The inverse scattering problem at fixed energy based on the Marchenko equation for an auxiliary Sturm–Liouville operator

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Abstract

A new approach is proposed to the solution of the quantum mechanical inverse scattering problem at a fixed energy. The method relates the fixed energy phase shifts to those arising in an auxiliary Sturm–Liouville problem via the interpolation theory of the Weyl–Titchmarsh $m$-function. Then a Marchenko equation is solved to obtain the potential. As an illustration test results are shown including the reconstructions of the piecewise constant and Coulomb-type potentials. A byproduct of the new framework is a demonstration of the connection found between the Gelfand–Levitan and Marchenko formalisms.

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1. Introduction

Inverse scattering theory based on the spectral problem of the $s$-wave Schrödinger equation has been worked out in the 1950s [1–3] and developed further in the 1980s with the aim of applying it to problems in atomic, nuclear and subnuclear physics [4, 5]. This type of inverse scattering theory provides the fixed-$l$ potentials derived from input spectral data (eigenvalues and normalization constants) as well as scattering phase shifts $\delta_l(k)$ known for all energy $E = (\hbar k)^2/(2m)$.

Another type of inverse method was developed in the 1960s [6–8] to recover fixed energy (or fixed-$k$) potentials from a set of phase shifts $\{\delta_{l_{\text{max}},0,1,\ldots}\}$ given at a particular wave number $k$. For practical analysis of the measured scattering angular distribution, the modified Newton–Sabatier (mNS) method proved to be a powerful procedure [9, 10]. Also the Cox–Thompson method, developed in the last decade for practical problems, offers results with nice physical
properties such as the non-singular behavior of the potential at the origin and demanding only a finite set of input data \([11, 12]\) to recover the potentials.

In this paper a third type of inverse method will be presented. It belongs to the fixed energy category requiring a set of phase shifts at one energy but uses spectral information belonging to an auxiliary problem resulting from a Liouville transformation. The new method bears a resemblance to a recently proposed procedure by Horvath and Apagyi (HA) \([13]\) (developed further and generalized in \([14]\)). However, whereas the latter obtained results from the Gelfand–Levitan (GL) equation by solving a moment problem, our present method makes use of the Marchenko integral equation in connection with the auxiliary spectral problem.

Because in all physical problems the potential can be known beyond a finite radius \(r = a < \infty\), it is enough for a practical inverse scattering method to seek the inverse potential \(q(r)\) within a finite range \(0 < r < a\) (beyond which for instance \(q(r > a) \equiv 0\) is assumed). The HA method applies a variable transformation \(r = a \exp(-x)\) and thereby casts the finite interval \([0, a]\) in \(r\) to the half line \([\infty, 0]\) in \(x\). The inverse potential is obtained from the derivative of the transformation kernel \(K(x, x)\) which is determined from the GL equation within the interval \([x, 0]\). This means that the potential \(q(r')\) will be known in the interval \([r, a]\) corresponding to the transformed interval \([x, 0]\). In order that the potential be known at the origin \(r = 0\), the kernel \(K(x, x)\) should be calculated accurately as \(x \to \infty\). This, however, is difficult in view of the restricted number of input data.

If one tries, in contrast to the HA method, to solve the inverse problem by using the Marchenko integral equation, then one obtains the transformation kernel \(K(x, x)\) within the interval \([\infty, x]\) which suggests that a more accurate potential value can be expected at the origin \(r = 0\) than in the case of the HA method. As we will see, this task is feasible by straightforward numerical evaluation of certain integrals. The basis of the theory remains the same as in the HA method, i.e. the recognition of the fact that the input set of fixed energy phase shifts \(\{\delta_l\}_{l=0,1,\ldots,\lambda_{\text{max}}}\) is related to the \(m\)-function of the auxiliary (Liouville-transformed) inverse spectral problem. While the HA method leads to the solution of a moment problem where the moments are calculated also from the input phase shifts, the present procedure requires the Jost function to be determined for the auxiliary problem. Restricting ourselves to the simple case when there exists no bound state in the auxiliary spectral problem, we present some illuminating examples and point out the necessary future development related to the generic case.

