Realistic phase shift and mixing parameters for elastic neutron-deuteron scattering: Comparison of momentum space and configuration space methods

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Eigenphase shift and mixing parameters for elastic nd scattering below the breakup threshold are compared as determined by the Faddeev theory and the correlated hyperspherical harmonic method. The AV14 NN potential is used. The agreement is very good and the numbers can be considered as benchmarks.

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I. INTRODUCTION

Scattering of nuclei as composite objects upon each other, each one carrying nonzero spin, can yield a complicated S matrix, which allows for coupling of different channel spins and different orbital angular momenta. The complex spin dependence of the NN interaction acting within and between the nucleon clusters yields an effective cluster-cluster potential, which depends in general in a complicated manner on the channel spins and the orbital angular momenta. Due to the complexity of the NN interaction and the few- or many-nucleon systems, little is known theoretically about the strengths and presence of the various couplings. The ignorance is reflected, for instance, in older phase shift analysis (PSA) for pd elastic scattering. This is the simplest system of composite particle scattering, where only one of the interacting bodies is composite. All sorts of assumptions have been made in those PSA's: no mixing of states of different orbital angular momenta and channel spin conservation, or mixing of angular momenta but still channel spin conservation, or finally the general case (see Ref. [1] and references therein). Above the nd breakup threshold all phase shift and mixing parameters will even become complex. Again up to now no theoretical guidance exists about what should be reasonable magnitudes of the imaginary parts and again various sorts of *ad hoc* assumptions have been made [1]. Recently a PSA for pd elastic scattering at $E_p^{\rm lab} = 3$ MeV appeared [2] based on new measurements of various spin observables. That PSA was compared to results of a Faddeev calculation and in general a reasonable agreement could be established. The theory, however, was based only on a rank-1 separable approximation to the Paris potential. This was enforced by the wish to include the pp Coulomb force. Certainly this has to be improved in the future, since a closer look into the comparison of the PSA values with that theory exhibits quite some differences. Nowadays with the possibility to treat the NN force in the $3N$ system with all its complexity one would like to pin down the phases much more precisely, especially since there still exists an outstanding discrepancy between theory and experiment in elastic Nd scattering: the low energy analyzing power A_y [3].

Here in this article we would like to compare for one NN potential, AV14 [4], theoretical nd phase shift and mixing parameters achieved by two basically different theoretical methods: the Faddeev equations in momentum space [5] and the pair correlated hyperspherical harmonic (PHH) basis method [6] in configuration space. The results can be considered as benchmarks for nd elastic scattering and using NN forces with their full complexity.

Previous calculations [7] for nd phase shifts and the simple s-wave MT(I-III) potentials will also be confirmed.

In Sec. II we briefly present the two theoretical methods and the definition of the phase shift and mixing parameters related to the S matrix. Our results are shown in Sec. III. We end with a brief outlook in Sec. IV.

II. THEORETICAL FORMULATIONS

We briefly review the two approaches used in this article, the Faddeev one and the pair correlated hyperspherical harmonic basis method. The Faddeev equations [5,8] read

$$\psi = \psi_0 + G_0 t P \psi \ . \tag{2.1}$$

For a conserved total three-body angular momentum $\mathcal{J}$ and a given parity the driving term ψ_0 can be chosen as

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$$\psi_0(\vec{x},\vec{y}) = \sum_\lambda \sum_{l=0,2} \varphi_l(x) j_\lambda(q_0 y) \times \{\{Y_l(\hat{x})\chi_1\}_{j=1}\{Y_\lambda(\hat{y})\chi_{1/2}\}_J\}^{\mathcal{JM}} . \quad (2.2)$$

Here $\vec{x}$ and $\vec{y}$ are the usual Jacobi vectors in configuration space [5], $\varphi_l(x)$ ($l = 0, 2$) the s- and d-wave components of the deuteron, $j_\lambda(q_0 y)$ the spherical Bessel function related to a fixed orbital angular momentum λ of the projectile nucleon with respect to the deuteron, and the rest are obvious angular momentum states in j-J coupling. The relative momentum q_0 of the projectile is given by

$$E = E_d + \frac{3}{4m} q_0^2 , \quad (2.3)$$

where $E_d < 0$ is the deuteron energy and m the nucleon mass. The free $3N$ propagator G_0 acts on the NN t-matrix t in the integral kernel and that piece can be rewritten as GV, where $G \equiv (E + i\epsilon - H_0 - V)^{-1}$ and V is the NN force. Then using spectral decompositions and performing one integration, the Green function G can easily be found to have the following form in the subspace of a fixed $\mathcal{JM}$ and restricted to the deuteron channel:

$$G^d = \sum_{l=0,2} \varphi_l(x) \sum_{\lambda J} \{\{Y_l(\hat{x})\chi_1\}_{j=1}\{Y_\lambda(\hat{y})\chi_{1/2}\}_J\}^{\mathcal{JM}} \times \frac{4m}{3}\frac{1}{yy'}(-1)^{\lambda+1}\frac{1}{q_0} u_\lambda(q_0 y_<) w_\lambda^{(+)}(q_0 y_>) \times \sum_{l'=0,2} \varphi_{l'}(x') \{\{Y_{l'}^*(\hat{x}')\chi_1^\dagger\}_{j=1} \times \{Y_\lambda^*(\hat{y}')\chi_{1/2}^\dagger\}_J\}^{\mathcal{JM}} \quad (2.4)$$

