An algebraic form of the Marchenko inversion.
Partial waves with orbital momentum $l \geq 0$

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We present a generalization of the algebraic method for solving the Marchenko equation (fixed-$l$ inversion) for any values of the orbital angular momentum $l$. We expand the Marchenko equation kernel in a separable form using a triangular wave set. The separable kernel allows a reduction of the equation to a system of linear equations. We obtained a linear expression of the kernel expansion coefficients in terms of the Fourier series coefficients of $q(1 - S(q))$ function ($S(q)$ is the scattering matrix) depending on the momentum $q$. The linear expression is valid for any orbital angular momentum $l$. The kernel expansion coefficients are determined by the scattering data in the finite range $0 \leq q \leq \pi/h$. In turn, the thus defined Marchenko kernel of the equation allows one to find the potential function of the radial Schrödinger equation with $h$-step accuracy.

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I. INTRODUCTION

The inverse problem (IP) of quantum scattering is essential for many physical applications. One of the most important such applications is the interparticle potential extraction from scattering data. The fixed-$l$ IP considered here is usually solved within the framework of Marchenko, Krein, and Gelfand-Levitan theories \cite{1-7}. Development of accurate and unambiguous methods for solving this problem remains a fundamental challenge \cite{8-12}. The ill-posedness of the IP significantly complicates its numerical solution.

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. Marchenko was successfully applied by H.V. von Geramb and H. Kohlhoff to recover nucleon-nucleon partial wave potentials from partial-wave analysis (PWA) data up to the inelastic threshold ($E_{lab} \approx 280$ MeV) \cite{13,14}. They used rational fraction expansions of partial $S$-matrices. This expansion allows one to obtain an analytical solution to the Marchenko equation (Bargmann-type potentials). Optical model nucleon-nucleon partial potentials were recovered from PWA data up to 3 GeV using a similar approach \cite{13,14}. It is not clear whether such a procedure converges with an increase in the $S$-matrix approximation accuracy. We approximate the integral kernel by a separable series in the triangular single wave set. Thus, the Marchenko equation is solved analytically as in Refs. \cite{13,14}. The expansion coefficients of the integral kernel are obtained from the Fourier series coefficients of the function $q(1 - S(q))$ on a finite range $0 \leq q \leq \pi/h$ of the momentum $q$. The $h$ value determines a required accuracy of the potential function.

II. MARCHENKO EQUATION IN AN ALGEBRAIC FORM

The radial Schrödinger equation is

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

The Marchenko equation \cite{2,3} is a Fredholm integral equation of the second kind:

$$F(x, y) + L(x, y) + \int_x^{+\infty} L(x, t) F(t, y) dt = 0 \tag{2}$$

The kernel function is defined by the following expression

$$F(x, y) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} h_i^+(qx)[1 - S(q)]h_i^+(qy) dq$$

$$+ \sum_{j=1}^{n} h_j^+ (\tilde{q}_j, x) M_j^2 h_j^+ (\tilde{q}_j, y)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} h_i^+(qx)Y(q)h_i^+(qy) dq \tag{3}$$

where $h_i^+(z)$ is the Riccati-Hankel function, and

$$Y(q) = \left[ 1 - S(q) - i \sum_{j=1}^{n} M_j^2 (q - \tilde{q}_j)^{-1} \right], \tag{4}$$

Experimental data entering the kernel are

$$\{ S(q), (0 < q < \infty), \tilde{q}_j, M_j, j = 1, \ldots, n \}, \tag{5}$$

where $S(q) = e^{2i\delta(q)}$ 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 $q \geq 0$; $\tilde{q}_j^2 = E_j \leq 0, E_j$ is $j$-th bound state energy ($-\tilde{u}_j \geq 0$); $M_j$ is $j$-th bound state asymptotic constant.

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The potential function of Eq. \((1)\) is obtained from the solution of Eq. \((2)\)

\[ V(r) = -2 \frac{dL(r,r)}{dr} \]  

(6)

Many methods for solving Fredholm integral equations use series expansion of the equation kernel. [23–30]. We also use this approach.