In section 2 the formalism will be outlined. Here an interesting (and hitherto seemingly overlooked) connection between the GL and Marchenko equations is also discussed together with an adopted approximation of the \(m\)-function. Section 3 contains the illustrative examples of the piecewise constant and Coulomb-type potentials. For the former analytic solutions are known for the auxiliary (transformed) problem, while for the latter such information is not available. Nevertheless, in all cases we also present the results which are obtained without the use of the analytic solutions. These examples can help us to assess the accuracy of the underlying numerical procedure and the approximations used. Finally, section 4 is devoted to the discussion and conclusion.

2. Theory

Consider the radial Schrödinger equation (in units of \(\hbar^2/2m = 1\))

\[
r^2 \left[ \frac{d^2}{dr^2} + q(r) - k^2 \right] \psi(r) = -l(l+1)\psi(r), \quad r \in (0, a),
\]

which, after a Liouville-transformation

\[
y(x, -(l+1/2)^2) = r^{-1/2} \psi(r), \quad r = a e^{-x},
\]

where \(a\) is related to the physical radius \(a \equiv \exp(x_0)\) by the relation \(x_0 = \ln(a)\).
takes the form of a standard Sturm–Liouville (SL) or \( s \)-wave Schrödinger eigenvalue equation
\[
\left[ -\frac{d^2}{dx^2} + Q(x) \right] y(x, \lambda) = \lambda y(x, \lambda) \quad x \in (0, \infty)
\]  
(3)
with the transformed potential
\[
Q(x) = r^2(q(r) - k^2), \quad r = a e^{-x}.
\]  
(4)
The \( m \)-function of the SL operator
\[
\left[ -\frac{d^2}{dx^2} + Q(x) \right]
\]
is known at the point values \( \lambda = -(l + 1/2)^2, \ l = 0, 1, 2, \ldots, l_{\text{max}} \), in terms of the phase shifts \( \delta_l \) generated by the potential \( q(r) \) (with \( q(r > a) = 0 \)) at a fixed wave number \( k \), because the following relation \[13\] holds:
\[
m(-(l + 1/2)^2) = \frac{y'(0, -(l + 1/2)^2)}{y(0, -(l + 1/2)^2)} = \frac{\lambda y(0, -(l + 1/2)^2)}{y(0, -(l + 1/2)^2)}
\]
\[
= -ka \frac{J_{l+1/2}(ka) - \tan \delta_{l+1/2}(ka)}{J_{l+1/2}(ka) - \tan \delta_{l+1/2}(ka)}.
\]  
(5)

The Marchenko equation reads
\[
\mathcal{F}(x + y) + \mathcal{K}(x, y) + \int_x^\infty \mathcal{K}(x, t) \mathcal{F}(t + y) \, dt = 0 \quad (x \leq y)
\]  
(6)
for the transformation kernel \( \mathcal{K}(x, y) \) from which the wavefunction can be obtained by the Povzner–Levitan representation as
\[
y(x, \lambda) = \frac{1}{\sqrt{\lambda}} \sin(\sqrt{\lambda} x) + \frac{1}{\sqrt{\lambda}} \int_x^\infty \mathcal{K}(x, y) \sin(\sqrt{\lambda} y) \, dy.
\]  
(7)
This assumes a Dirichlet boundary condition
\[
y(0, \lambda) = 0, \quad y'(0, \lambda) = 1,
\]  
(8)
and implies the relation
\[
Q(x) = -2 \frac{d\mathcal{K}(x, x)}{dx}
\]  
(9)
between the potential and the transformation kernel which can be obtained upon insertion of (7) into (3).