Here u_λ and $w_\lambda^{(+)}$ are Riccati-Bessel functions [9]. From that follows easily the asymptotic form of the Faddeev component $\psi(\vec{x},\vec{y})$ in the deuteron channel:

$$\psi(\vec{x},\vec{y}) \to \sum_{l=0,2} \varphi_l(x) \sum_{\lambda' J'} \{\{Y_\lambda(\hat{x})\chi_1\}_{j=1}\{Y_\lambda(\hat{y})\chi_{1/2}\}_J\}^{\mathcal{JM}} \times \left[\delta_{\lambda\lambda'}\delta_{JJ'}\frac{1}{2iq_0 y}\left(e^{i(q_0 y - 1/2\lambda\pi)} - e^{-i(q_0 y - 1/2\lambda\pi)}\right) - \frac{4m}{3}\frac{e^{i(q_0 y - 1/2\lambda'\pi)}}{q_0 y} f_{\lambda' J',\lambda J}\right] . \quad (2.5)$$

The transition amplitudes f between different orbital angular momenta λ and total angular momenta J of the third nucleon (not the one in the deuteron) are

$$f_{\lambda' J',\lambda J} \equiv \int d\vec{x}' \int d\vec{y}' \frac{u_{\lambda'}(q_0 y')}{y'} \sum_{l''} \varphi_{l''}(x') \times \{\{Y_{l'}^*(\hat{x}')\chi_1^\dagger\}_{j=1}\{Y_{\lambda'}^*(\hat{y}')\chi_{1/2}^\dagger\}_{J'}\}^{\mathcal{JM}} \times \langle \vec{x}'\vec{y}'|VP\psi\rangle . \quad (2.6)$$

The quantity P is the sum of a cyclic and anticyclic permutation of three objects, which typically occurs in a Faddeev equation [5].

Clearly (2.5) defines the S matrix as [9]

$$S^{\mathcal{J}}_{\lambda' J',\lambda J} \equiv \delta_{\lambda'\lambda}\delta_{J'J} - 2i\frac{4m}{3} f_{\lambda' J',\lambda J} . \quad (2.7)$$

The asymptotic behavior can also be chosen differently by replacing the square bracket in (2.5) by

$$[\,] \to [\,]_{\rm sw} = \delta_{\lambda'\lambda}\delta_{J'J} j_\lambda(q_0 y) - K_{\lambda' J',\lambda J} n_{\lambda'}(q_0 y) , \quad (2.8)$$

where n_λ is again a Riccati-Bessel function, defined through its asymptotic behavior

$$n_\lambda(z) \to -\frac{1}{z}\cos(z - \tfrac{1}{2}\lambda\pi) . \quad (2.9)$$

It then easily follows (using a matrix notation) that the matrix $\mathbf{S}$ is related to the matrix $\mathbf{K}$ by

$$\mathbf{S} = (1 + i\mathbf{K})(1 - i\mathbf{K})^{-1} . \quad (2.10)$$

The index sw in (2.8) stands for standing wave, as is obvious from the asymptotic form.

Using standard normalizations for momentum states $|q\lambda m\rangle$ and configuration space states $|y\lambda m\rangle$ one finds

$$\langle y\lambda' m'|q\lambda m\rangle = \sqrt{\frac{2}{\pi}} i^\lambda j_\lambda(qy)\delta_{\lambda'\lambda}\delta_{m'm} \quad (2.11)$$

and consequently

$$f_{\lambda' J',\lambda J} = q_0\sqrt{\frac{\pi}{2}} i^{\lambda'} \sum_{l''} \langle \varphi q_0 (l''1)1(\lambda' \tfrac{1}{2})J'\mathcal{JM}|VP\psi\rangle . \quad (2.12)$$

We used the notation of a partial wave projected momentum space basis vector [5].

Let us now relate the elastic scattering amplitudes f to the form that we use in our momentum space treatment [10]. Summarizing all the discrete quantum numbers in (2.12) into α, one has

$$\sum_{l''}\langle \varphi q_0\alpha|VP\psi\rangle = \sum_{l''}\langle \varphi q_0\alpha|(E - \overleftarrow{H}_0)P\psi\rangle = \sum_{l''}\langle \varphi q_0\alpha|P(E - H_0)\psi\rangle . \quad (2.13)$$

The first equality is due to the Schrödinger equation for the asymptotic channel state $|\varphi q_0\alpha\rangle$ and $\overleftarrow{H}_0$ denotes a differentiation to the left. Because of the permutation operator P there are no surface terms in the partial integration, which means that H_0 acts to the right. Then we insert the Faddeev equation (2.1) and get

$$\sum_{l''}\langle\varphi q_0\alpha|P(E-H_0)\psi\rangle$$

$$=\sum_{l''}\langle\varphi q_0\alpha|P(E-H_0)|\psi_0+G_0tP\psi\rangle$$
$$=\sum_{l''}\langle\varphi q_0\alpha|PG_0^{-1}|\psi_0\rangle+\sum_{l''}\langle\varphi q_0\alpha|PtP\psi\rangle\ . \quad (2.14)$$

Defining T by

$$tP\psi\equiv T\psi_0\ , \quad (2.15)$$

we end up with

$$\sum_{l''}\langle\varphi q_0\alpha|VP\psi\rangle=\sum_{l''}\langle\varphi q_0\alpha|PG_0^{-1}+PT|\psi_0\rangle \quad (2.16)$$

and

$$T\psi_0=tP\psi_0+tPG_0T\psi_0\ . \quad (2.17)$$

The last equation is the one that we use in our momentum space treatment [10] of nd scattering. The operator T generates the full breakup operator U_0 directly via [5]

$$U_0=(1+P)T\ . \quad (2.18)$$

In Eq. (2.16) we encounter the operator

$$U\equiv PG_0^{-1}+PT \quad (2.19)$$

for elastic nd scattering. Since the driving term (2.2) has the momentum representation

