NN potentials from inverse scattering in the $J$-matrix approach.

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Abstract

An approximate inverse scattering method [5, 6] has been used to construct separable potentials with the Laguerre form factors. As an application, we invert the phase shifts of proton-proton in the $^{1}S_{0}$ and $^{3}P_{2} - ^{3}F_{2}$ channels and neutron-proton in the $^{3}S_{1} - ^{3}D_{1}$ channel elastic scattering. In the latter case the deuteron wave function of a realistic $np$ potential was used as input.

1 Introduction

Low-rank separable potentials greatly simplify many-body computations. The main sources of separable nucleon-nucleon ($NN$) potentials are the inverse scattering methods (see [1] and references therein). On the other hand the model effective two-particles interactions (see e.g. [2]) constructed with use of a realistic $NN$ potential (e.g. [3]) as input are also of separable form.

Recently a novel method was proposed for the treating of three-body problems including Coulomb forces [4]. In the framework of this approach the potential operator of the short-range part of full interaction is expanded with use of Coulomb-Sturmian (Laguerre) functions. Whereas Coulomb interaction is kept in the Green’s operator involved in Lippman-Schwinger equation. Instead of separable potentials (of relatively high rank) resulting from a realistic $NN$ interaction, the potentials obtained by means of inverse scattering technique [5, 6] within so-called $J$-matrix method can be applied in the three-body calculations [4].

The $J$-matrix method [5, 6, 7] is equivalent to the potential separable expansion approach [10, 11]; here too the potential $V$ is approximated by its projection $V^{N}$ onto the finite subspace spanned by the first $N$ (Laguerre or oscillator) basis functions. However in the $J$-matrix method the Schrödinger equation rather than Lippman-Schwinger one is solved in the square integrable basis representation. In the $J$-matrix approach an auxiliary function have been introduced resulting from discrete representation of the full Green’s operator [12]. This function (or matrix in the multichannel scattering case), so-called $P$-matrix, plays in our inversion scheme a part similar to that of the $R$-matrix in the potential reconstruction in the framework of finite-difference analogue of $R$-matrix scattering theory [13]. In particular, information requisite for the potential construction can also be obtained from the poles and residues of the $P$-matrix.

As an application of our method, we invert phase shifts of the proton-proton and neutron-proton elastic scattering. In the $NN$ potential construction an attempt have been made to account for the deuteron wave function [3] using the phase-equivalent transformation [14, 8].

In Sect. 2 we outline the $J$-matrix formalism for the solution of multichannel scattering problem. In Sect. 3 we briefly present the inversion procedure in the Laguerre form factors case, and describe the taking account for deuteron wave function technique within our method. We then apply the method to the $NN$ elastic scattering in Sect. 4. In Sect. 5 we summarize our conclusions.
2 Elements of the $J$-matrix formalism

The formalism is spelled out in detail in [12] for treating the problem of multichannel scattering from the potentials of the form

$$\hat{V} = \sum_{\alpha, \beta = 1, 2} |\alpha\rangle V^{\alpha \beta} \langle \beta|,$$

where the partial wave potentials $V^{\alpha \beta}$ are given by the expansion

$$V^{\alpha \beta} = \frac{\hbar^2}{2\mu} \sum_{n=0}^{N_{\alpha} - 1} \sum_{n'=0}^{N_{\beta} - 1} \phi_n^{(\alpha)} \langle n_{\alpha, n'}^{\alpha \beta} | V^{\alpha \beta} | n'_{\alpha, n'}^{\alpha \beta} \phi_n^{(\beta)} \rangle.$$

Here, the $\alpha$ and $\beta$ denote sets of quantum numbers including the values of the orbital momenta $l_\alpha$ and $l_\beta$, and

$$|\phi_n^{(\alpha)}\rangle = \frac{n!}{r(n + 2l_\alpha + 1)!} (a_\alpha r)^{l_\alpha + 1} e^{-a_\alpha r/2} L_{2n+1}^{2l_\alpha+1}(a_\alpha r),$$

are the functions bi-orthogonal to the Laguerre basis functions $|\phi_n^{(\alpha)}\rangle$ in the channel $\alpha$

$$|\phi_n^{(\alpha)}\rangle = (a_\alpha r)^{l_\alpha + 1} e^{-a_\alpha r/2} L_{2n+1}^{2l_\alpha+1}(a_\alpha r),$$

i.e. $\langle \phi_n^{(\alpha)} | \phi_{n'}^{(\alpha)} \rangle = \delta_{nn'}$. Here, $a_\alpha$ is a scaling parameter, $\mu$ is the reduced mass of the system. We confine ourselves to the elastic scattering case, in which the energy $\epsilon \equiv k^2 = 2\mu/\hbar^2 E$ is the same in the two channels.