The input function \( \mathcal{F}(x) \) to the Marchenko equation (6) contains contributions of the bound states (discrete spectrum) and scattering states (continuous spectrum)
\[
\mathcal{F}(x) = \sum_{j=1}^B \frac{1}{m_j} e^{-\lambda_j x} + \frac{1}{2\pi} \int_{-\infty}^{\infty} \left( 1 - e^{2i\Delta(\kappa)} \right) e^{ikx} \, dk
\]  
(10)
where \( B \) denotes the number of the bound states supported by the potential \( Q(x) \), and \( \lambda_j < 0, m_j > 0 \) denote, respectively, the eigenvalues and normalization constants of the eigenfunctions \( y(x, \lambda_j) \) belonging to the Schrödinger equation (3). The phase function \( \Delta(\kappa) \) corresponds to the \( (s \)-wave) phase shift arising when a particle with wave number \( \kappa \) is scattered by the hypothetical potential \( Q(x) \).

\( \Delta(\kappa) \) is related to the modulus of the Jost function \( f^+(\kappa) = |f^+(\kappa)| \) by the dispersion relation \[15\]
\[
\Delta(\kappa) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\log |f^+(\kappa')| \, dk'}{k' - \kappa},
\]  
(11)
The modulus, in turn, is connected to the \( m \)-function by
\[
|f^+(\kappa)|^2 = \lim_{\varepsilon \to 0^+} \frac{1}{\text{Im} \, m(\kappa^2 + i\varepsilon)}, \quad \kappa > 0.
\] (12)
The latter equality can easily be proved by using the reflection principle \( m(z) = m(\overline{z}) \) and the Wronskian property
\[
f^-(f^+)' - (f^-)' f^+ = 2ik
\]
of the two linearly independent Jost functions \( f^\pm \).

In summary, if the \( m \)-function is known near the positive half axis of its argument, then one can determine the potential \( Q \) (or \( q \)).

2.1. Connection to the Regge–Loeffel–Sabatier–Levitan framework

Let us transform back both the input and transformation kernels into the \( r \)-space. Performing the transformation \( x = -\log \frac{r}{a} \) and using the notations
\[
\tilde{K} (r, r') = K \left( -\log \frac{r}{a}, -\log \frac{r'}{a} \right)
\]
\[
\tilde{F} (r, r') = F \left( -\log \frac{r}{a} - \log \frac{r'}{a} \right)
\]
we obtain from the Marchenko integral equation (6) the following equation of the GL type\(^2\):
\[
\tilde{F} (r, r') + \tilde{K} (r, r') + \int_0^r \tilde{K} (r, r'') \tilde{F} (r'', r') \frac{dr''}{r'} = 0 \quad (r \geq r').
\] (15)
The (wanted) fixed energy potential can also be calculated as
\[
q (r) = \frac{2}{r} \frac{d \tilde{K} (r, r)}{dr} + k^2.
\] (16)
Note that equations (15) and (16) are exactly the same as those appearing in the Regge–Loeffel–Sabatier–Levitan framework of inverse scattering theory at fixed energy (see chapter 5 of [15] where \( \tilde{F} (r, r') = F_{\lambda_1, k_{\lambda_1}} (r, r') \) with \( k = 1 \)). These authors discussed that their method requires the fixed energy phases \( \delta_l \) for \( l \in i\mathbb{R} \) (an obviously non-physical domain) and at the time when a relevant extrapolation theory was not available. In contrast, our new method relates the exact input kernel to the fixed energy phase shifts through the \( m \)-function of the auxiliary Schrödinger operator, a function whose extrapolation/interpolation is now possible.

2.2. Interpolation of the \( m \)-function

Returning to equation (12), we see that the \( m \)-function must be evaluated at argument values which are different from those offered by the input data as showed by equation (5). Therefore, we must use interpolation theories for calculating the \( m \)-function. These interpolation theories all rely upon a consequence of Simon’s representation of the \( m \)-function [16], which states that the \( m \)-function can be represented essentially by a Laplace transform. For both the Fourier and the Laplace transforms there are known interpolation formulas; here the latter, a recent work of Rybkin and Tuan [17], will be adopted for our purposes.

