Energy-independent complex $^1S_0$ NN potential from the Marchenko equation

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We present a new algebraic method for solving the inverse problem of quantum scattering theory based on the Marchenko theory (fixed-l inversion). We applied a triangular wave set for the Marchenko equation kernel expansion in a separable form. The separable form allows a reduction of the Marchenko equation to a system of linear equations. For the zero orbital angular momentum l, a linear expression of the kernel expansion coefficients is obtained in terms of the Fourier series coefficients of $q(1 - S(q))$ function [$S(q)$ is the scattering matrix] depending on the momentum q and determined by the scattering data in the finite range $0 \leqslant q \leqslant \pi/h$. It is shown that this Fourier series defines the potential function of the corresponding radial Schrödinger equation with h-step accuracy. Based on the developed method, a numerical algorithm is obtained for reconstructing complex partial potentials from scattering data on a finite range of q. The reconstructed potentials describe with a required accuracy a partial S matrix that is unitary below the threshold of inelasticity and nonunitary (absorptive) above the threshold. The developed procedure is applied to analyze the $^1S_0$ NN data up to 3 GeV. We show that these data are described by energy-independent complex partial potential.

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I. INTRODUCTION

The inverse problem of quantum scattering is essential for various physical applications such as the interparticle potential extraction from scattering data and similar problems. The main approaches to solving the fixed-l inversion problem are Marchenko, Krein, and Gelfand-Levitan theories [1–7]. The ill-posedness of the inverse problem complicates its numerical solution. The development of robust methods for solving the problem remains a fundamental challenge for applications [8–12]. Previously, Marchenko theory was successfully applied to reconstruct nucleon-nucleon partial potentials from partial-wave analysis (PWA) data up to the inelastic threshold ($E_{\text{lab}} \approx 280$ MeV) [13,14] using rational fraction expansions of partial S matrices. In this case, the kernel of the Marchenko equation is represented as finite separable series of the Riccati-Hankel functions products, and the Marchenko equation is solved analytically. The partial potentials are also expressed through these functions (Bargman-type potentials). A similar approach was used later to reconstruct optical model nucleon-nucleon partial potentials from PWA data up to 3 GeV [15,16]. However, the convergence of such a procedure with an increase in the S-matrix approximation accuracy is not apparent.

This paper considers a new algebraic method for solving the fixed-l inverse problem of quantum scattering theory. We derive the method from the Marchenko theory. To this end, we propose a novel numerical solution of the Marchenko equation based on the integral kernel approximation as a separable series in the triangular and rectangular wave sets. Thus, we solve the Marchenko equation with a separable kernel, which can be performed analytically as in Refs. [13–16]. For the kernel expansion in the series we propose, we show that the expansion coefficients can be obtained from the Fourier series coefficients of the function $q(1 - S(q))$ on a finite range ($0 \leqslant q \leqslant \pi/h$) of the momentum q. The convergence of the procedure is demonstrated numerically by decreasing the value of h. Thus we show that the kernel approximation may be calculated directly from the scattering data on the finite range of q. The developed method is based on the Fourier series expansion of a continuous function, and the theory of the Fourier series substantiates its convergence with decreasing step h.

The concept of optical potential (OP) is a useful tool in many branches of nuclear physics. NN potentials are used as an input for (semi)microscopic construction of OPs for description of nuclei and nuclear reactions [17–21]. The commonly used NN potentials in such approaches are real and only describe the NN PWA data below the inelastic threshold. The use of complex partial NN potentials describing the PWA data at energies above the threshold is necessary (in the absence of a microscopic theory) to describe nuclear reactions with energies of the NN relative motion above the threshold [16]. There are different models of such optical partial NN potentials. In Ref. [15], an algorithm was presented for constructing a partial potential, with an energy-independent real potential r-space function modified by an energy-dependent

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complex r-independent multiplier. In Ref. [22], an algorithm for constructing a separable partial potential was presented. In this algorithm, the separable part of the potential modifies the r-space real part of the potential. In both algorithms, the modifying part is absent below the threshold, and the potential is real. The real partial potential gives the real wave function to within an r-independent factor. Such a limitation for a realistic OP is excessive. Thus, the problem arises of constructing optical model partial potential that is complex at all energies, even below the inelasticity threshold. Such a possibility exists. For example, the phase-equivalent Krein transformations make it possible to obtain an energy-independent complex potential giving a unitary matrix [2].