The elements $u_{\alpha \beta}(k, r)$ of the $2 \times 2$ matrix as the solution of the Schrödinger equation are represented in the $J$-matrix method in the form of the expansion

$$u_{\alpha \beta}(k, r) = \sum_{n=0}^{\infty} |\phi_n^{(\alpha)}\rangle b_n^{(\alpha \beta)}(k),$$

whose coefficients $b_n^{(\alpha \beta)}$ obey the relations [12]:

$$b_n^{(\alpha \beta)}(k) = \begin{cases} \sum_{\alpha'} P_{n, N_{\alpha'} - 1}^{\alpha, \alpha'}(\epsilon) J_{N_{\alpha'} - 1}^{(\alpha')} (\alpha') b_{N_{\alpha'}}^{(\alpha') \beta}(k), & n \leq N_\alpha - 1, \\ S_n^{(\alpha)}(k) \delta_{\alpha \beta} + C_n^{(\alpha)}(k) K_{\alpha \beta}, & n \geq N_\alpha - 1. \end{cases}$$

Here, $K_{\alpha \beta}$ are the elements of the $K$-matrix, $P_{n, n'}^{\alpha, \beta}$ are the elements of the matrix

$$P = (\hbar^2 - h)^{-1},$$

where $h$ is the matrix of the Hamiltonian $\hat{h} = \hat{h}_0^{(1)} + \hat{h}_0^{(2)} + \frac{2\mu}{\hbar^2} \hat{V}$ calculated in the basis $\{|\alpha\rangle |\phi_n^{(\alpha)}\rangle, n = 0, N_\alpha - 1, \alpha = 1, 2\}$. $R$ is the block-diagonal overlap matrix involving the symmetric tridiagonal submatrices $R_n^{(\alpha)}$ [15]:

$$R_n^{(\alpha)} = \frac{2}{d_\alpha} (n + l_\alpha + 1) \frac{(n + 2l_\alpha + 1)!}{n!},$$

$$R_{n+1, n}^{(\alpha)} = R_{n, n+1}^{(\alpha)} = -\frac{1}{d_\alpha} (n + 2l_\alpha + 2)!. $$
The matrix $h_0^{(α)}$ of free Coulomb Hamiltonian

$$h_0^{(α)} = -\frac{d^2}{dr^2} + \frac{l_α(l_α + 1)}{r^2} + \frac{2\tau k}{r}, \quad (9)$$

where $\tau = \frac{Ze^2\mu}{\hbar^2 k}$, is also symmetric and tridiagonal [13]:

$$[h_0^{(α)}]_{n,n} = \frac{a_0^2}{4} R_n^{(α)} + 2\tau k \frac{(n + 2l_α + 1)!}{n!}, \quad (10)$$

$$[h_0^{(α)}]_{n,n+1} = [h_0^{(α)}]_{n+1,n} = -\frac{a_0^2}{4} R_n^{(α)},$$

$J_{N_α-1,N_α}$ are the elements of so called $J-$matrix [11]:

$$J_{n,n'}^{(α)}(k) = [h_0^{(α)}]_{n,n'} - k^2 R_n^{(α)}. \quad (11)$$

In what follows, $h$ denotes an $N \times N$-matrix ($N = N_1 + N_2$) whose elements $h_{ij}$ are defined in accordance with the rule $h_{ij} = h_{n,n'}^{α,β}$ if $i = n + \sum_{α' < α} N_{α'} + 1$ and $j = n' + \sum_{α' < β} N_{α'} + 1$.

With the spectral decomposition of the matrix $h' = ZΛZ^*$ (where superscript * denotes transposition) of the Hamiltonian $\hat{h}$ calculated in the orthonormalized basis $\{|α⟩\,|ψ_n^{α}⟩\}$, $n = 0, N_α - 1$, $α = 1, \frac{1,2}{\Lambda}$, where $Z$ is the orthogonal matrix of eigenvectors, and $Λ$ is the diagonal matrix of the eigenvalues $\{λ_j\}$ of the matrix $h'$, expression (7) can be written as [13]

$$P = D^*Z [I - Λ]^{-1} Z^* D. \quad (12)$$

Here, $I$ is the identity matrix, $D$ is the block-diagonal matrix involving the $N_α \times N_α$ submatrices $D^{(α)}$, $α = 1, 2$ of the transformation to the orthonormal basis $\{|ψ_n^{(α)}⟩\}$, $n = 0, N_α - 1$, i. e.

$$|ψ_n^{(α)}⟩ = \sum_{j=1}^{N_α} D^{(α)}_{n+1,j} |φ_j^{(α)}⟩. \quad (13)$$

$C_n^{(α)}$ and $S_n^{(α)}$ coincide respectively with the real and image part of the solution $C_n^{(α)(+)}$ of the discrete analogue of the Coulomb Schrödinger equation [11]

$$C_n^{(α)(+)}(k) = \frac{n! e^{iσ_α e^{(θ_α - π/2)τ}} e^{-i(n+1)θ_α}}{Γ(n + l_α + 2 + iτ) (2 \sin θ_α)^{l_α}} \times 2F_1(-l_α + iτ, n + 1; n + l_α + 2 + iτ; e^{-2iθ_α}). \quad (14)$$

Here, $σ_α = argΓ(iτ + l_α + 1)$, $e^{iθ_α} = (i(q_α - \frac{1}{2})/(i(q_α + \frac{1}{2})$, $q_α = k/a_α$. For $Z = 0$ hypergeometric function $2F_1$ in Eq. (14) degenerates into a polynomial of degree $l_α$ in $e^{-2iθ_α}$.