$$\langle p'q'\alpha'|\psi_0\rangle=i^{-\lambda}\delta_{\lambda'\lambda}\delta_{J'J}\frac{\delta(q'-q_0)}{q'^2}\sqrt{\frac{\pi}{2}}\varphi_l(p')\ , \quad (2.20)$$

we find

$$f_{\lambda'J',\lambda J}=q_0\frac{\pi}{2}i^{\lambda'-\lambda}U^{\mathcal{J}}_{\lambda'J',\lambda J}\ , \quad (2.21)$$

where

$$U^{\mathcal{J}}_{\lambda'J',\lambda J}\equiv\sum_{l'l}\int dp'p'^2\varphi_{l'}(p')\int dp\ p^2\varphi_l(p)$$
$$\times\langle p'q_0(l'1)1(\lambda'\tfrac{1}{2})J'\mathcal{J}\mathcal{M}|U|pq_0$$
$$\times(l1)1(\lambda\tfrac{1}{2})J\mathcal{J}\mathcal{M}\rangle\ . \quad (2.22)$$

Thus we end up with the unitary S matrix

$$S^{\mathcal{J}}_{\lambda'J',\lambda J}=\delta_{\lambda'\lambda}\delta_{J'J}-\frac{4\pi}{3}iq_0mi^{\lambda'-\lambda}U^{\mathcal{J}}_{\lambda'J',\lambda J}\ . \quad (2.23)$$

The fact that this expression defines a unitary S matrix follows, of course, also directly from the well known relations for three-body transition operators [5]. They lead to the equivalent statement

$$\left(U^{\mathcal{J}}_{\lambda'J',\lambda J}\right)^*-U^{\mathcal{J}}_{\lambda'J',\lambda J}$$
$$=\frac{4\pi}{3}q_0mi\sum_{\lambda''J''}\left(U^{\mathcal{J}}_{\lambda'J',\lambda J}\right)^*U^{\mathcal{J}}_{\lambda'J',\lambda J}\ . \quad (2.24)$$

Note that as a consequence of this relation the phase factor $i^{\lambda'-\lambda}$ can be dropped without loosing unitarity. Such a definition would be natural if one started from the unitarity relation for the transition operator U [5]. Here, however, we shall stick to the usual definition (2.7), connected to the asymptotic behavior in configuration space.

In one of the approaches of the authors (Bochum group) one solves Eq. (2.17) in momentum space and determines then the $U^{\mathcal{J}}_{\lambda'J',\lambda J}$ matrix elements via quadrature [see Eqs. (2.19) and (2.22)].

Now we follow Seyler [11] and use the channel spin representation. The channel spin in our case is the sum of deuteron and nucleon spins $\vec{j}_d$, and $\vec{s}_N$, respectively:

$$\vec{\Sigma}\equiv\vec{j}_d+\vec{s}_N\ . \quad (2.25)$$

Using the channel spin obviously requires the following recoupling:

$$U^{\mathcal{J}}_{\lambda'\Sigma',\lambda\Sigma}=\sum_{J'}\sum_{J}\sqrt{\hat{J}'\hat{\Sigma}'}(-1)^{\mathcal{J}-J'}\begin{Bmatrix}\lambda' & \frac{1}{2} & J'\\ j_d & \mathcal{J} & \Sigma'\end{Bmatrix}$$
$$\times\sqrt{\hat{J}\hat{\Sigma}}(-1)^{\mathcal{J}-J}\begin{Bmatrix}\lambda & \frac{1}{2} & J\\ j_d & \mathcal{J} & \Sigma\end{Bmatrix}U^{\mathcal{J}}_{\lambda'J',\lambda J}\ . \quad (2.26)$$

These new quantities obey exactly the same unitarity relations (2.24) as the previous U's.

In the other approach of the authors (Pisa group) one works in configuration space and uses the pair correlated hyperspherical harmonic basis method, briefly described below [6,12]. In this approach the wave function of the system for an nd scattering state is written as a sum of two terms (for the details, see Ref. [6] and references therein)

$$\Psi=\Psi_C+\Psi_A\ . \quad (2.27)$$

The first term Ψ_C describes the system when the three nucleons are close to each other, and goes to zero when the two clusters are well apart. It can be written as a sum of three Faddeev-like amplitudes,

$$\Psi_C=\psi_C(\mathbf{x}_i,\mathbf{y}_i)+\psi_C(\mathbf{x}_j,\mathbf{y}_j)+\psi_C(\mathbf{x}_k,\mathbf{y}_k)\ . \quad (2.28)$$

Each amplitude corresponds to a total angular momentum $\mathcal{J}\mathcal{M}$ and total isospin TT_z; therefore, if we use the L-S coupling, the following channel expansion is obtained:

$$\psi_C(\mathbf{x}_i,\mathbf{y}_i)=\sum_{\alpha=1}^{N_c}\Phi^C_\alpha(x_i,y_i)\mathcal{Y}_\alpha(jk,i)\ , \quad (2.29a)$$

$$\mathcal{Y}_\alpha(jk,i)=\{\{Y_{\ell_\alpha}(\hat{x}_i)Y_{\lambda_\alpha}(\hat{y}_i)\}_{L_\alpha}\{s^{jk}_\alpha s^i_\alpha\}_{S_\alpha}\}^{\mathcal{J}\mathcal{M}}$$
$$\times\{t^{jk}_\alpha t^i_\alpha\}^{TT_z}\ . \quad (2.29b)$$