Thus, we shall use the following interpolation formula for the \( m \)-function (special case of theorem 5 of [17]):
\[
m (\lambda) \approx i \sqrt{\lambda} + \sum_{n=0}^{\lambda_{\text{max}}} c_n (-i \sqrt{\lambda}) \sum_{m=0}^{n} \omega_m (m (-\omega_m^2) + \omega_m)
\] (17)
\(^2\) Note that equation (15) can be transformed to the standard GL form by a further transformation of \( \tilde{F} \) and \( \tilde{K} \).
with \( \omega_n = m + \frac{1}{2} \) and

\[
c_n(x) = (2n+1)\left(\frac{1}{2} - x\right)_n, \quad a_{nm} = \frac{(-n)_m (n+1)_m}{(m!)^2}.
\]

(18)

\((x)_n\) is the Pochhammer symbol:

\[
(x)_n = x(x+1) \cdots (x+n-1), \quad (x)_0 = 1.
\]

The interpolation formula applies for locally absolute integrable potentials. Its domain of convergence depends on the specific features of the potential and we suppose it to be valid on the whole complex \( \lambda \)-plane throughout the subsequent numerical examples.

3. Applications

As an illustration of the above theory we show first examples where solutions of the transformed problem are known analytically. Such are the cases of the constant potentials and the step potentials. Then we exhibit some results for cases where the solution of the transformed problem is not at hand, and thus the interpolation formula (17) must be applied.

The selected example for the latter case is the shifted truncated Coulomb potential problem, whose reconstruction is known to be a challenging exercise for any method developed to solve the inverse problem of quantum mechanical scattering theory [18].

3.1. Constant potentials

Let us reconstruct first the constant potential

\[
q(r) = \begin{cases} q_0 & \text{for } r \leq a \\ 0 & \text{for } r > a \end{cases}
\]

(20)

which generates the transformed potential

\[
Q(x) = -se^{-2x}, \quad s = a^2(k^2 - q_0).
\]

(21)

The solution of the transformed Schrödinger equation (3) becomes

\[
\psi(x) = C_1 J_{\kappa}(\sqrt{s}e^{-x}) + C_2 J_{-\kappa}(\sqrt{s}e^{-x})
\]

(22)

from which the \( m \)-function being the logarithmic derivative of the unique \( L^2 \) solution at the origin takes the form

\[
m(\lambda) = \frac{\psi'(0)}{\psi(0)} = -\sqrt{s} \frac{J_{-\kappa}(\sqrt{s})}{J_{-\kappa}(\sqrt{s})}.
\]

(23)

The \( (s) \)-wave phase shift belonging to equation (3) can be expressed from (22) as \( \kappa = \sqrt{\lambda} \)

\[
\Delta(k) = \text{tanh}^{-1}\left(1 - \frac{4^{s-k^2} \Gamma(i\kappa^2 + 1)J_{-\kappa}(\sqrt{s})}{\Gamma(1-i\kappa)J_{-\kappa}(\sqrt{s})}ight).
\]

(24)

Now, we are in the position to perform the calculation at three different levels. Either we can use the exact \( m \)-function (23) or the exact phase function (24) or the interpolation formula (17) for an approximate calculation of the \( m \)-function using the set of input phase shifts \( \{\delta_l\} \). Results of the three performances are depicted in figure 1 (left panel) for two constant potentials with \( q_0 = 1.2 \) and \( a = 1 \) (dashed lines), and \( q_0 = 0.5 \) and \( a = 0.75 \) (continuous lines). The wave number in each case is chosen to be \( k = 1 \). Eleven input phase shifts \( (n_{\text{max}} = 10) \) were used when the interpolation formula was applied (see figure 1).
Figure 1. Recovery of the constant (20) with parameters $q_0 = 1.2$, $a = 1$ (dashed lines) and $q_0 = 0.5$, $a = 0.75$ (continuous lines) and step (25) potentials using exact input $m$-function (upper row), exact phase shift functions (middle row) and fixed energy phase shifts (lower row). The HA results are shown as a dotted line. (For further details see the text.)

Apparently, while there is no practical difference between the calculations performed at the levels with exact $m$-function and $\Delta$-function, the weakest point appears to be the use of the interpolation formula. As a comparison we have included in figure 1 as a dotted line the result given by the HA method without bound states [14]. One can observe that in the case of the HA method there appear nonphysical oscillations as the radius goes to zero, proving the superiority of the new procedure at the zero bound state level.