The symmetric $2 \times 2$ $K$-matrix corresponding to the potential (11), (2) has the form [15]:

$$K = -[C_{N-1} - \mathcal{P}JC_N]^{-1} [S_{N-1} - \mathcal{P}JS_N], \quad (15)$$

where

$$[C_{N-1} - \mathcal{P}JC_N]_{α,β} = C_{N_{α-1}}^{(α)}(k) δ_{α,β} - \mathcal{P}_{α,β}(ε) J_{N_{β-1},N_{β}}^{(β)}(k) C_{N_β}^{(β)}(k), \quad (16)$$

$$[S_{N-1} - \mathcal{P}JS_N]_{α,β} = S_{N_{α-1}}^{(α)}(k) δ_{α,β} - \mathcal{P}_{α,β}(ε) J_{N_{β-1},N_{β}}^{(β)}(k) S_{N_β}^{(β)}(k),$$

$\mathcal{P}_{α,β}(ε) ≡ P_{α,β}^{α,β}$ are the elements of so called $\mathcal{P}$-matrix.
3 Description of the method

By choosing the orthonormal basis functions \( \{|\psi_n^{(a)}\rangle\} \) (13) in the form

\[
|\psi_n^{(a)}\rangle = \left( \frac{a_\alpha n!}{(n + 2l_\alpha + 2)!} \right)^{1/2} (a_\alpha r)^{l_\alpha + 1} e^{-a_\alpha r/2} J_n^{2l_\alpha + 2}(a_\alpha r),
\]

which is to say that the matrices \( D^{(a)} \) are defined by the expressions

\[
D_{i,j}^{(a)} = \begin{cases} d_{i-1}^{(a)}, & i \geq j, \\ 0, & i < j, \end{cases}
\]

where

\[
d_n^{(a)} = \left( \frac{a_\alpha n!}{(n + 2l_\alpha + 2)!} \right)^{1/2},
\]

we derive the following expressions for the \( P \)-matrix elements

\[
\begin{align*}
P_{11}(\epsilon) &= \left(d_{N_1-1}^{(1)}\right)^2 \sum_{j=1}^{N} \frac{Z_{N_1,j}^2}{\epsilon - \lambda_j}, \\
P_{22}(\epsilon) &= \left(d_{N_2-1}^{(2)}\right)^2 \sum_{j=1}^{N} \frac{Z_{N_2,j}^2}{\epsilon - \lambda_j}, \\
P_{12}(\epsilon) &= P_{21}(\epsilon) = d_{N_1-1}^{(1)} d_{N_2-1}^{(2)} \sum_{j=1}^{N} \frac{Z_{N_1,j} Z_{N_2,j}}{\epsilon - \lambda_j}.
\end{align*}
\]

It should be noted that the elements \( P_{\alpha,\beta}(\epsilon) \) (20) decay \( (\sim \epsilon^{-1}) \) at the energies \( \epsilon > \lambda_N \), and the same is true for the \( K \)-matrix elements (15). On this basis, we set ourselves the task of the construction of the potential (1), (2) descriptive of the \( K \)-matrix in an energy interval \([0, \epsilon_0]\) and the system bound spectrum. In the case of arbitrary \( K \)-matrix behaviour it is suggested that \( \epsilon_0 < \lambda_N \).

The expressions (20) for the \( P \)-matrix are similar in structure to those for the \( R \)-matrix (16). This analogue have inspired us [6] to implement the technique used within the finite-difference analogue of the \( R \)-matrix scattering theory [13] for the retrieval of information requisite for the potential constructing from the \( K \)-matrix. For this purpose we fix some values of \( a_\alpha, N_\alpha \) and define functions

\[
\begin{align*}
\tilde{P}_{11}(\epsilon) &= \frac{1}{\Delta(k) J_{N_1-1,N_1}^{(1)}(k)} \left\{ \left(S_{N_1-1}^{(1)}(k) + C_{N_1-1}^{(1)}(k)K_{11}\right) \left(S_{N_2}^{(2)}(k) + C_{N_2}^{(2)}(k)K_{22}\right) - C_{N_1-1}^{(1)}(k)C_{N_2}^{(2)}(k)K_{12}^2 \right\}, \\
\tilde{P}_{22}(\epsilon) &= \frac{1}{\Delta(k) J_{N_2-1,N_2}^{(2)}(k)} \left\{ \left(S_{N_2-1}^{(2)}(k) + C_{N_2-1}^{(2)}(k)K_{22}\right) \left(S_{N_1}^{(1)}(k) + C_{N_1}^{(1)}(k)K_{11}\right) - C_{N_2-1}^{(2)}(k)C_{N_1}^{(1)}(k)K_{12}^2 \right\}, \\
\tilde{P}_{12}(\epsilon) &= \tilde{P}_{21}(\epsilon) = \frac{-k K_{12}}{\Delta(k) J_{N_1-1,N_1}^{(1)}(k) J_{N_2-1,N_2}^{(2)}(k)},
\end{align*}
\]