Each channel is specified by the quantum numbers $\ell_\alpha,\lambda_\alpha,L_\alpha,s^{jk}_\alpha,t^{jk}_\alpha,S_\alpha$ with $\ell_\alpha+s^{jk}_\alpha+t^{jk}_\alpha$ odd to ensure antisymmetrization. The number of channels N_c taken into account in the expansion can be increased until convergence is reached. The corresponding bidimensional amplitude Φ^C_α is expanded in terms of the PHH basis

$$\Phi_\alpha^C(x_i,y_i)=\rho^{\ell_\alpha+\lambda_\alpha}f_\alpha(x_i)\times\left[\sum_{K=K_0}^{K_\alpha}u_K^\alpha(\rho)\ {}^{(2)}P_K^{\ell_\alpha,\lambda_\alpha}(\phi_i)\right]\ , \quad (2.30)$$

where we have introduced the hyperspherical coordinates

$$x_i=\rho\ \cos\phi_i\ ,\quad y_i=\rho\ \sin\phi_i\ . \quad (2.31)$$

In Eq. (2.30) the one-dimensional functions $f_\alpha(x_i)$ are the pair correlation factors included to give the proper behavior of the system when the two particles (j,k) are close to each other [12,13]. ${}^{(2)}P_K^{\ell_\alpha,\lambda_\alpha}(\phi_i)$ is a hyperspherical polynomial [14] and $u_K^\alpha(\rho)$ are the unknown hyperradial functions which satisfy the conditions $u_K^\alpha(\rho)\to 0$ when $\rho\to\infty$.

The second term Ψ_A of Eq. (2.27) has to describe the asymptotic configurations of the system when the two clusters are far from each other. In this asymptotic region, the wave function Ψ reduces to Ψ_A, which must therefore be the appropriate asymptotic solution of the Schrödinger equation. Ψ_A can also be decomposed in three Faddeev-like amplitudes and each of them is written as a linear combination of the following functions:

$$\Omega^o_{\lambda\Sigma\mathcal{J}}(\mathbf{x}_i,\mathbf{y}_i)=\sum_{l_\alpha=0,2}\varphi_{l_\alpha}(x_i)\mathcal{R}^o_\lambda(q_0y_i)\times\{\{\{Y_{l_\alpha}(\hat{x}_i)s_\alpha^{jk}\}_1\otimes s^i\}_\Sigma\otimes Y_\lambda(\hat{y}_i)\}^{\mathcal{J}\mathcal{M}}\times\{t_\alpha^{jk}t^i\}^{TT_z}\ , \quad (2.32)$$

where $\varphi_{l_\alpha}(x_i)$ is the deuteron wave function component in the waves with $l_\alpha=0,2$, and the coupling is given in the channel spin representation [11]. An asymptotic state will be labeled as ${}^{(2\Sigma+1)}\lambda_\mathcal{J}$, the corresponding phase shift as $\delta^\mathcal{J}_{\Sigma\lambda}$, and the parity Π of the state is given by $(-1)^\lambda$.

The functions $\mathcal{R}^o_\lambda(q_0y_i)$ of Eq. (2.32) can be taken as the regular ($o\equiv R$) and irregular ($o\equiv I$) radial solutions of the two-body nd Schrödinger equation without nuclear interaction.

With the above definitions, the ith Faddeev-like amplitude for the asymptotic wave function is written as

$$\Omega_{\lambda\Sigma\mathcal{J}}(\mathbf{x}_i,\mathbf{y}_i)=\Omega^R_{\lambda\Sigma\mathcal{J}}(\mathbf{x}_i,\mathbf{y}_i)+\sum_{\lambda'\Sigma'}{}^\mathcal{J}\tilde{K}^{\Sigma\Sigma'}_{\lambda\lambda'}\Omega^I_{\lambda'\Sigma'J}(\mathbf{x}_i,\mathbf{y}_i)\ , \quad (2.33)$$

where the matrix elements ${}^\mathcal{J}\tilde{K}^{\Sigma\Sigma'}_{\lambda\lambda'}$ give the relative weight between the regular and the irregular components. They are closely related to the corresponding $\mathbf{K}$ matrix elements (following Delves [15], in Ref. [6] this matrix was called $\mathbf{R}$):

$$\mathbf{K}^\mathcal{J}_{\lambda\Sigma,\lambda'\Sigma'}=q_0^{\lambda+\lambda'+1}\ {}^\mathcal{J}\tilde{K}^{\Sigma\Sigma'}_{\lambda\lambda'}\ . \quad (2.34)$$

By definition of the $\mathbf{K}$ matrix its eigenvalues are $\tan\delta^\mathcal{J}_{\Sigma\lambda}$. This $\mathbf{K}$ matrix is identical to the one defined in Eq. (2.8).

The total wave function corresponding to an asymptotic state ${}^{(2\Sigma+1)}\lambda_\mathcal{J}$ is written, in this approach, as

$$\Psi_{\lambda\Sigma\mathcal{J}}=\sum_{i=1,3}[\psi_C(\mathbf{x}_i,\mathbf{y}_i)+\Omega_{\lambda\Sigma\mathcal{J}}(\mathbf{x}_i,\mathbf{y}_i)]=\sum_{i=1,3}\left[\psi_C(\mathbf{x}_i,\mathbf{y}_i)+\Omega^R_{\lambda\Sigma\mathcal{J}}(\mathbf{x}_i,\mathbf{y}_i)+\sum_{\lambda'\Sigma'}{}^\mathcal{J}\tilde{K}^{\Sigma\Sigma'}_{\lambda\lambda'}\Omega^I_{\lambda'\Sigma'\mathcal{J}}(\mathbf{x}_i,\mathbf{y}_i)\right]\ . \quad (2.35)$$

The unknown quantities in the wave function (2.35) are the hyperradial functions and the $\mathbf{K}$ matrix elements which can be determined by means of the Kohn variational principle [6,15], stating that the $\mathbf{K}$ matrix elements, considered as functionals of the wave function, must be stationary with respect to variations of all the trial parameters. These functionals are

$$[{}^\mathcal{J}\tilde{K}^{\Sigma\Sigma'}_{\lambda\lambda'}]={}^\mathcal{J}\tilde{K}^{\Sigma\Sigma'}_{\lambda\lambda'}-\langle\Psi_{\lambda'\Sigma'\mathcal{J}}|H-E|\Psi_{\lambda\Sigma\mathcal{J}}\rangle\ . \quad (2.36)$$

The variation of the diagonal functionals with respect to the hyperradial functions $u_K^\alpha(\rho)$ gives a set of second order inhomogeneous differential equations. The variation with respect to the $\mathbf{K}$ matrix elements gives a set of algebraic equations, whose solution represents their optimum choice [6].