3.2. Step potential

As a next example we reconstruct the step potential

$$q(r) = \begin{cases} 
q_1 & \text{for } r \leq r_0 \\
q_2 & \text{for } r_0 \leq r \leq a \\
0 & \text{for } r > a,
\end{cases}$$

with parameters $q_1 = 1.25$, $q_2 = 1.125$, $r_0 = 1$, $a = 2$. The transformed potential looks like

$$Q(x) = \begin{cases} 
-s_2 e^{-2x} & \text{for } x \leq x_0 \\
s_1 e^{-2x} & \text{for } x > x_0,
\end{cases}$$

and the transformed Schrödinger equation (3) admits the solution

$$\psi(x) = \begin{cases} 
C_1 J_{i\sqrt{s_2}}(\sqrt{s_2} e^{-x}) + C_2 J_{-i\sqrt{s_2}}(\sqrt{s_2} e^{-x}), & x \leq x_0, \\
D_1 J_{i\sqrt{s_1}}(\sqrt{s_1} e^{-x}) + D_2 J_{-i\sqrt{s_1}}(\sqrt{s_1} e^{-x}), & x \geq x_0.
\end{cases}$$

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From this the $m$-function takes the form
\[
m(\lambda) = \frac{J_{\lambda}(\sqrt{\lambda})W[1,2]}{J_{\lambda}(\lambda)W[1,2]} - \frac{J_{-\lambda}(\sqrt{\lambda})W[1,2]}{J_{-\lambda}(\lambda)W[1,2]}
\]
(28)
where
\[
W[1, 2] = W[J_{\lambda}(\lambda)W[1, 2] \cdot J_{\lambda}(\lambda)e^{\lambda})], \quad J_{\lambda}(\lambda) = J_{\lambda}(\sqrt{\lambda})
\]
(29)
with the Wronskian $W[f, g](x) = f(x)g(x) - f'(x)g(x)$. The $s$-wave phase function can be written as ($\lambda = \sqrt{\lambda}$)
\[
\Delta(\lambda) = i \tanh^{-1} \left( \frac{1 + \frac{4s_\lambda^{\lambda+1}G_{\lambda+1}}{1 - i}}{1 - \frac{4s_\lambda^{\lambda+1}G_{\lambda+1}}{1 - i}} \right).
\]
(30)
with
\[
H = \frac{J_{-i\lambda}(\sqrt{\lambda})W[1, 2]}{J_{-i\lambda}(\sqrt{\lambda})W[1, 2]} - \frac{J_{i\lambda}(\sqrt{\lambda})W[1, 2]}{J_{i\lambda}(\sqrt{\lambda})W[1, 2]}
\]
(31)

The results obtained at $k = 1$ are depicted in figure 1 (right panel) at various levels of approximation indicated. Also in this case, the less satisfactory result is obtained by the use of the interpolation formula (with $l_{\text{max}} = 20$) and, as a comparison, the result of the HA method is shown by a dotted line. Compared to the HA the new method again seems to be better.

3.3. Shifted truncated Coulomb potential

We now reconstruct the shifted truncated Coulomb potential defined by
\[
q(r) = \begin{cases} 
A/r - A/a & \text{for } r \leq a \\
0 & \text{for } r > a
\end{cases}
\]
(32)
with the parameters $a = 2$ and $A = 1$. Requiring a continuous logarithmic derivative of the associated wavefunctions leads to the formula for the input phase shifts
\[
\delta_i = \tan^{-1} \left( \frac{u_i'(ka) - C_iu_i(ka)}{v_i'(ka) - C_iv_i(ka)} \right),
\]
(33)
\[
C_i = \frac{k_B F_i(k_Ba, \eta)}{F_i(k_Ba, \eta)},
\]
(34)
with $k_B^2 = k^2 + A/a$, $\eta = A/(2k_B)$, and the usual $u_i$, $v_i$ Riccati–Bessel and $F_i$ Coulomb wavefunctions.