where

\[
\Delta(k) = \left(S_{N_1}^{(1)}(k) + C_{N_1}^{(1)}(k)K_{11}\right) \left(S_{N_2}^{(2)}(k) + C_{N_2}^{(2)}(k)K_{22}\right) - C_{N_1}^{(1)}(k)C_{N_2}^{(2)}(k)K_{12}^2.
\]
by inverting expression (15) relative to the $\mathcal{P}$-matrix elements. We set, in view of Eq. (21),

$$
\lambda_j = \tilde{\lambda}_j, \quad Z_{N_1,j} = \left( d_{N_1-1}^{(1)} \right)^{-1} \sqrt{\frac{\text{Res} \mathcal{P}_{11}(\epsilon)}{\epsilon - \tilde{\lambda}_j}},
$$

$$
Z_{N_2,j} = \left( d_{N_2-1}^{(2)} \right)^{-1} \frac{\text{Res} \mathcal{P}_{12}(\epsilon)}{\epsilon - \tilde{\lambda}_j} \sqrt{\frac{\text{Res} \mathcal{P}_{11}(\epsilon)}{\epsilon - \tilde{\lambda}_j}}, \quad j = 1, p,
$$

(25)

where $\{\tilde{\lambda}_j < \epsilon_0, j = 1, p\}$ are the “internal” poles of the functions $\tilde{\mathcal{P}}_{\alpha,\beta} (21)-(24)$.

An search for optimal combinations $a_{\alpha}, N_{\alpha}$ is an important constituent of the method. Assuming that the absolute values of the off-diagonal elements of the $K$-matrix are negligibly small, this problem can be solved in every channel $\alpha = 1, 2$ separately. For this purpose, on every step of variational procedure involving $[3]$ in which the rational approximant

$$
\mathcal{P}_{\alpha}(\epsilon) = \left( d_{N_{\alpha}-1}^{(\alpha)} \right)^2 \sum_{j=1}^{N_{\alpha}} \frac{\left( Z_{N_{\alpha},j}^{(\alpha)} \right)^2}{\epsilon - \lambda_j^{(\alpha)}},
$$

(26)
on the interval $[0, \epsilon_0]$ of the function

$$
\tilde{\mathcal{P}}_{\alpha}(\epsilon) = \frac{1}{J_{N_{\alpha}-1, N_{\alpha}}^{(\alpha)}(\epsilon)} \frac{\tilde{C}_{N_{\alpha}-1}^{(\alpha)}(k)}{C_{N_{\alpha}}^{(\alpha)}(k)},
$$

(27)

is constructed. Going to the next step, we increase $a_{\alpha}$ and decrease $N_{\alpha}$. The condition that remainder of the approximation (14) be small is criteria for going to new combination $a_{\alpha}, N_{\alpha}$.

$N_{\alpha}$ is bounded below by the requirement that the residues of $\tilde{\mathcal{P}}_{\alpha}$ be positive, or by the equivalent condition that the roots of the denominators of the functions $\tilde{\mathcal{P}}_{\alpha}$ alternate those of the numerators (3). It is evident from asymptotic expressions for the solutions $S_n^{(\alpha)}, C_n^{(\alpha)}$ as $n \to \infty$ ($k$ is bounded) (15):

$$
S_n^{(\alpha)}(k) = -n^{-(l_\alpha+1)} \sin \left\{ \sigma_\alpha - (n + l_\alpha + 1) \theta_\alpha - \tau \ln(2 n \sin \theta_\alpha) + \frac{\pi l_\alpha}{2} \right\},
$$

$$
C_n^{(\alpha)}(k) = -n^{-(l_\alpha+1)} \cos \left\{ \sigma_\alpha - (n + l_\alpha + 1) \theta_\alpha - \tau \ln(2 n \sin \theta_\alpha) + \frac{\pi l_\alpha}{2} \right\},
$$

(28)

$$
\tilde{C}_n^{(\alpha)}(k) = -n^{-(l_\alpha+1)} \sin \left\{ \sigma_\alpha - (n + l_\alpha + 1) \theta_\alpha - \tau \ln(2 n \sin \theta_\alpha) + \frac{\pi l_\alpha}{2} + \delta_\alpha \right\},
$$

that if $N_{\alpha}$ is large enough to fulfill the condition

$$
\left| \frac{d}{dk} \{ \sigma_\alpha - (N_{\alpha} + l_\alpha) \theta_\alpha - \tau \ln[2 (N_{\alpha} - 1) \sin \theta_\alpha] \} \right| > \left| \frac{d \delta_\alpha}{dk} \right|,
$$

(29)

the roots separation holds.

The parameters $a_{\alpha}, N_{\alpha}$ obtained above are used in the coupled-channel case. Once the “internal” parameters has been fixed (25), $r = N - p$ “external” triplets $\{\lambda_j > \epsilon_0, Z_{N_1,j}, Z_{N_2,j}, j = p + 1, N\}$ remain unknown. Since the rows $\{Z_{N_1,j}\}$ and $\{Z_{N_2,j}\}$ of the orthogonal matrix $\mathbf{Z}$ must meet the orthonormalization conditions

$$
\sum_{j=1}^N Z_{N_1,j}^2 = \sum_{j=1}^N Z_{N_2,j}^2 = 1, \quad \sum_{j=1}^N Z_{N_1,j} Z_{N_2,j} = 0,
$$

(30)
it is evident that the minimal \( r \) is equal to 2.