Finally we come to the S matrix parametrization as given by Seyler [11]. With the exception of the $\mathcal{J}=\frac{1}{2}$ case (which is two dimensional), the S matrix $S^\mathcal{J}_{\lambda'\Sigma',\lambda\Sigma}$ is three dimensional and describes, for the two possible parities $\Pi=(-1)^{\mathcal{J}\pm\frac{1}{2}}$, the following coupling:

$$\mathbf{S}=\begin{pmatrix} S^\mathcal{J}_{\mathcal{J}\mp\frac{3}{2}\ \frac{3}{2},\mathcal{J}\mp\frac{3}{2}\ \frac{3}{2}} & S^\mathcal{J}_{\mathcal{J}\mp\frac{3}{2}\ \frac{3}{2},\mathcal{J}\pm\frac{1}{2}\ \frac{1}{2}} & S^\mathcal{J}_{\mathcal{J}\mp\frac{3}{2}\ \frac{3}{2},\mathcal{J}\pm\frac{1}{2}\ \frac{3}{2}} \\ S^\mathcal{J}_{\mathcal{J}\pm\frac{1}{2}\ \frac{1}{2},\mathcal{J}\mp\frac{3}{2}\ \frac{3}{2}} & S^\mathcal{J}_{\mathcal{J}\pm\frac{1}{2}\ \frac{1}{2},\mathcal{J}\pm\frac{1}{2}\ \frac{1}{2}} & S^\mathcal{J}_{\mathcal{J}\pm\frac{1}{2}\ \frac{1}{2},\mathcal{J}\pm\frac{1}{2}\ \frac{3}{2}} \\ S^\mathcal{J}_{\mathcal{J}\pm\frac{1}{2}\ \frac{3}{2},\mathcal{J}\mp\frac{3}{2}\ \frac{3}{2}} & S^\mathcal{J}_{\mathcal{J}\pm\frac{1}{2}\ \frac{3}{2},\mathcal{J}\pm\frac{1}{2}\ \frac{1}{2}} & S^\mathcal{J}_{\mathcal{J}\pm\frac{1}{2}\ \frac{3}{2},\mathcal{J}\pm\frac{1}{2}\ \frac{3}{2}} \end{pmatrix}\ . \quad (2.37)$$

The matrix can be diagonalized:

$$\mathbf{S}=\mathbf{U}^Te^{2i\Delta}\mathbf{U}\ , \quad (2.38)$$

where Δ is the diagonal matrix of eigenphases $\delta^\mathcal{J}_{\Sigma\lambda}$ and $\mathbf{U}$ can be chosen as

$$\mathbf{U}=\mathbf{vwx} \quad (2.39)$$

with

$$\mathbf{v}=\begin{pmatrix}1&0&0\\0&\cos\epsilon&\sin\epsilon\\0&-\sin\epsilon&\cos\epsilon\end{pmatrix}\ , \quad (2.40)$$

$$\mathbf{w}=\begin{pmatrix}\cos\xi&0&\sin\xi\\0&1&0\\-\sin\xi&0&\cos\xi\end{pmatrix}\ , \quad (2.41)$$

$$\mathbf{x}=\begin{pmatrix}\cos\eta&\sin\eta&0\\-\sin\eta&\cos\eta&0\\0&0&1\end{pmatrix}\ . \quad (2.42)$$

The actual determination of the mixing parameters leads to some ambiguities. The eigenvectors related to the eigenvalue problem (2.38) build up the three rows of $\mathbf{U}$. This can be done in six ways. Moreover, there is arbitrariness in the choice of the overall sign for each eigenvector. Clearly, these various $\mathbf{U}$'s lead to quite different mixing parameters. A convention is required and for weak mixing the following one appears to be natural: we choose the one which grows steadily out of an S matrix, which is already diagonal and to which belongs $\mathbf{U} = \mathbf{1}$. Therefore we arrange the three eigenvectors in $\mathbf{U}$ (occurring as rows) in such a way that the dominant component stands in the diagonal and has a positive sign. For the nd scattering investigated below the dominant component for each eigenvector is always very close to 1. This convention uniquely defines $\mathbf{U}$ and, consequently, the mixing parameters.

III. RESULTS

Let us first reconfirm s-wave phase shifts for the MT(I-III) potentials, which have been determined by the Iowa/Los Alamos [7] group through Faddeev calculations in configuration space. Our results in comparison to the ones in [7] are displayed in Table I. The agreement is perfect.

We used the realistic AV14 NN potential and determined, by both the methods described in this article, the eigenphase shift and mixing parameters for $\mathcal{J}^\Pi = \frac{1}{2}^\pm \cdots \frac{5}{2}^\pm$ and $\frac{7}{2}^+$ at the nucleon laboratory energies $E_{\rm lab} = 1, 2$ and 3 MeV below the nd breakup threshold.[1] The results are displayed in Table II. We see an essentially perfect agreement, which demonstrates the maturity of both methods. Since we do not include the pp Coulomb force, we cannot compare directly to the recent phase shift analysis [2]. It is also interesting to note that for $\mathcal{J}^\Pi = \frac{1}{2}^+$, the quantum numbers of the triton, the phase shift $\delta^{\frac{1}{2}}_{\frac{1}{2},0}$ is correlated to the ground state energy. For this reason, it is necessary to include the NN force up to $j_{\max} = 3$ in the momentum space approach and $N_c = 14$ in the configuration space approach in order to get fully converged results. Some of the eigenphase shift and mixing parameters are also displayed in Fig. 1.

