A discrete version of the inverse scattering problem and the $J$-matrix method

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Abstract

The problem of the Hamiltonian matrix in the oscillator and orthogonalized Laguerre basis construction from a given $S$-matrix is treated in the context of the algebraic analogue of the Marchenko method.

1. Introduction

The $J$-matrix [1] theory of scattering is based on the fact that the $\ell$th partial wave kinetic energy or the Coulomb Hamiltonian $H^0$ is represented in a certain square-integrable basis set by an infinite symmetric tridiagonal matrix. In the harmonic oscillator and the Laguerre basis sets $\{\phi_n^\ell\}_{n=0}^\infty$ the eigenvalue problem for $H^0$ can be solved analytically. The $J$-matrix method yields an exact solution to a model scattering Hamiltonian where the given short-range potential is approximated by truncating in a finite subset $\{\phi_n^\ell\}_{n=0}^{N-1}$.

In [2, 3] an inverse scattering formalism within the $J$-matrix method has been proposed, where the matrix $\|V_{n,m}\|$ of the potential

$$V_\ell(r, r') = \hbar \omega \sum_{n,m=0}^{N-1} \phi_n^\ell(x) V_{n,m} \phi_m^\ell(x')$$

(1)

with the oscillator form factors

$$\phi_n^\ell(x) = (-1)^n \sqrt{\frac{2n!}{\rho \Gamma(n + \ell + \frac{1}{2})}} x^{\ell+1} e^{-x^2/2} L_n^{\ell+1/2}(x^2)$$

(2)

is determined from a given $S$-matrix. Here, $x = r/\rho$ is the relative coordinate in units of the oscillator radius $\rho = \sqrt{\hbar/\mu \omega}$, where $\mu$ is the reduced mass.

Obviously a correlation can be made between the $J$-matrix method and a discrete model of quantum mechanics, within which a finite-difference Schrödinger equation is used. As a result, the $J$-matrix versions of the Gel’fand–Levitan–Marchenko method algebraic analogue can be formulated. For instance, the $J$-matrix method formally and computationally is quite

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similar to the $R$-matrix theory. It is this analogy that the previous $J$-matrix version of inverse scattering theory [2–4] (see also [5]) leans upon. Within the $J$-matrix approach the discrete representation of the Green function in finite subspace of the basis functions $\{\phi_n^{(\ell)}\}_{n=0}^{N-1}$

$$G(\epsilon) = (\epsilon I - h)^{-1}$$  

(3)

is used. Here, $I$ is identity matrix and $h$ is the truncated Hamiltonian matrix of order $N$ in the oscillator basis (2). We measure the energy $E$ in the units of the oscillator basis parameter $\hbar\omega$, \(\text{i.e. } E = \hbar\omega \epsilon\) and $\epsilon = q^2/2$, where $q$ is the dimensionless momentum: $q = k\rho$. In particular, the element $[G(\epsilon)]_{N-1,N-1} \equiv \mathcal{P}_N(\epsilon)$ can be presented in the two rational forms [2, 6]:

$$\mathcal{P}_N(\epsilon) = \prod_{j=0}^{N-2} (\epsilon - \mu_j) \prod_{j=0}^{N-1} (\epsilon - \lambda_j)$$  

(4)

where $\{\lambda_j\}_{j=0}^{N-1}$ and $\{\mu_j\}_{j=0}^{N-2}$ satisfy the interlacing property

$$\lambda_0 < \mu_0 < \lambda_1 < \cdots < \lambda_{N-2} < \mu_{N-2} < \lambda_{N-1},$$

and [7]

$$\mathcal{P}_N(\epsilon) = \sum_{j=0}^{N-1} \frac{Z_{N-1,j}^2}{\epsilon - \lambda_j}.$$  

(5)

Here, $\{Z_{N-1,j}\}_{j=0}^{N-1}$ are the elements of the $N$th row of the eigenvector matrix $Z$ of the truncated Hamiltonian matrix $h$. The sets $\{\lambda_j\}_{j=0}^{N-1}$, $\{\mu_j\}_{j=0}^{N-2}$ and $\{\lambda_j\}_{j=0}^{N-1}$, $\{Z_{N-1,j}\}_{j=0}^{N-1}$ are derived from the $S$-matrix which is intimately connected with $\mathcal{P}_N$ (see equation (39)). Note that both sets of the spectral parameters determine a unique (apart from the off-diagonal elements sign) Hamiltonian matrix $h$ of a Jacobi form [8, 9]

$$\|h_{n,m}\| = \begin{pmatrix}
a_0 & b_1 & & & \\
b_1 & a_1 & b_2 & & \\
& a_2 & b_3 & & \\
& & b_3 & \times & \\
& & & & b_{N-1}
\end{pmatrix}.$$  

(6)

Hence, the sought potential matrix $\|V_{n,m}\|$ is also of a Jacobi form. Recall that the kinetic energy operator

$$H^0 = \frac{\hbar^2}{2\mu} \left( \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} \right)$$  

(7)

matrix representation $\|T_{n,m}^\ell\| = \frac{1}{\sqrt{\mu}} \|H_{n,m}^0\|$ in the harmonic oscillator basis (2) is symmetric tridiagonal [1, 7]:

$$T_{n,n}^\ell = \frac{1}{2} (2n + \ell + \frac{3}{2}),$$

$$T_{n,n+1}^\ell = T_{n+1,n}^\ell = -\frac{1}{2} \sqrt{(n+1) \left(n + \ell + \frac{1}{2}\right)}.$$  