The values of the “external” parameters \( \{ \lambda_j \} \), as a rule, lie in the energy range that is far removed from the right limit of the interval \([0, \epsilon_0]\). If the assumption is made that for this energies the phase shifts and the mixing parameter are negligible, for the parameters \( \{ \lambda_j > \epsilon_0 \} \) the “external” parameters \( \{ \lambda_j^{(a)} \} \) obtained in the construction of the rank \( N_\alpha \) potential in every channel \( \alpha = 1, 2 \) can be used.

There is for every bound state with the energy \( \epsilon_\nu = -\kappa_\nu^2 \) a corresponding parameter \( \lambda_\nu \): \( \epsilon_\nu < \lambda_\nu < \lambda_1 \), which fits the equation (31):

\[
\det \left[ C_{N-1}^{(+)} - PJC_N^{(+)} \right] = 0,
\]

where

\[
\left[ C_{N-1}^{(+)} - PJC_N^{(+)} \right]_{\alpha, \beta} = C_{N,\alpha-1}^{(a)(+)}(i\kappa_\nu) \delta_{\alpha, \beta} - P_{\alpha, \beta}(\epsilon_\nu) J_{N,\beta-1, N,\beta}^{(\beta)}(i\kappa_\nu) C_{N,\beta}^{(\beta)(+)}(i\kappa_\nu).
\]

Eq. (31) is similar to the equation (10, 11)

\[
\det \left[ I - G^{(0)(+)}(i\kappa_\nu) V \right] = 0,
\]

where

\[
\left[ G^{(0)(+)}(i\kappa_\nu) \right]_{\alpha, \beta}^{\alpha', \beta'} = \delta_{\alpha', \beta'} \frac{\langle \phi_{\alpha} | \hat{G}^{(0)(+)}(i\kappa_\nu) | \phi_{\beta'} \rangle}{\langle \phi_{\beta'} | \hat{G}^{(0)(+)}(i\kappa_\nu) | \phi_{\alpha} \rangle}
\]

are the matrix elements of the Coulomb Green’s operator. In spite of the fact that Eq. (31) possesses the redundant roots \( \kappa = a_\alpha/2 \) of multiplicity \( N_\alpha \), it is preferable to Eq. (33), since the desired potential matrix \( V \) not enters explicitly into Eq. (31).

**Phase-equivalent transformation**

From Eq. (20) follows the expression that relates the matrices of the phase-equivalent potentials (for comparison see [14, 6]) corresponding to fixed values of \( a_\alpha, N_\alpha \):

\[
V(Q) = D^{-1}QZ_0 \Lambda \left( D^{-1}QZ_0 \right)^* - h_0.
\]

Here, \( \Lambda \) and \( Z_0 \) are fixed diagonal and orthogonal \( \mathcal{N} \times \mathcal{N} \)-matrices respectively; \( Q \) is arbitrary orthogonal matrix of the form

\[
Q = \begin{pmatrix}
\begin{array}{cccc}
1 & & & \\
& 0 & & \\
& & 0 & \\
& & & 0
\end{array}
& \begin{array}{cccc}
\begin{array}{c}
\vdots
\end{array} & \begin{array}{cc}
\begin{array}{c}
\ddots
\end{array} & \begin{array}{c}
\ddots
\end{array}
\end{array} & \begin{array}{c}
\vdots
\end{array} & \begin{array}{c}
\vdots
\end{array}
\end{array}
& \begin{array}{cccc}
\begin{array}{c}
\vdots
\end{array} & \begin{array}{cc}
\begin{array}{c}
\ddots
\end{array} & \begin{array}{c}
\ddots
\end{array}
\end{array} & \begin{array}{c}
\vdots
\end{array} & \begin{array}{c}
\vdots
\end{array}
\end{array}
\end{pmatrix}
\begin{array}{c}
\begin{array}{c}
N_1 \text{-th column}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
N \text{-th column}
\end{array}
\end{array}
\end{pmatrix}
\end{array}
\end{pmatrix}

(36)

\( h_0 \) is the block-diagonal matrix of the free Hamiltonian involving submatrices \( h_0^{(\alpha)} \) (10). Thus, the eigenvalues \( \{ \lambda_j \} \) and rows \( \{ Z_{N_i, j} \}, \{ Z_{N, j} \} \) of the eigenvectors matrix \( Z \) of the truncated
Hamiltonian matrix $h'$ specify the potential (1), (2) $V$ to within the orthogonal matrix $Z$ construction method from given $N_1$-th and $N$-th rows. Once this method has been fixed (e.g. (3)), and the corresponding matrix has been denoted by $Z_0$, the uncertainty of sought-for potential can be concentrated in the arbitrary orthogonal matrix $Q$ (36).

It should be noted that from (20) it also follows that the $P$-matrix is invariant under exchange of $Z_{N_1,j}$ and $Z_{N,j}$ signs.