TABLE I. Comparison of nd s-wave eigenphase shifts $\delta_{\Sigma\lambda}$ (in degrees) for the MT(I-III) NN potentials, determined by solving the Faddeev equations in momentum space (Bochum) and in configuration space (Iowa/Los Alamos [7]) and by the pair correlated hyperspherical harmonic basis method (Pisa).

$E_{\rm lab}$ (MeV)	$\delta_{\Sigma\lambda}$	Bochum	Pisa	Iowa/Los Alamos [7]
0.75	$\delta_{\frac{1}{2}0}$	−12.1	−12.12	−12.1
0.75	$\delta_{\frac{3}{2}0}$	−42.4	−42.37	−42.4
1.5	$\delta_{\frac{1}{2}0}$	−20.7	−20.66	−20.7
1.5	$\delta_{\frac{3}{2}0}$	−55.9	−55.86	−55.8

[1]Phase shift values and mixing parameters for higher $\mathcal{J}^\Pi$ values can be received from the authors on request. They are in general much smaller than 1.

At zero energy only the s-wave scattering lengths survive, the doublet ($\Sigma = \frac{1}{2}$) and the quartet ($\Sigma = \frac{3}{2}$) ones. They are defined as the limits $q_0 \to 0$ of the eigenphases

$$\delta^{\frac{1}{2}}_{\frac{1}{2}0}(q_0) \to -^2a q_0 \ , \tag{3.1}$$

$$\delta^{\frac{3}{2}}_{\frac{3}{2}0}(q_0) \to -^4a q_0 \ , \tag{3.2}$$

and equivalently by

$$^{2\Sigma+1}a = \frac{2\pi}{3} m U^{\mathcal{J}}_{\Sigma\lambda=0,\Sigma\lambda=0}|_{q_0=0} \tag{3.3a}$$

in the momentum space Faddeev approach, or by

$$^{2\Sigma+1}a = -^{\mathcal{J}}\tilde{K}^{\Sigma\Sigma}_{00}|_{q_0-0} \tag{3.3b}$$

in the configuration space approach.

In the momentum space approach we solve Eqs. (2.17) directly at $E = E_d$, where no singularities are present and which is as easy as a bound state calculation. For more details see the Appendix.

Some of the phase shift and mixing parameters given in Table II have been calculated before in the configuration space approach [6]. The present calculation has been performed by extending the Hilbert space. This explains the small difference between some parameters given in Ref. [6] and those presented here.

The scattering lengths have been calculated before [6,16], and our numbers, shown in Table III, agree with each other and with the ones in [16]. Due to the wrong ^{3}H binding energy given by the AV14 potential the doublet scattering length, which is correlated to the binding energy, deviates from the experimental value of 0.65 ± 0.04 fm. The quartet case is less sensitive and theory agrees quite well with the experimental value of 6.35 ± 0.02 fm. In the doublet case one has to add a three-nucleon force to bring [6,16] binding energy and scattering length to the experimental values.

IV. OUTLOOK

We displayed the formalisms for extracting the partial wave projected S matrix in elastic nd scattering, in both momentum and configuration space treatments. The results found in both methods and using the realistic AV14 NN potential agree very well. The two methods are essentially different; in momentum space the Faddeev equations have been solved, while in configuration space the Kohn variational principle has been applied. The almost perfect agreement in the calculated phase shift and mixing parameters fixes the actual accuracy in the theoretical predictions of these quantities.

The next step to be done will be the inclusion of the pp

Coulomb force in order to make contact with the experimental *pd* data [2] at those rather low energies. This has already been started in our configuration space approach [6,17]. Another step is to go beyond the *nd* breakup threshold, where all the phase shift and mixing parameters will acquire imaginary parts. This can easily be done in our momentum space approach. At these energies theory appears to be needed to guide the phase shift analysis with respect to choices of reasonable magnitudes of the imaginary parts. Finally one can study the dependence of the mixing parameters on the NN force input parameters (central, spin-orbit, tensor forces) and the deuteron properties. Investigations are planned.

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TABLE II. Comparison of *nd* eigenphase shift $\delta^{\mathcal{J}}_{\Sigma\lambda}$ and mixing parameters (in degrees), determined in a momentum space (Bochum) and a configuration space (Pisa) method for the AV14 NN potential.