We introduce auxiliary functions:

\[ F_m(z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{iqz}Y(q)dq}{q^m}, \]  

(7)

and

\[ \hat{K}_{y,t}K_{x,t}F_{2t}(x+y) = \sum_{n_1,n_2=0}^{t} \frac{(2l-n_1)!(2l-n_2)!}{n_1!(l-n_1)!n_2!(l-n_2)!} (-2x)^{n_1-l}(2y)^{n_2-l}F_{2l-n_1-n_2}(x+y) \]

\[ = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{h}_1^\pm(qx)Y(q)\hat{h}_1^\pm(qy)dq \equiv F(x,y). \]  

(11)

Assuming the finite range \(R\) of the bounded potential function, we approximate \(F_m(x+y)\) as follows:

\[ F_m(x+y) \approx \sum_{k=-2N}^{2N} f_{m,k}H_k(x+y) \]  

(12)

\[ \approx \sum_{k,j=0}^{N} \Delta_k(x)f_{m,k+j}\Delta_j(y) \]  

(13)

where \(f_{m,k} \equiv F_m(kh)\), \(h\) is some step, and \(R = Nh\). The used basis sets are

\[ H_0(x) = \begin{cases} 1 & \text{if } 0 \leq x \leq h, \\ 0 & \text{otherwise} \end{cases} \]

\[ H_n(x) = H_0(x-hn). \]  

(14)

\[ \Delta_0(x) = \begin{cases} 1 - |x-0.25|/h & \text{if } |x-0.25| \leq h, \\ 0 & \text{otherwise} \end{cases} \]

\[ \Delta_n(x) = \Delta_0(x-hn). \]  

(15)

We use bases set \(\Delta_0(x)\Delta_j(y)\) shifted by vector \((0.25h,0.25h)\) compared to the set used previously [17,18]. The basis sets are illustrated in the (Fig. 1).Decreasing the step \(h\), one can approach \(F_m(x+y)\) arbitrarily close at all points with both sets. Coefficients \(f_{m,k}\) are same for both approximations.

The Fourier transform of the basis set Eq. \((12)\) is

\[ \hat{H}_k(q) = \int_{-\infty}^{+\infty} H_k(x)e^{-iqx}dx = \frac{t(e^{-iqh}-1)}{qe^{iqh}}. \]  

(16)

then

\[ \frac{d^kF_m(z)}{dz^k} = i^kF_{m-k}(z), \]  

(8)

We use transformations

\[ \hat{K}_{z,t}f(z) = z^{t+1} \left( \frac{1}{2} \frac{d}{dz} \right) \left[ z^{-1}f(z) \right] \]

\[ \equiv (-1)^t \sum_{n=0}^{\infty} \frac{(2l-n)!}{n!(l-n)!} (-2z)^{-n-l}e^{iqz}f(z). \]  

(9)

Thus \((22),\) Eqs. 10.1.23-10.1.26

\[ \hat{K}_{z,t}e^{\pm iqz} = q^t\hat{h}_t^\pm(qz). \]  

(10)

The Fourier transform of Eq. \((11)\) yields

\[ \frac{Y(q)}{q^m} \approx \sum_{k=-2N}^{2N} f_{m,k}\hat{H}_k(q) = \sum_{k=-2N}^{2N} f_{m,k} \frac{t(e^{-iqh}-1)}{qe^{iqh}}. \]  

(17)

We rearrange the last relationship

\[ Y(q)/q^{m-1} = t \sum_{k=-2N}^{2N} f_{m,k} (e^{-iqh}-1)e^{-iqhk} \]

\[ = t \sum_{k=-2N+1}^{2N} (f_{m,k-1} - f_{m,k}) e^{-iqhk} + t(-f_{m,-2N}) e^{iqh2N} \]

\[ + t(f_{m,2N}) e^{-iqh(2N+1)}. \]  

(18)

Thus, the left side of the expression is represented as a Fourier series on the interval \(-\pi/h \leq q \leq \pi/h\).

\[ f_{m,k-1} - f_{m,k} = \frac{ih}{2\pi} \int_{-\pi/h}^{\pi/h} Y(q)e^{iqhk}dq. \]  

(19)

for \(k = -2N,\ldots,2N\). We solve the system \((19)\) recursively from \(k = 2N+1\) \((f_{m,2N+1} = 0)\) for fixed \(m:\)

\[ f_{m,k} = \frac{ih}{2\pi} \int_{-\pi/h}^{\pi/h} e^{iq(k+1)} \left(1 - e^{iq(2N-k+1)}\right) \frac{Y(q)dq}{(1-e^{iqh})q^{m-1}}. \]  