**Taking into account the bound state wave function**

The components $u_\alpha$ of the bound state wave function are represented in the form of expansion

$$u_\alpha(i\kappa, r) = \sum_{n=0}^{\infty} b_n^{(\alpha)}(i\kappa) |\phi_n^{(\alpha)}\rangle, \quad \alpha = 1, 2,$$  

(37)

where the coefficients $b_n^{(\alpha)}$ for $n_\alpha \geq N_\alpha - 1$ are given by (12):

$$b_n^{(\alpha)}(i\kappa) = S_\alpha C_n^{(\alpha)(+)}(i\kappa).$$  

(38)

Notice that the parameters $\{\lambda_j, Z_{N_1,j}, Z_{N,j}, j = 1, N\}$ determine the asymptotic properties of the bound state wave function. Really, from the equation (18)

$$[C_N^{(+)} - PJC_N^{(+)}] S = 0,$$  

(39)

it follows that

$$\tilde{\eta} \equiv \frac{S_2}{S_1} = \frac{C_{N_1-1}^{(1)(+)}(i\kappa) - P_{11}(\varepsilon) J_{N_1-1, N_1}^{(1)}(i\kappa) C_{N_1}^{(1)(+)}(i\kappa)}{P_{12}(\varepsilon) J_{N_2-1, N_2}^{(2)}(i\kappa) C_{N_2}^{(2)(+)}(i\kappa)}.$$  

(40)

To derive the expression for $S_1$, let us define two auxiliary $N$-component vectors:

$$x_j = \frac{b_j^{(1)}(i\kappa) - b_j^{(1)}(i\kappa)}{S_1 d_j^{(1)}}, \quad j = 1, N_1 - 1, \quad x_{N_1} = \frac{C_{N_1-1}^{(1)(+)}(i\kappa)}{d_j^{(1)}},$$  

$$x_j = \frac{b_j^{(2)}(i\kappa) - b_j^{(2)}(i\kappa)}{S_1 d_j^{(2)}}, \quad j = N_1 + 1, N - 1, \quad x_N = \frac{\tilde{\eta} C_{N_2-1}^{(2)(+)}(i\kappa)}{d_j^{(2)}},$$  

(41)

and

$$g_j = -\frac{1}{\kappa^2 + \lambda_j} \left\{Z_{N_1,j} d_{N_1-1}^{(1)} J_{N_1-1, N_1}^{(1)}(i\kappa) C_{N_1}^{(1)(+)}(i\kappa) + \tilde{\eta} Z_{N,j} d_{N_2-1}^{(2)} J_{N_2-1, N_2}^{(2)}(i\kappa) C_{N_2}^{(2)(+)}(i\kappa) \right\}, \quad j = 1, N.$$  

(42)

With the help of (11), (12), we can rewrite (9), (38) as

$$x = Z g.$$  

(43)

Since $Z$ is the orthogonal matrix, the vector $x$ norm is equal to that of $g$:

$$x^* x = g^* g.$$  

(44)
Notice that the functions $u_\alpha$ can be rewritten in the form:

$$u_1(i\kappa, r) = S_1 \left\{ \sum_{n=0}^{N_1-2} x_{n+1} \left| \psi_n^{(1)} \right\rangle + \tilde{u}_1(i\kappa, r) \right\},$$

$$u_2(i\kappa, r) = S_1 \left\{ \sum_{n=0}^{N_2-2} x_{N_1+n+1} \left| \psi_n^{(2)} \right\rangle + \tilde{\eta} \tilde{u}_2(i\kappa, r) \right\},$$

where

$$\tilde{u}_\alpha(i\kappa, r) = u_\alpha^{(0)}(i\kappa, r) - \sum_{n=0}^{N_\alpha-2} \frac{C_n^{(\alpha)+(i\kappa)} - C_{n+1}^{(\alpha)+(i\kappa)}}{d_n^{(\alpha)}} \left| \psi_n^{(\alpha)} \right\rangle,$$

$$u_\alpha^{(0)}(i\kappa, r) = \sum_{n=0}^{\infty} C_n^{(\alpha)+(i\kappa)} \left| \phi_n^{(\alpha)} \right\rangle = \sum_{n=0}^{\infty} \frac{C_n^{(\alpha)+(i\kappa)} - C_{n+1}^{(\alpha)+(i\kappa)}}{d_n^{(\alpha)}} \left| \psi_n^{(\alpha)} \right\rangle.$$  

Substitution of Eq. (44-46) into the unit norm of the wave function condition

$$\int_0^\infty |u_1(i\kappa, r)|^2 dr + \int_0^\infty |u_2(i\kappa, r)|^2 dr = 1$$

(47)

gives:

$$S_1^{-2} = g^* g - \left| \frac{C_{N_1-1}^{(1)+(i\kappa)}}{d_{N_1-1}^{(1)}} \right|^2 - \left| \frac{\tilde{\eta} C_{N_2-1}^{(2)+(i\kappa)}}{d_{N_2-1}^{(2)}} \right|^2 + \int_0^\infty |\tilde{u}_1(i\kappa, r)|^2 dr + \int_0^\infty |\tilde{\eta} \tilde{u}_2(i\kappa, r)|^2 dr.$$  

(48)

In the framework of our method the phase-equivalent transformation (35), (36) is a tool for the influence on the potential (1), (2) off-shell behaviour. If we only be interested in describing the bound state wave function properties, we may vary the first $N_\alpha - 1$ coefficients of the expansions (37) in view of the condition (44). For $N \geq 4$, the resulting set \( \{ b_n^{(\alpha)}, n = 0, N_\alpha - 2 \} \) does not uniquely specify (see (43)) the matrix $Q = \begin{pmatrix} I & II \\ III & IV \end{pmatrix}$, since its unknown submatrix $Q_{12}$ is of order $N - 2$.