		$E_{\rm lab}$ = 1 MeV		$E_{\rm lab}$ = 2 MeV		$E_{\rm lab}$ = 3 MeV	
J^Π	$\delta_{\Sigma\lambda}$	Bochum	Pisa	Bochum	Pisa	Bochum	Pisa
$\frac{1}{2}^+$	$\delta_{\frac{3}{2}2}$	−0.999	−1.00	−2.57	−2.58	−3.91	−3.91
	$\delta_{\frac{1}{2}0}$	−17.8	−17.7	−28.0	−27.9	−34.9	−34.9
	η	1.03	1.04	1.20	1.21	1.25	1.26
$\frac{1}{2}^-$	$\delta_{\frac{1}{2}1}$	−4.20	−4.20	−6.66	−6.67	−7.54	−7.54
	$\delta_{\frac{3}{2}1}$	12.4	12.4	20.5	20.5	25.0	25.0
	ϵ	3.73	3.73	5.37	5.38	7.23	7.24
$\frac{3}{2}^+$	$\delta_{\frac{3}{2}0}$	−47.2	−47.2	−61.3	−61.3	−70.5	−70.5
	$\delta_{\frac{1}{2}2}$	0.579	0.579	1.54	1.55	2.41	2.42
	$\delta_{\frac{3}{2}2}$	−1.07	−1.08	−2.77	−2.77	−4.22	−4.22
	ϵ	0.651	0.651	0.716	0.717	0.779	0.783
	ξ	0.544	0.546	1.01	1.01	1.43	1.44
	η	−0.113	−0.113	−0.246	−0.245	−0.386	−0.385
$\frac{3}{2}^-$	$\delta_{\frac{3}{2}3}$	0.124	0.125	0.502	0.501	0.942	0.943
	$\delta_{\frac{1}{2}1}$	−4.14	−4.15	−6.50	−6.52	−7.21	−7.25
	$\delta_{\frac{3}{2}1}$	14.3	14.3	22.7	22.7	26.3	26.3
	ϵ	−1.31	−1.29	−1.96	−1.94	−2.75	−2.72
	ξ	−0.186	−0.182	−0.273	−0.272	−0.265	−0.268
	η	−1.11	−1.10	−2.30	−2.30	−3.78	−3.77
$\frac{5}{2}^+$	$\delta_{\frac{3}{2}4}$	−0.0153	−0.0151	−0.0923	−0.0926	−0.211	−0.211
	$\delta_{\frac{1}{2}2}$	0.574	0.575	1.53	1.53	2.38	2.38
	$\delta_{\frac{3}{2}2}$	−1.14	−1.14	−2.98	−2.98	−4.57	−4.57
	ϵ	−0.286	−0.285	−0.306	−0.311	−0.323	−0.331
	ξ	−0.286	−0.287	−0.516	−0.520	−0.727	−0.733
	η	−0.873	−0.872	−1.58	−1.58	−2.17	−2.16
$\frac{5}{2}^-$	$\delta_{\frac{3}{2}1}$	13.4	13.3	22.0	21.9	26.3	26.2
	$\delta_{\frac{1}{2}3}$	−0.0644	−0.0645	−0.258	−0.258	−0.478	−0.477
	$\delta_{\frac{3}{2}3}$	0.130	0.131	0.523	0.523	0.969	0.969
	ϵ	0.470	0.467	0.493	0.491	0.518	0.513
	ξ	0.417	0.416	0.734	0.732	0.993	0.993
	η	−0.132	−0.132	−0.258	−0.257	−0.365	−0.364
$\frac{7}{2}^+$	$\delta_{\frac{3}{2}2}$	−1.06	−1.06	−2.73	−2.73	−4.14	−4.15
	$\delta_{\frac{1}{2}4}$	0.00792	0.00783	0.0480	0.0481	0.110	0.110
	$\delta_{\frac{3}{2}4}$	−0.0160	−0.0159	−0.0966	−0.0969	−0.220	−0.219
	ϵ	0.377	0.361	0.383	0.383	0.367	0.370
	ξ	0.452	0.453	0.838	0.846	1.21	1.21
	η	−0.152	−0.152	−0.317	−0.318	−0.484	−0.490

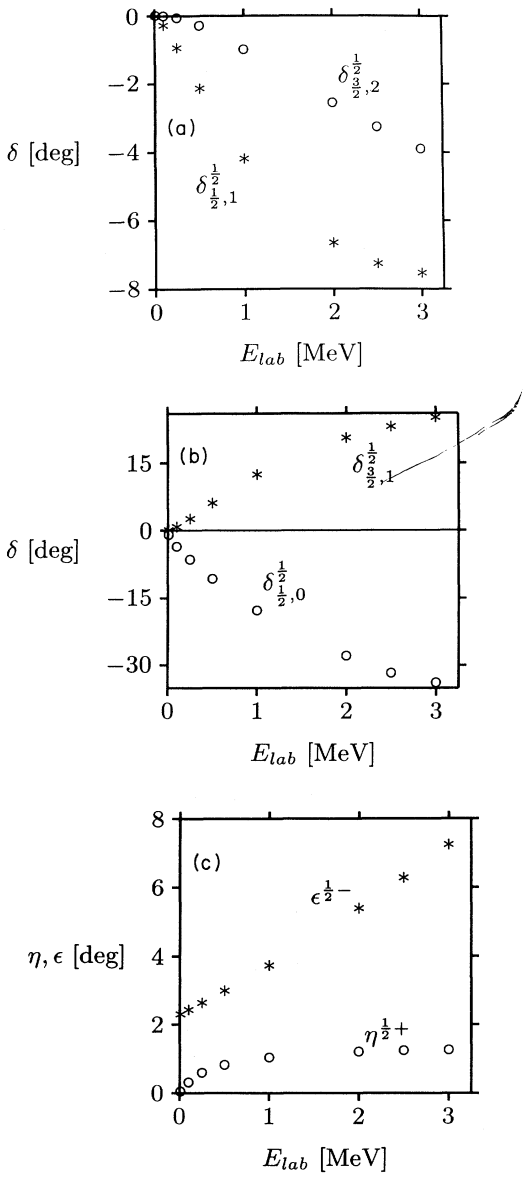

FIG. 1. Eigenphase shift and mixing parameters for $\mathcal{J}^{\Pi} = \frac{1}{2}^{\pm}$ for nd scattering using the AV14 NN potential.

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TABLE III. nd doublet and quartet scattering lengths for the AV14 NN potential.