The direct application of the fixed-l inversion theories to the reconstruction of a potential which is phase equivalent to the effective potential describing reactions of composite particles seems impossible. The reconstructed potential must reproduce the unitary S matrix below the inelastic threshold. In addition, it must reproduce an absorptive, nonunitary S matrix above the threshold. These requirements seem to be incompatible with energy-independent potentials derived from fixed-l inversion theories. However, for the shallow threshold (elastic nD scattering, the binding energy of the deuteron $E_{\text{c.m.}} \approx 2.226$ MeV), it was shown that Marchenko theory is applicable and produces energy-independent complex partial nD potentials [23,24]. To approximate the S-matrix unitary below the threshold and nonunitary (absorptive) above the point, they used a rational parametrization similar to that used for the case of a unitary matrix in Refs. [13–16]. Verification of the Marchenko theory in this particular case in a numerical experiment is not convincing. We analyzed the Marchenko theory [2,3] and found that most of the theory applies not only to $S(q)$-matrices unitary for $0 \leqslant q < -\infty$ but also to nonunitary S matrices. The Marchenko equation and our algebraic form of the Marchenko equation allow us to reconstruct energy-independent complex local partial potential from a partly unitary and partly nonunitary S matrix. We applied the developed formalism to analyze the ${}^1S_0\, NN$ data (up to $E_{\text{lab}} \approx 3$ GeV) and showed that these data are described by energy-independent complex partial potential. In the considered case, the inelasticity threshold is high ($E_{\text{lab}} \approx 280$ MeV), and it is not easy to achieve the required accuracy of the S-matrix rational parametrization used in Refs. [23,24]. The Fourier series theory ensures the convergence of our numerical procedure with an increase of the S-matrix approximation accuracy. Our results contradict conclusions of [25] for the NN interaction where they state that "... the optical potential with a repulsive core exhibits a strong energy dependence whereas the optical potential with the structural core is characterized by a rather adiabatic energy dependence..." On the contrary, we reconstructed from the scattering data local and energy-independent NN soft core OP.

II. MARCHENKO EQUATION IN AN ALGEBRAIC FORM

We write the radial Schrödinger equation in the form

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - V(r) + q^2\right)\psi(r,q) = 0. \tag{1}$$

Initial data for the Marchenko method [1] are

$$\{S(q), (0 < q < \infty), \tilde{q}_j, M_j, j = 1, \ldots, n\}, \tag{2}$$

where $S(q) = e^{2\imath\delta(q)}$ is a scattering matrix dependent on the momentum q. The S matrix defines asymptotic behavior at $r \to +\infty$ of regular at $r = 0$ solutions of Eq. (1) for $q \geqslant 0$; $\tilde{q}_j^2 = E_j \leqslant 0, E_j$ is jth bound state energy ($-\imath\tilde{q}_j \geqslant 0$); M_j is jth bound state asymptotic constant. The Marchenko equation is a Fredholm integral equation of the second kind:

$$F(x,y) + L(x,y) + \int_x^{+\infty} L(x,t)F(t,y)dt = 0. \tag{3}$$

We write the kernel function as

$$\begin{aligned} F(x,y) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} h_l^+(qx)[1 - S(q)]h_l^+(qy)dq \\ &\quad + \sum_{j=1}^{n_b} h_l^+(\tilde{q}_j x)M_j^2 h_l^+(\tilde{q}_j y) \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} h_l^+(qx)Y(q)h_l^+(qy)dq, \end{aligned} \tag{4}$$

where

$$Y(q) = \left[1 - S(q) - i\sum_{j=1}^{n_b} M_j^2(q - \tilde{q}_j)^{-1}\right]. \tag{5}$$