(20)
FIG. 1. The basis set \( H_n \equiv H_n(x+y) \) (Eq. (14)) is shown as trapezoid (triangle for \( n = 0 \) ) domains where \( H_n(x+y) = 1 \), and elsewhere \( H_n(x+y) = 0 \). The domains are bounded by lines \( x = 0 \), \( y = 0 \), and \( x + y = h(n-1) \). The basis set \( \Delta_i(x)\Delta_j(y) \) (Eq. (15)) is shown as projections (points) of the corresponding regular square pyramids apexes on the \( xy \)-plane. \( \Delta_i(x)\Delta_j(y) = 1 \) at \( x = (0.25+i)h, y = (0.25+j)h \) (apex of the \( ij \)-pyramid). The pyramids bases are \((2h \times 2h)\) squares on the \( xy \)-plane with sides parallel to the \( x \) and \( y \) axes. On sides of the corresponding square (as well as outside them) \( \Delta_i(x)\Delta_j(y) = 0 \).

Thus, the range of known scattering data defines value of \( h \) and, therefore, the inversion accuracy.

We solve Eq. (2) substituting

\[
L(x, y) \approx \sum_{j=0}^{N} P_j(x) \Delta_j(y) \tag{24}
\]

Substitution of Eqs. (21) and (24) into Eq. (2), and linear independence of the basis functions give

\[
\sum_{m=0}^{N} \left( \delta_{jm} + \sum_{n=0}^{N} \left[ \int_{max((m+0.25)h,(n+0.25)h)}^{max((m+0.25)h,(n+0.25)h)} \Delta_m(t) \Delta_n(t) \, dt \right] F_{n,j} \right) P_m(x) = - \sum_{k=0}^{N} \Delta_k(x) F_{k,j} \tag{25}
\]

We define

\[
\zeta_{n \, m \, p} = \int_{(p+0.25)h}^{max((m+0.25)h,(n+0.25)h)} \Delta_m(t) \Delta_n(t) \, dt = \frac{h}{6} \left( 2 \delta_{n \, m} (2 \eta_{n \geq p+1}) + \delta_{n(m-1)} \delta_{n(p+1)} + \delta_{n(m+1)} \eta_{n \geq p} \right) \tag{26}
\]
where $\delta_{kp}$ are the Kronecker symbols $\delta_{kp}$, and

$$\eta_a = \begin{cases} 1 & \text{if } a \text{ is true}, \\ 0 & \text{otherwise}, \end{cases}$$

(27)

Since $\Delta_k(hp) \equiv \delta_{kp}$, we finally get a system of equations

$$\sum_{m=0}^{N} \left( \delta_{jm} + \sum_{n=p}^{N} \zeta_{nm} F_{nj} \right) P_{p,m} = -F_{pj},$$

(28)

for $P_k(h(p + 0.25)) \equiv P_{p,k} \ (p, k = 0, \ldots, N) \ (j, p = 0, \ldots, N)$.

Solution of Eq. 28 gives $P_{p,k}$. We calculate potential values at points $r = hp \ (p = 0, \ldots, N)$ from Eq. 28 by some finite difference formula.

III. RESULTS AND CONCLUSIONS

We tested the developed approach by restoring the potential function $V(r) = -3 \exp(-3r/2)$ from the corresponding scattering data. Results are presented in Figs. 2-3 where $h = 0.04$, $R = 4$. The input $S$-matrix was calculated at points shown in Fig. 2 up to $q = 8$. The $S$-matrix was interpolated by a quadratic spline in the range $0 < q < 8$. The $S$-matrix was approximated as asymptotic $S(q) \approx \exp(-2i\alpha/q)$ for $q > 8$, where $\alpha$ was calculated at $q = 8$.

Thus, we presented a general solution of the quantum scattering inverse problem for the any orbital angular momentum $l$. The algorithm of the solution is as follows. We set the step value $h$, which determines a required accuracy of the potential. From the experimental data, we determine $P_{k,j}$ using Eqs. 23. Solution of Eqs. 28 gives values of $P_{k}(hp) \ (p = 0, \ldots, N)$. The values of the potential function $V$ are determined by some finite difference formula. Expressions 21-28 give a method for the Marchenko equation’s numerical solution for an arbitrary orbital angular momentum $l$.

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