}) = \sqrt{\frac{E+m}{2m}} \left(\frac{1}{\frac{\sigma \cdot \mathbf{q}}{E+m}} \right). \quad (\text{D7})$$

$$\begin{aligned} O_{ps} = & \left(1 + \frac{2m}{E'+E} \right) [(\mathbf{p}' \cdot \mathbf{p})^2 - p'^2 p^2] w_2 + \left(1 + \frac{2m}{E'+E} \right) w_4 + \frac{1}{4} \left\{ -(W' - W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 - 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_5 \\ & + \frac{1}{4} \left\{ -(W' + W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 + 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_6, \end{aligned} \quad (\text{D10})$$

$$O_s = -[W' W - (\mathbf{p}' \cdot \mathbf{p})]^2 w_1 - [W' W - (\mathbf{p}' \cdot \mathbf{p})] w_3 + w_4, \quad (\text{D11})$$

$$\begin{aligned} O_{vv} = & \{ [W' W + (\mathbf{p}' \cdot \mathbf{p})]^2 + W'^2 p^2 + W^2 p'^2 + 2W' W (\mathbf{p}' \cdot \mathbf{p}) \} w_1 \\ & + \left\{ -\frac{1}{2} (W'^2 + W^2) (p'^2 + p^2) + 2W' W (\mathbf{p}' \cdot \mathbf{p}) + \frac{1}{2} \left(1 + \frac{2m}{E'+E} \right) [p'^4 + p^4 - 2(\mathbf{p}' \cdot \mathbf{p})^2] \right\} w_2 \\ & - [3W' W + (\mathbf{p}' \cdot \mathbf{p})] w_3 - \left(2 + \frac{2m}{E'+E} \right) w_4 - \frac{1}{4} \left\{ -(W' - W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 - 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_5 \\ & - \frac{1}{4} \left\{ -(W' + W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 + 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_6, \end{aligned} \quad (\text{D12})$$

$$\begin{aligned} O_{vt} = & \left\{ W'^2 p^2 + W^2 p'^2 - \frac{W' - W}{2m} (W'^2 p^2 - W^2 p'^2) 2W' W [2W' W + (\mathbf{p}' \cdot \mathbf{p})] - \frac{W' + W}{m} [W'^2 W^2 - (\mathbf{p}' \cdot \mathbf{p})^2] \right\} w_1 \\ & + \left\{ 2W' W (\mathbf{p}' \cdot \mathbf{p}) - \frac{1}{2} (W'^2 + W^2) (p'^2 + p^2) + \frac{1}{2} \left(1 + \frac{2m}{E'+E} \right) [p'^4 + p^4 - 2(\mathbf{p}' \cdot \mathbf{p})^2] \right. \\ & \left. - \frac{1}{2m(E'+E)} [W'^2 p^4 + W^2 p'^4 - (W'^2 + W^2) (\mathbf{p}' \cdot \mathbf{p})^2] \right\} w_2 - \left[2W' W + \frac{W' + W}{m} (\mathbf{p}' \cdot \mathbf{p}) \right] w_3 \end{aligned}$$

Each vertex is multiplied with a form factor

$$F_\alpha^2[(\mathbf{p}' - \mathbf{p})^2] = \left[\frac{\Lambda_\alpha^2 - m_\alpha^2}{\Lambda_\alpha^2 + (\mathbf{p}' - \mathbf{p})^2} \right]^{2n}, \quad (\text{D8})$$

where the values of n and the cutoff parameters Λ_α are given in Table II.

Note that for the three isovector mesons (π , δ , and ρ) contributing to the Bonn B potential, expressions (D2)–(D6) are additionally multiplied by the isospin factor $\tau(1) \cdot \tau(2)$.

In Ref. [7], this potential was presented in a different operator form. However, in that work one of the six operators was chosen to be $\sigma_1 \cdot (\mathbf{p} + \mathbf{p}') \sigma_2 \cdot (\mathbf{p}' - \mathbf{p}) + \sigma_1 \cdot (\mathbf{p}' - \mathbf{p}) \sigma_2 \cdot (\mathbf{p} + \mathbf{p}')$, which is an operator that violates time reversal invariance. In practice, this operator is always multiplied with the term $(p'^2 - p^2)$, which also violates time reversal invariance. Therefore, the entire term is invariant as it should be. In principle, it is not desirable to work with symmetry violating operators, thus we prefer to use the operators from Eq. (2.2) and rewrite