### 4 Results

As an application, we invert the $NN$ elastic scattering data. A set of Nijmegen phase shifts in the $0 - 350$ MeV energy range is taken as input to calculate the potentials. The obtained $pp$ potentials parameters in the channels $^1S_0$ and $^3P_2 - ^3F_2$ are listed in Table I. In Fig. 1 we
show the phase shifts resulting from the Nijmegen partial wave analysis \([3]\) (crosses) and the phase shifts obtained from our potentials (solid line).

In the \(1S_0\) channel for a chosen \(a\) and \(N\) the pair of unknown “external” parameters \(\lambda_4, Z_{4,4}\) has been obtained. Since the \(Z_{4,4}\) value is fixed by the normalization of the vector \(\{Z_{4,j}\}\) condition, only free parameter \(\lambda_4\) remains.

In the channel \(^3P_2 - ^3F_2\) the absolute values of the phase shift \(\delta_3\) are very small. For the relative deviations of the \(\delta_3\) values from ones of \([3]\) to be comparable to those for the phase shift \(\delta_1\), the value of \(N_2\) must be chosen sufficiently large (see Table I). For a chosen combination of the \(a_{\alpha}, Na_{\alpha}\), we obtain three triplets of the “external” parameters \(\{\lambda_j, Z_{2,j}, Z_{8,j}, j = 6, 7, 8\}\). The values of \(\lambda_6\) and \(\lambda_7\) are obtained by making it equal to \(\lambda_4^{(1)}\) and \(\lambda_5^{(2)}\) calculated in the potentials construction in the uncoupled channels \(^3P_2\) and \(^3F_2\) respectively. The parameters \(\lambda_8, Z_{2,8}, Z_{8,8}\) values were calculated in a similar way to those of the “internal”; to do this the phase shifts are extrapolated with functions which decay asymptotically. Finally, the orthonormalization conditions \([9]\) allow the free parameters number to be reduced to one. For the latter we used \(Z_{2,7}\).

The obtained values for the \(np\) potential parameters in the channel \(^3S_1 - ^3D_1\) are given in Table II. The phase shifts and the mixing parameter corresponding to our potential are represented by solid lines in Fig. 2.

Here, we also have obtained three triplets \(\{\lambda_j, Z_{2,j}, Z_{8,j}, j = 6, 7, 8\}\) of the “external” parameters. The values \(\lambda_6\) and \(\lambda_7\) are equal to \(\lambda_4^{(2)}\) and \(\lambda_4^{(1)}\) obtained in the uncoupled channels \(^3D_1\) and \(^3S_1\) respectively. Next, orthonormalization conditions \([9]\) have reduced the unknown parameters number to four, three of which \(Z_{4,7}, Z_{4,8}, Z_{8,8}\) are variable. Further, the combination of \(Z_{4,8}, Z_{8,8}\) has an effect on the phase shift \(\delta_0\) and mixing parameter \(\tau_1\) behaviour in the neighborhood of \(\epsilon = 0\), whereas \(Z_{4,7}\) is responsible for \(\tau_1\) curve form at the right of the interval \([0, \epsilon_0]\). Then the parameter \(\lambda_8\) fits Eq. \([9]\) with the deuteron binding energy \(\varepsilon = -\kappa^2 = -0.536401 \text{ fm}^{-2}\).

The deuteron wave function of the potential Nijm II \([3]\) is employed as input in the \(np\) potential constructing. It is seen from \([13]\), \([14]\) and the relation \(u_s^{(0)}(ik, r) \rightarrow e^{-\kappa r}\) that the asymptotic \(S\)-state normalization \(A_S\) is equal to \(S_1\), i.e. depends on the module of the vector \(g\) \([12]\) (see \([18]\)). The last component \(g_8\) containing the parameters \(Z_{4,8}, Z_{8,8}\), \(\lambda_8\) makes a major contribution to the vector \(g\) norm (see Table III). \(A_S\) is found to be the most sensitive to the change in \(Z_{4,8}\), whereas the \(D/S\)-state ratio \(\eta (\eta = -\bar{\eta}\) \([11]\), since \(u_D^{(0)}(ik, r) \rightarrow -e^{-\kappa r}\) is strongly dependent on the value of \(Z_{8,8}\).