Solution of Eq. (3) gives the potential of Eq. (1):

$$V(r) = -2\frac{dL(r,r)}{dr}. \tag{6}$$

There are many computational approaches for the solution of Fredholm integral equations of the second kind. Many of the methods use an equation kernel's series expansion [26–32]. We also use this technique. Assuming the finite range R of the bounded potential function, we approximate the kernel function as

$$F(x,y) \approx \sum_{k,j=0}^{N} \Delta_k(x)F_{k,j}\Delta_j(y), \tag{7}$$

where $F_{k,j} \equiv F(kh, jh)$, and the basis functions are

$$\begin{aligned} \Delta_0(x) &= \begin{Bmatrix} 0 & \text{for} & |x| > h, \\ 1 + x/h & \text{for} & -h \leqslant x \leqslant 0, \\ 1 - x/h & \text{for} & 0 < x \leqslant h; \end{Bmatrix} \\ \Delta_n(x) &= \Delta_0(x - hn), \end{aligned} \tag{8}$$

where h is some step, and $R = Nh$. Decreasing the step h, one can approach the kernel arbitrarily close at all points. As a result, the kernel is presented in a separable form. We solve Eq. (3) substituting

$$L(x,y) \approx \sum_{j=0}^{N} P_j(x)\Delta_j(y). \tag{9}$$

Substitution of Eqs. (7) and (9) into Eq. (3), and taking into account the linear independence of the basis functions, gives

$$\sum_{m=0}^{N}\left(\delta_{jm}+\sum_{n=0}^{N}\left[\int_x^\infty \Delta_m(t)\Delta_n(t)dt\right]F_{n,j}\right)P_m(x) = -\sum_{k=0}^{N}\Delta_k(x)F_{k,j}. \tag{10}$$

We need values of $P_k(hp)\equiv P_{p,k}$ $(p,k=0,\ldots,N)$. In this case integrals in Eq. (10) may be calculated

$$\zeta_{nmp}=\int_{ph}^{\infty}\Delta_m(t)\Delta_n(t)dt=\frac{h}{6}(2\delta_{nn}(\delta_{np}+2\eta_{n\geqslant p+1}) + \delta_{n(m-1)}\eta_{n\geqslant p}+\delta_{n(m+1)}\eta_{m\geqslant p}). \tag{11}$$

Here, along with the Kronecker symbols δ_{kp}, symbols η_a are introduced, which are equal to one if the logical expression a is true, and are equal to zero otherwise. Considering also that $\Delta_k(hp)\equiv\delta_{kp}$, we finally get a system of equations

$$\sum_{m=0}^{N}\left(\delta_{jm}+\sum_{n=0}^{N}\zeta_{nmp}F_{n,j}\right)P_{pm}=-F_{p,j} \tag{12}$$

for each j, $p=0,\ldots,N$. Solution of Eq. (12) gives $P_k(hp)\equiv P_{p,k}$. Potential values at points $r=hp$ $(p=0,\ldots,N)$ are determined from Eq. (6) by some finite difference formula.

Next, we consider the case $l=0$, for which $h_l^+(qx)=e^{\imath qx}$ and

$$F(x,y)=F(x+y)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{\imath q(x+y)}Y(q)dq. \tag{13}$$

We approximate the kernel as follows:

$$F(x,y)=F(x+y)\approx\sum_{k=-2N}^{2N}F_{0,k}H_k(x+y), \tag{14}$$

where $F_{0,k}\equiv F(kh)$ as in Eq. (7) for $l=0$, and the used basis set is

$$H_0(x)=\begin{cases}0 & \text{for} \quad x<0,\\ 1 & \text{for} \quad 0\leqslant x\leqslant h,\\ 0 & \text{for} \quad x>h,\end{cases}$$
$$H_n(x)=H_0(x-hn). \tag{15}$$

The Fourier transform of the basis set Eq. (15) is

$$\tilde{\mathrm{H}}_k(q)=\int_{-\infty}^{\infty}\mathrm{H}_k(x)e^{-\imath qx}dx=\frac{\imath(e^{-\imath qh}-1)}{q}e^{-\imath qhk}. \tag{16}$$

The function $Y(q)$ may be presented as

$$Y(q)=\sum_{k=-2N}^{2N}F_{0,k}\tilde{\mathrm{H}}_k(q)=\sum_{k=-2N}^{2N}F_{0,k}\frac{\imath(e^{-\imath qh}-1)}{q}e^{-\imath qhk}. \tag{17}$$