$$\begin{aligned} & \sigma_1 \cdot (\mathbf{p} + \mathbf{p}') \sigma_2 \cdot (\mathbf{p}' - \mathbf{p}) + \sigma_1 \cdot (\mathbf{p}' - \mathbf{p}) \sigma_2 \cdot (\mathbf{p} + \mathbf{p}') \\ & = \frac{-4(\mathbf{p} \times \mathbf{p}')^2}{p'^2 - p^2} \sigma_1 \cdot \sigma_2 + \frac{(\mathbf{p} - \mathbf{p}')^2}{p'^2 - p^2} \sigma_1 \cdot (\mathbf{p} + \mathbf{p}') \sigma_2 \cdot (\mathbf{p} + \mathbf{p}') \\ & + \frac{(\mathbf{p} + \mathbf{p}')^2}{p'^2 - p^2} \sigma_1 \cdot (\mathbf{p} - \mathbf{p}') \sigma_2 \cdot (\mathbf{p} - \mathbf{p}') \\ & + \frac{4}{p'^2 - p^2} \sigma_1 \cdot (\mathbf{p} \times \mathbf{p}') \sigma_2 \cdot (\mathbf{p} \times \mathbf{p}'), \end{aligned} \quad (\text{D9})$$

which is an identity for $(\mathbf{p} + \mathbf{p}')(\mathbf{p}' - \mathbf{p}) = p'^2 - p^2 \neq 0$. Inserting Eq. (D9) into the expressions given in Ref. [7] cancels the factor $p'^2 - p^2$, and one obtains the following expressions for the operators O_α from Eqs. (D2)–(D6) in terms of the operators $w_j \equiv w_j(\sigma_1, \sigma_2, \mathbf{p}', \mathbf{p})$ from Eq. (2.2):

$$\begin{aligned} O_{ps} = & \left(1 + \frac{2m}{E'+E} \right) [(\mathbf{p}' \cdot \mathbf{p})^2 - p'^2 p^2] w_2 + \left(1 + \frac{2m}{E'+E} \right) w_4 + \frac{1}{4} \left\{ -(W' - W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 - 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_5 \\ & + \frac{1}{4} \left\{ -(W' + W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 + 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_6, \end{aligned} \quad (\text{D10})$$

$$\begin{aligned} O_s = & -[W' W - (\mathbf{p}' \cdot \mathbf{p})]^2 w_1 - [W' W - (\mathbf{p}' \cdot \mathbf{p})] w_3 + w_4, \\ O_{vv} = & \{ [W' W + (\mathbf{p}' \cdot \mathbf{p})]^2 + W'^2 p^2 + W^2 p'^2 + 2W' W (\mathbf{p}' \cdot \mathbf{p}) \} w_1 \\ & + \left\{ -\frac{1}{2} (W'^2 + W^2) (p'^2 + p^2) + 2W' W (\mathbf{p}' \cdot \mathbf{p}) + \frac{1}{2} \left(1 + \frac{2m}{E'+E} \right) [p'^4 + p^4 - 2(\mathbf{p}' \cdot \mathbf{p})^2] \right\} w_2 \\ & - [3W' W + (\mathbf{p}' \cdot \mathbf{p})] w_3 - \left(2 + \frac{2m}{E'+E} \right) w_4 - \frac{1}{4} \left\{ -(W' - W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 - 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_5 \\ & - \frac{1}{4} \left\{ -(W' + W)^2 + \left(1 + \frac{2m}{E'+E} \right) [p'^2 + p^2 + 2(\mathbf{p}' \cdot \mathbf{p})] \right\} w_6, \end{aligned} \quad (\text{D12})$$

$$\begin{aligned}
& + \left\{ -\frac{W' + W}{m} + \frac{1}{2m(E' + E)} [W'^2 + W^2 - 2m(W' + W)] \right\} w_4 \\
& - \frac{1}{4} \left\{ -(W' - W)^2 + \left(1 + \frac{2m}{E' + E} \right) [p'^2 + p^2 - 2(\mathbf{p}' \cdot \mathbf{p})] - \frac{1}{m(E' + E)} [W'^2 p^2 + W^2 p'^2 - (W'^2 + W^2)(\mathbf{p}' \cdot \mathbf{p})] \right\} w_5 \\
& - \frac{1}{4} \left\{ -(W' + W)^2 + \left(1 + \frac{2m}{E' + E} \right) [p'^2 + p^2 + 2(\mathbf{p}' \cdot \mathbf{p})] - \frac{1}{m(E' + E)} [W'^2 p^2 + W^2 p'^2 + (W'^2 + W^2)(\mathbf{p}' \cdot \mathbf{p})] \right\} w_6,
\end{aligned} \tag{D13}$$