Because in this case there is no analytic result to the $m$-function or phase function $\Delta$ of the transformed problem (3), we have only the possibility to apply the Rybkin–Tuan formula (17) for calculating the $m$-function. The calculation has been performed at two different settings of the wave number $k = 0.8$ and $k = 1.0$. The corresponding input phase shifts calculated from equation (33) are listed in table 1. The results exhibited in figure 2 show an improvement of the procedure with increasing energy as more input phase shifts are involved, according to the semiclassical thumb rule $l_{\text{max}} \approx k_a$. Although the reproductions show a generic departure from the exact result in both cases (attributed to the shortcomings with use of the interpolation formula (17)), the trends are captured well. Here we cannot make a consistent comparison to the HA results because of the difference in the bound states of the auxiliary problem (1 and 0 bound states are generated in the HA and the present method, respectively).
4. Discussion and conclusion

Using the Marchenko integral equation (6) a new fixed energy method was presented to solve the inverse problem of quantum mechanical scattering theory by recovering potentials bounded to a finite range \( r \in [0, a] \). The method consists of Liouville-transforming the radial variable and the radial wavefunction (see equation (2)), and thus casting the inverse problem of scattering at fixed energy to the inverse spectral problem of a Sturm–Liouville operator on the half line \( x \in [\infty, 0] \). The possibility of doing this is based on the observation that the set of input phase shifts can be related to the \( m \)-function of the transformed problem [13].

In [13, 14] the GL equation has been used for solving the transformed problem, from which one recovers the potential in the interval \( \lim_{r \to a} [r, a] \). However, one is frequently interested in the behavior of the potential at the origin \( r = 0 \); therefore, in this work we propose usage of the Marchenko equation, because it recovers the potential (after back-transforming it) in the interval \( \lim_{r \to 0} [0, r] \). In view of the finite number of input data it has been assumed that the present method recovers the potential at the origin more accurately than the one proposed in [13] (HA method). This assumption is based on the following argument. The HA method has been formulated to accommodate the usage of input phase shifts by solving a moment problem; there is no room (yet, in the present stage of the formalism) to offer any entry points for the usage of exact (intermediate) input data, such as the \( m \)-function and/or the \( \Delta \) phase function. The moment problem can only be solved approximately even if these intermediate quantities were at hand. This feature and the requirement of knowledge of the transformation kernel on the (infinite) half line leads the HA method always to produce a worse (re)construction of the potential at the origin.

By studying simple examples we have shown that it is indeed so. In the cases where we know the exact \( m \)-function (or phase-function), the present procedure is capable to recover the potential at the origin exactly while the HA method is not.

The present method is conducted on a path paved by analytical formulas derived from standard scattering and spectral theory. It offers explicit entry points for applying exact
intermediate input data (if known). However, in proportion to the moment problem of [13], the present technique also needs to use approximations in realistic situations. The determination of the \( m \)-function from the input data phase shifts \( \{ \delta_l \} \) (related to the wanted fixed energy potential \( q(r) \)) can be done through the application of the interpolation theory of the \( m \)-function, an up-to-date topic of mathematical physics. We have adopted the theory worked out by Rybkin and Tuan [17], which is an important development based on an earlier study [19].

Closer inspection of their formula (17) reveals that, strictly speaking, it might not be applicable to our purpose: the choice \( \omega_m = m + 1/2 \) in their framework is only permitted for cases when the norm of the potential \( Q \) is small enough and even then the domain of convergence of equation (17) is such that it excludes the vicinity of the positive real half-line. However these restrictions originate from bounds on the domain of convergence of Simon’s formula for the \( m \)-function (overestimating the potential by a constant) and are expected to be relaxed when the true exponential decay of \( Q \) is taken into account. The fact that our numerical examples recover reasonable results (see figures 1 and 2) indicates this. At the same time we recognize that an important development of the present inverse method relies upon the more thorough examination of Simon’s representation and the interpolation theory of the \( m \)-function.

Another important development of the present method would be the inclusion of the intermediate bound states into the procedure. This could be done within the above formalism but we left this investigation to a future work.

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