The last relationship may be rearranged as

$$qY(q)=\imath\sum_{k=-2N}^{2N}F_{0,k}(e^{-\imath qh}-1)e^{-\imath qhk}=i\sum_{k=-2N+1}^{2N}(F_{0,k-1}-F_{0,k})e^{-\imath qhk}+\imath(-F_{0,-2N})e^{\imath qh2N}+\imath(F_{0,2N})e^{-\imath qh(2N+1)}. \tag{18}$$

Thus, the left side of the expression is represented as a Fourier series on the interval $-\pi/h\leqslant q\leqslant\pi/h$. Taking into account that $Y(-q)=Y^*(q)$, we get

$$\left.\begin{aligned}&-F_{0,-2N}=\tfrac{h}{\pi}\textstyle\int_0^{\pi/h}\mathrm{Im}(Y(q)e^{-\imath qh2N})qdq;\\ &F_{0,k-1}-F_{0,k}=\tfrac{h}{\pi}\textstyle\int_0^{\pi/h}\mathrm{Im}(Y(q)e^{\imath qhk})qdq \text{ for } k=-2N+1,\ldots,2N-1;\\ &F_{0,2N}=\tfrac{h}{\pi}\textstyle\int_0^{\pi/h}\mathrm{Im}(Y(q)e^{\imath qh(2N+1)})qdq.\end{aligned}\right\} \tag{19}$$

The system (19) is solved recursively from $F_{0,2N}$. Thus, the range of known scattering data defines the step value h and, therefore, the inversion accuracy. Calculation results for the potential function $V(r)=-3\exp(-3r/2)$ are presented in Figs. 1 and 2, where $h=0.04$, $R=4$. S matrix was calculated at points shown in Fig. 1 up to $q=8$. The S matrix was interpolated by a quadratic spline in the range $0<q<8$. For $q>8$ the S matrix was approximated as asymptotic $S(q)\approx\exp(-2iA/q)$ for $q>8$, where A was calculated at $q=8$.

III. ENERGY-INDEPENDENT COMPLEX $^1S_0$ NN POTENTIAL

Realistic potentials derived unambiguously from inverse theories should describe scattering data from zero to infinite energy. It seems that it is only possible if the available scattering data approach the asymptotic region below the relativistic region. It is unnecessary because relativistic two-particle potential models may be presented in the nonrelativistic form [33]. Another problem is the presence of closed channels whose characteristics are not known. It is usually assumed (for example, for an NN system) that below the inelasticity threshold, effects of closed channels can be neglected, and a real NN potential may describe the interaction of nucleons. This assumption is a consequence of the ingrained misconception that a complex potential corresponds to a nonunitary matrix. One can only assert that the S matrix is unitary for a real potential.

We have carefully analyzed the Marchenko theory [2,3] and found that it applies not only to unitary S matrices but

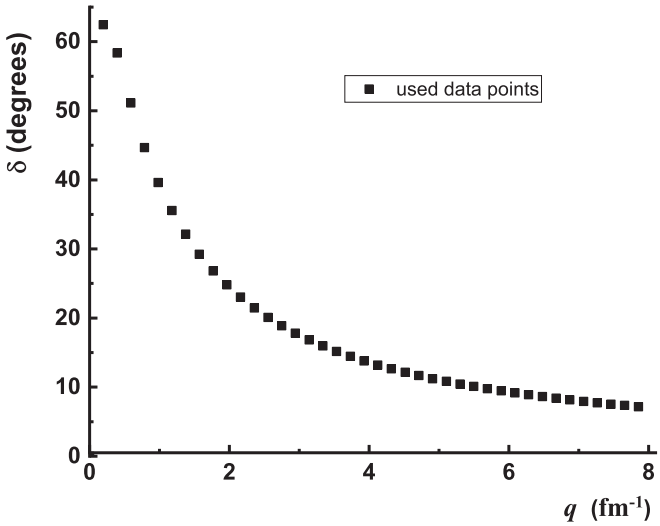

FIG. 1. Data used to reconstruct $V(r) = V_0 \exp(-ar)$, where $V_0 = -3$ fm$^{-2} = -124.5$ MeV, $a = 1.5$ fm^{-1}. Units correspond to the NN system.