$$\begin{aligned}
O_{tt} = & \left\{ [W'W + (\mathbf{p}' \cdot \mathbf{p})]^2 + 2 \left(2 - \frac{W' + W}{m} \right) [W'^2 W^2 - (\mathbf{p}' \cdot \mathbf{p})^2] + \left\{ 3 + \frac{3[W'W - m(W' + W)] + (\mathbf{p}' \cdot \mathbf{p})}{2m^2} \right\} [W'W - (\mathbf{p}' \cdot \mathbf{p})]^2 \right. \\
& + \left[1 + \frac{(W' - W)^2}{4m^2} \right] (W'^2 p^2 + W^2 p'^2) + 2 \left[1 - \frac{(W' - W)^2}{4m^2} \right] W'W(\mathbf{p}' \cdot \mathbf{p}) - \frac{W' - W}{m} (W'^2 p^2 - W^2 p'^2) \Big\} w_1 \\
& + \left\{ 2 \left[1 - \frac{(W' - W)^2}{4m^2} \right] W'W(\mathbf{p}' \cdot \mathbf{p}) - \left[1 + \frac{(W' - W)^2}{4m^2} \right] \left(1 + \frac{2m}{E' + E} \right) (\mathbf{p}' \cdot \mathbf{p})^2 \right. \\
& - \left[1 + \frac{(W' - W)^2}{4m^2} \right] \left(\frac{m^2 + E'E}{E' + E} + m \right) (W' p^2 + W p'^2) - \frac{1}{m(E' + E)} [W'^2 p^4 + W^2 p'^4 - (W'^2 + W^2)(\mathbf{p}' \cdot \mathbf{p})^2] \Big\} w_2 \\
& + \left\{ -W'W - (\mathbf{p}' \cdot \mathbf{p}) + 2 \left(2 - \frac{W' + W}{m} \right) (\mathbf{p}' \cdot \mathbf{p}) - 2 \left[1 - \frac{(W' - W)^2}{4m^2} \right] W'W \right. \\
& + \left\{ 3 + \frac{3[W'W - m(W' + W)] + (\mathbf{p}' \cdot \mathbf{p})}{2m^2} \right\} [W'W - (\mathbf{p}' \cdot \mathbf{p})] \Big\} w_3 - \left\{ 4 + \frac{3[W'W - m(W' + W)] + (\mathbf{p}' \cdot \mathbf{p})}{2m^2} \right. \\
& - 2 \left(2 - \frac{W' + W}{m} \right) + \left[1 + \frac{(W' - W)^2}{4m^2} \right] \left(1 + \frac{2m}{E' + E} \right) - \frac{1}{m(E' + E)} (W'^2 + W^2) \Big\} w_4 \\
& - \frac{1}{2} \left\{ \left[1 - \frac{(W' - W)^2}{4m^2} \right] W'W - \frac{1}{m(E' + E)} [W'^2 p^2 + W^2 p'^2 - (W'^2 + W^2)(\mathbf{p}' \cdot \mathbf{p})] \right. \\
& + \frac{1}{2} \left[1 + \frac{(W' - W)^2}{4m^2} \right] \left[\left(1 + \frac{2m}{E' + E} \right) [p'^2 + p^2 - 2(\mathbf{p}' \cdot \mathbf{p})] - W'^2 - W^2 \right] \Big\} w_5 \\
& - \frac{1}{2} \left\{ - \left[1 - \frac{(W' - W)^2}{4m^2} \right] W'W - \frac{1}{m(E' + E)} [W'^2 p^2 + W^2 p'^2 + (W'^2 + W^2)(\mathbf{p}' \cdot \mathbf{p})] \right. \\
& + \frac{1}{2} \left[1 + \frac{(W' - W)^2}{4m^2} \right] \left[\left(1 + \frac{2m}{E' + E} \right) [p'^2 + p^2 + 2(\mathbf{p}' \cdot \mathbf{p})] - W'^2 - W^2 \right] \Big\} w_6. \tag{D14}
\end{aligned}$$

The values of the parameters are given in Table II.

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