	Bochum	Pisa	Los Alamos [16]
^2a(fm)	1.200	1.196	1.200
^4a(fm)	6.388	6.380	6.372

APPENDIX

In our standard manner [10] for solving Eq. (2.17) we use a different state $|\psi_0\rangle$, namely,

$$|\psi_0\rangle \to |\phi\rangle = |\varphi_d m_d t_d\rangle |\vec{q_0} m_N t_N\rangle \ , \tag{A1}$$

composed of the deuteron with magnetic and isospin quantum numbers m_d and t_d, respectively, and the projectile state with corresponding quantum numbers.

This leads to the partial wave representation ($\hat{q_0} \equiv \hat{e_z}$)

$$\begin{aligned} |\phi\rangle = \sum_{\mathcal{J}} \sum_{l=0,2} \sum_{\lambda J} \int dp\ p^2 \varphi_l(p) \\ \times |pq_0(l1)1(\lambda\tfrac{1}{2})J\mathcal{J} m_d + m_N(0\tfrac{1}{2})\tfrac{1}{2} t_N\rangle \\ \times (1J\mathcal{J}, m_d m_n)(\lambda\tfrac{1}{2}J, 0m_N)\sqrt{\frac{\hat{\lambda}}{3\pi}} \end{aligned} \tag{A2}$$

$$\equiv \sum_{\mathcal{J}} \sum_{\lambda J} |\phi_{\lambda J}\rangle (1J\mathcal{J}, m_d m_n)(\lambda\tfrac{1}{2}J, 0m_N)\sqrt{\frac{\hat{\lambda}}{4\pi}} \tag{A3}$$

(note $\hat{\lambda} \equiv 2\lambda + 1$). Consequently, the solution of (2.17) for a fixed $\mathcal{J}$ can be written as

$$\begin{aligned} \langle pq\alpha|T|\phi\rangle = \sum_{\lambda' J'} \langle pq\alpha|T|\phi_{\lambda' J'}\rangle (1J'\mathcal{J}, m_d m_n) \\ \times (\lambda'\tfrac{1}{2}J', 0m_N)\sqrt{\frac{\hat{\lambda}'}{4\pi}} \end{aligned} \tag{A4}$$

or

$$\begin{aligned} \langle pq\alpha|T|\phi_{\lambda' J'}\rangle = \sqrt{4\pi}\frac{\sqrt{\hat{\lambda}'}}{\hat{\mathcal{J}}} \sum_{m_d m_N} (1J'\mathcal{J}, m_d m_n) \\ \times (\lambda'\tfrac{1}{2}J', 0m_N)\langle pq\alpha|T|\phi\rangle \ . \end{aligned} \tag{A5}$$

Using now (2.19) and one of the representations of the permutation operator P [5] the amplitudes $U^{\mathcal{J}}_{\lambda' J', \lambda J}$ of Eq. (2.22) can be written as

$$\begin{aligned} U^{\mathcal{J}}_{\lambda' J', \lambda J} = \int_{-1}^{1} dx \sum_{l' l} \frac{\varphi_{l'}(\pi)}{\pi^{l'}} G_{\alpha'_d \alpha_d}(q_0 q_0 x) \frac{\varphi_l(\pi)}{\pi^l} \left(E - \frac{2q_0^2}{m} - \frac{q_0^2 x}{m} \right) + \int_{-1}^{1} dx \int_0^{\infty} dq'' q''^2 \sum_{l'} \frac{\varphi_{l'}(\pi_1)}{\pi_1^{l'}} \\ \times \left\{ \sum_{\alpha'' \neq \alpha_d} G_{\alpha'_d \alpha''}(q_0 q'' x) \frac{\langle \pi_2 q'' \alpha''|T|\phi_{\lambda J}\rangle}{\pi_2^{l''}} + \sum_{\alpha'' = \alpha_d} G_{\alpha'_d \alpha''}(q_0 q'' x) \frac{1}{\pi_2^{l''}} \frac{\langle \pi_2 q'' \alpha''|\hat{T}|\phi_{\lambda J}\rangle}{E - (3/4m)q''^2 - E_d + i\epsilon} \right\} . \end{aligned} \tag{A6}$$

Here

$$\pi = q_0\sqrt{\tfrac{5}{4}+x}\ ,$$
$$\pi_1 = \sqrt{q''^2+\tfrac{1}{4}q_0^2+q''q_0x}\ , \tag{A7}$$
$$\pi_2 = \sqrt{q_0^2+\tfrac{1}{4}q''^2+q_0q''x}\ .$$

In the $\hat{T}$ amplitude the deuteron pole has been extracted (see [10] for more details). The set of quantum numbers α_d includes those of the deuteron.

In the case of zero energy nucleon-deuteron scattering ($q_0 = 0$) this expression simplifies to

$$U^{\mathcal{J}}_{\lambda'J',\lambda J} = 2E_d\delta_{\lambda 0}\delta_{\lambda' 0}g^{00000}_{\alpha'_d\alpha d}\sum_{l'l}\frac{\varphi_{l'}(\pi)}{\pi^{l'}}\frac{\varphi_l(\pi)}{\pi^l}\bigg|_{\pi\to 0} + \delta_{\lambda' 0}\sum_{l'}\sum_{\alpha''}2^{l''+1}g^{0l'0l''0}_{\alpha'_d\alpha''}\int_0^\infty dq''q''^2\varphi_{l'}(q'')$$
$$\times\left\{\bar{\delta}_{\alpha''\alpha_d}\langle\tfrac{1}{2}q''q''\alpha''|T|\phi_{\lambda J}\rangle + \delta_{\alpha''\alpha_d}\frac{\langle\frac{1}{2}q''q''\alpha''|\hat{T}|\phi_{\lambda J}\rangle}{-(3/4m)q''^2}\right\}. \tag{A8}$$

The geometrical coefficient $g^{kl_1l_2l'_1l'_2}_{\alpha\alpha'}$ contained in $G_{\alpha\alpha'}$ is given in Eq. (A 19) of [5].

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