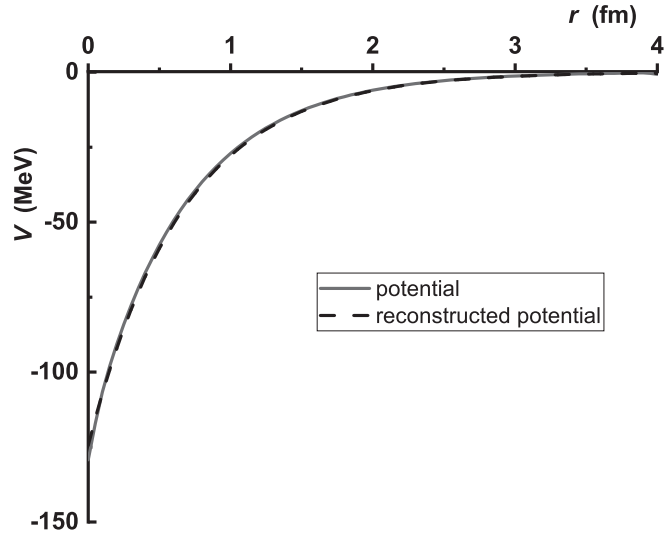

FIG. 2. Initial and reconstructed potentials: $V(r) = V_0 \exp(-ar)$, where $V_0 = -3$ fm$^{-2} = -124.5$ MeV, $a = 1.5$ fm^{-1}. Units correspond to the NN system.

also to nonunitary S matrices describing absorption. That is, the Marchenko theory Eqs. (1)–(6) and our algebraic form of the Marchenko Eqs. (7)–(18) allow to reconstruct local, and energy-independent OP from an absorptive S matrix and corresponding bound states' characteristics. We present an absorptive single partial channel S matrix on the q axis as

$$S(q) = \begin{cases} S_u(q) + S_n(q) & \text{for} \quad q > 0, \\ S_u^+(-q) - S_n^+(-q) & \text{for} \quad q < 0, \end{cases} \tag{20}$$

where superscript + means hermitian conjugation. For $q > 0$ we define

$$\begin{aligned} S_u(q) &= e^{2\imath\delta(q)}, \\ S_n(q) &= -\sin^2(\rho(q))e^{2\imath\delta(q)}, \end{aligned} \tag{21}$$

where $\delta(q)$ and $\rho(q)$ are phase shift and inelasticity parameter correspondingly. In this case we have instead of Eqs. (19) the following system:

$$\left.\begin{aligned} &-F_{0,-2N} = \tfrac{h}{\pi}\int_0^{\pi/h} q[\mathrm{Im}(Y_u(q)e^{-\imath qh2N}) - \imath\mathrm{Re}(S_n(q)e^{-\imath qh2N})]dq; \\ &F_{0,k-1} - F_{0,k} = \tfrac{h}{\pi}\int_0^{\pi/h} q[\mathrm{Im}(Y_u(q)e^{\imath qhk}) - \imath\mathrm{Re}(S_n(q)e^{\imath qhk})]dq \text{ for } k = -2N+1, \ldots, 2N-1; \\ &F_{0,2N} = \tfrac{h}{\pi}\int_0^{\pi/h} q[\mathrm{Im}(Y_u(q)e^{\imath qh(2N+1)}) - \imath\mathrm{Re}(S_n(q)e^{\imath qh(2N+1)})]dq, \end{aligned}\right\} \tag{22}$$

where

$$Y_u(q) = \left[1 - S_u(q) - i\sum_{j=1}^{n_b} M_j^2(q - \tilde{q}_j)^{-1}\right]. \tag{23}$$

IV. RESULTS AND CONCLUSIONS

We applied the developed formalism to analyze the $^1S_0$ NN data. As input data for the reconstruction, we used modern phase shift analysis data (SW16, single-energy solutions) up to 3 GeV [34,35]. We smoothed phase shift and inelasticity parameter data for $q > 3$ fm^{-1} by the following functions:

$$\begin{aligned} \delta(q) &\sim -54.56822/q^3 + 57.55296/q^2 - 15.36687/q, \\ \rho(q) &\sim 101.89881/q^3 - 80.13493/q^2 + 15.88984/q, \end{aligned} \tag{24}$$

where we fitted the coefficients by the least-squares method. Asymptotics (24) were used to calculate coefficients of Eqs. (19) with $h = 0.0125$ fm corresponding to $q_{\max} \approx 251.3$ fm^{-1}.