In order to get the right behaviour of the wave function in the interior domain we use the phase-equivalent transformation \([35]\), \([36]\). In so doing the vector \(x\) \([11]\) components \(\{x_1, x_2, x_3\}\) and \(\{x_5, x_6, x_7\}\) (which within the factor \(S_1\) are equal to the first three coefficients of the \(S\) and \(D\) waves expansions \([37]\) on the basis orthonormal functions \([17]\) ) are varied in view of Eq. \([14]\). In Fig. 3 the deuteron wave function \(S\) and \(D\) components (functions \(u_S\) and \(u_D\) respectively) of our potential with the parameters in Tables II, III are drawn (dotted line). There we compare them with the wave functions of the Nijm II potential \([3]\) (solid line). The deuteron parameters calculated with our wave function and those from the Nijm II potential are listed in Table IV.
5 Summary

Approximate inverse scattering method within $J$-matrix approach \cite{5,6} has been extended to the case of the Laguerre form factors. As a result the method has become applicable to the inversion of charge particles scattering. The $P$-matrix has a dominant role in our procedure. Similar to the $R$-matrix, the $P$-matrix contains requisite information for the potential constructing and on the other hand is uniquely determined by the $S$-matrix. Besides, the $P$-matrix determines the asymptotic normalization constants of the bound state wave functions.

In this work the phase-equivalent transformation \cite{14,6} has been modified to be valid for separable potentials with the Laguerre form factors. The phase-equivalent transformation was used for the description of the deuteron wave function of the realistic Nijm II \cite{3} nucleon-nucleon potential. In doing this, we were interested in the behaviour of the wave function in the internal domain rather than in fitting the values of the quadrupole moment $Q_d$ or the $D$-state probability $p_D$. The discrepancy between the deuteron wave functions of our potential and that of Nijm II potential can be removed by increasing of desired potential (1), (2) rank $N$.

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### Tables

**Table I.** $pp$ potentials parameters values in the channels $^1S_0$ and $^3P_2 - ^3F_2$.

| $j$ | $Z_{N,j}$ | $\lambda_j$ ($fm^{-2}$) | $Z_{N_1,j}$ | $Z_{N,j}$ | $\lambda_j$ ($fm^{-2}$) |
|-----|----------|-----------------------|-------------|---------|-----------------------|
| 1   | .1558523299 | .08517568687         | .002378372193 | -.2021238864 | .3171350908          |
| 2   | .4062499094  | .6366888556      | .00633410556 | .2927989544  | .7864286930          |
| 3   | .6517820375  | 2.999305831       | .02352440740 | -.3709560916 | 1.607103324          |
| 4   | .6211692507  | 22.               | .4982479821  | .0328828370  | 2.259459783          |
| 5   | .02790963713 | -.4402591159      | 3.146276272  |            |                      |
| 6   | .01090380937 | .4980705527       | 13.25       |            |                      |
| 7   | .8657366805  | .01462158020      | 16.20600628 |            |                      |
| 8   | .02742131063 | -.5409333126      |            |            |                      |

**Table II.** $np$ potential parameters values in the channel $^3S_1 - ^3D_1$.

| $j$ | $Z_{N_1,j}$ | $Z_{N,j}$ | $\lambda_j$ ($fm^{-2}$) |
|-----|-------------|----------|-----------------------|
| 1   | .02017320192 | -.2989525605 | .4678515858 |
| 2   | .3982489552  | .02212234580 | .6496845646 |
| 3   | .01890700216 | -.4605017812 | 1.501863086 |
| 4   | .6535995282  | .09501129016 | 3.492094508 |
| 5   | .1314698511  | -.5784348737 | 4.238758885 |
| 6   | .08780677309 | .5929301489  | 12.75       |
| 7   | .6152722974  | -.05339635194 | 35.         |
| 8   | .09943159709 | .006685636351 | -.03571632149 |
Table III. The components of the vectors $g$ (42) and $x$ (41) in $fm^{1/2}$.

| $j$ | $g_j$   | $x_j$ |
|-----|---------|-------|
| 1   | -.002345654140 | .6665 |
| 2   | -.1089332559  | -.69  |
| 3   | .0002896455277 | .341506600 |
| 4   | -.03560896022 | -.1757029190 |
| 5   | -.004683742390 | .265 |
| 6   | -.001726119865 | .025 |
| 7   | -.003354599822 | .045 |
| 8   | -.1067801341 | -.01049929153 |

Table IV. Deuteron properties: $D/S$-ratio $\eta$, asymptotic $S$-state normalization $A_S$ in $fm^{-1/2}$, $D$-state probability $p_D$ in $\%$, and quadrupole moment $Q_d$ in $fm^2$.

| $\eta$ | $A_S$ | $p_D$ | $Q_d$ |
|--------|-------|-------|-------|
| (this article) | .0252 | .8845 | 5.729 | .28185 |
| Nijm II | .0252 | .8845 | 5.635 | .2707 |
Figure captions

Fig. 1. $pp$ phase shifts in the channels $^1S_0$ and $^3P_2 - ^3F_2$ from the Nijmegen [3] partial-wave analysis (crosses) and the potential (1), (2) with the parameters listed in Table I (solid line).

Fig. 2. $np$ phase shifts in the channel $^3S_1 - ^3D_1$ from the Nijmegen [3] partial-wave analysis (crosses) and the potential (1), (2) with the parameters listed in Table II (solid line).

Fig. 3. The $S$ and $D$ components of the deuteron wave functions of the Nijm II potential [3] (solid line) and of the potential (1), (2) with the parameters listed in Tables II, III (dotted line).
Figure 1.
Figure 2.
Figure 3.