Results of our calculations show that these data are described by energy-independent complex partial potential (Figs. 3 and 4).

Thus, we presented a solution of the quantum scattering inverse problem for the zero orbital angular momentum, the

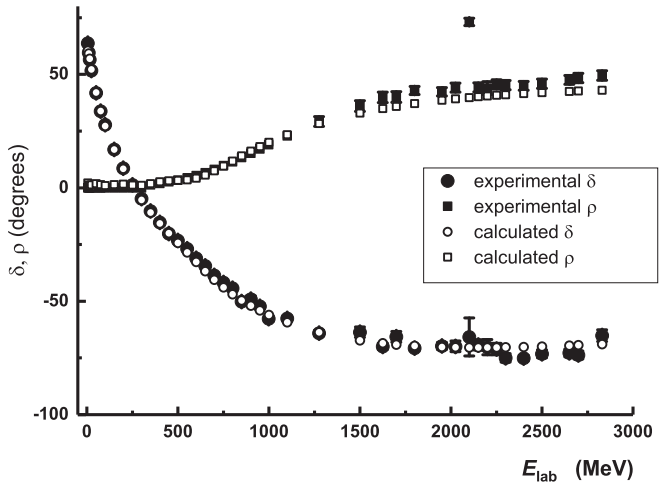

FIG. 3. Data used to reconstruct $^1S_0$ NN potential.

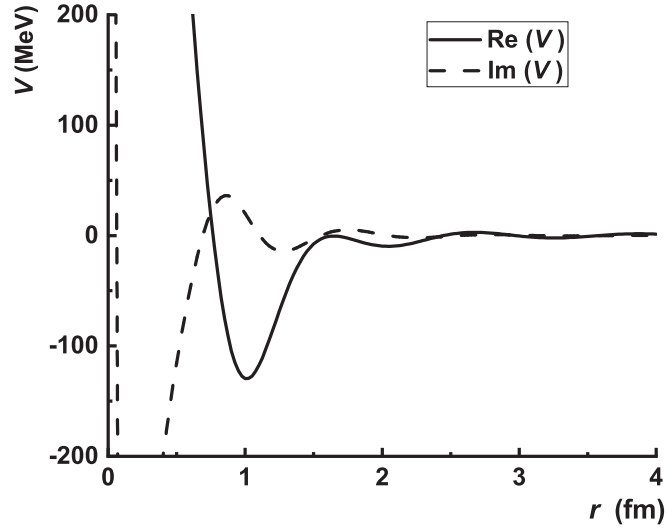

FIG. 4. Real and imaginary parts of the reconstructed $^1S_0$ NN potential.

algorithm of which is as follows. We set the step value h, which determines a required accuracy of the potential. From the scattering data, we determine $F_{0,k}$ from Eqs. (19) for unitary S matrix or from Eqs. (22) for nonunitary S matrix. Solution of Eqs. (12) gives values of $P_k(hp)$ $(p = 0, \ldots, N)$. Further, the values of the potential function (6) are determined by some finite difference formula. Expressions (7)–(14) give a method for the Marchenko equation's numerical solution for an arbitrary orbital angular momentum l, and may be generalized for a case of coupled channels.

Our results contradict conclusions of [25] claiming that the optical model $^1S_0$ NN potential with a repulsive core exhibits a strong energy dependence up to 3 GeV. On the contrary, we analyzed the $^1S_0$ NN data up to 3 GeV, and we showed that these data are described by optical model energy-independent partial potential with $\mathrm{Re}(\mathrm{V}(0)) \approx 14$ GeV and $\mathrm{Im}(V(0)) \approx 19$ GeV.

The reconstructed 1S0 NN complex potential may be requested from the author in the FORTRAN code.

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