(8)

Thus, the inverse scattering problem within the $J$-matrix approach admits the solution in the tridiagonal Hamiltonian matrix form. In this regard, the $J$-matrix method is similar to a discrete model of quantum mechanics, in the framework of which the Hamiltonian matrix representation is also symmetric tridiagonal. Note that the tridiagonal matrix representation of both the kinetic energy operator and the Hamiltonian is fundamental for a finite-difference analogue of the Gel’fand–Levitan equations (see, e.g., [10]) as well as for a discrete version
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[11] of the Marchenko equations. As shown below, the similarity between the \(J\)-matrix method and a finite-difference approach can be plainly extended to the inverse scattering formalism as well. In the present paper, in particular, an inverse scattering \(J\)-matrix approach via the Marchenko equations (JME) is given. In the appendix, a spectral function formula suitable for the Gel’fand–Levitan procedure in the oscillator basis case is also presented.

In JME the expansion coefficients \(c_n\) of the wavefunction \(\psi\) in terms of the \(L^2\) basis set play a role similar to that of the values \(\psi_n = \psi(x_n)\) at points \(x_n = n\Delta\) within the finite-difference inverse scattering approach. Here, the completeness relation for the solutions \(c_n\) of the Schrödinger equation discrete analogue is also exploited which involves an integration \(c_nc_m\) over the energy from zero to infinity. This raises the question as to whether the integrals converge. As shown below, taking account of the phase shift \(\delta_N(\ell)\) corresponding to the potential (1) of finite rank \(N\) asymptotic behaviour at large \(k\) provides the convergence of the integrals. Generally, with a potential (1) matrix of finite order \(N\) it is possible to reproduce the phase shift \(\delta_{\ell}\) only on a finite energy interval \([0, \epsilon_0]\) with \(\epsilon_0 < \lambda_{N-1}\). This is why the eigenvalue \(\lambda_{N-1}\) and the corresponding eigenvector component \(Z_{N-1,N-1}\) are the variational parameters within the previous \(J\)-matrix version [2–5] of the inverse scattering theory. By contrast, in JME the phase shift, even if modified in accordance with the \(\delta_N^{(\ell)}\) asymptotic feature, on infinite energy interval is used. As a result, JME has no variational parameters (apart from \(N\) and \(\rho\)).

The elements of the \(J\)-matrix method formalism are presented in section 2. In section 3, the inverse scattering \(J\)-matrix approach in the context of the Marchenko equations is formulated. The features of JME numerical realization are discussed in section 4. In section 5, JME is expanded to the Laguerre basis case. Here, we are dealing with the tridiagonal Hamiltonian matrix construction in an orthogonalized Laguerre basis set, in which the kinetic energy operator matrix is also tridiagonal. In section 6, we summarize our conclusions.

2. The direct problem

The oscillator-basis \(J\)-matrix formalism is discussed in detail elsewhere. We present here only some relations required for understanding the inverse scattering \(J\)-matrix approach. Within the \(J\)-matrix method, the radial wavefunction \(\psi(k,r)\) is expanded in an oscillator function (2) series

\[
\psi(k,r) = \sum_{n=0}^{\infty} c_n(k) \phi_n(x).
\]

In the assumption that the Hamiltonian matrix is of the form (6) the functions \(c_n\) are the solutions to the set of equations

\[
a_0c_0(k) + b_1c_1(k) = \epsilon c_0(k),
\]

\[
b_n c_{n-1}(k) + a_n c_n(k) + b_{n+1}c_{n+1}(k) = \epsilon c_n(k), \quad n = 1, 2, \ldots.
\]

The asymptotic behaviour of \(c_n(k)\) for \(k > 0\) as \(n \to \infty\) is given by

\[
c_n(k) = f_n(k) \equiv \frac{1}{2}\left[b_n^{(n)}(q) - S(k)c_n^{(n)}(q)\right].
\]
Here, the functions
\[ C_{n,\ell}(q) = C_{n,\ell}(q) \pm i S_{n,\ell}(q), \]
\[ S_{n,\ell}(q) = \sqrt{\pi \rho_n!} \frac{\Gamma(n + \ell + \frac{3}{2})}{\Gamma(n + \ell + \frac{1}{2})} q^{\ell} e^{-q^2/2} F\left(-n - \ell - 1/2, -\ell + 1/2; q^2\right), \]
\[ C_{n,\ell}(q) = \sqrt{\pi \rho_n!} \frac{\Gamma(\ell + 1/2)}{\pi q^\ell} e^{-q^2/2} F\left(-\ell, -\ell + 1/2, q^2\right). \]
(12)

obey the ‘free’ equations
\[ T_{\ell}^{n,n-1} e_n(q) + T_{\ell}^{n,n} e_n(q) + T_{\ell}^{n,n+1} e_{n+1}(q) = \epsilon e_n(q), \quad n = 1, 2, \ldots \]
(13)

where \( e_n(q) \) stands for either \( S_{n,\ell}(q) \) and \( C_{n,\ell}(q) \). \( S_{n,\ell} \) satisfy in addition the equation
\[ T_{\ell=0}^{0,0} S_{0,\ell}(q) + T_{\ell+1}^{0,1} S_{1,\ell}(q) = \epsilon S_{0,\ell}(q). \]
(14)

Besides, \( S_{n,\ell} \) meet the completeness relation
\[ 2 \pi \int_0^\infty dk S_{n,\ell}(q) S_{m,\ell}(q) = \delta_{n,m}. \]
(15)

The cosine-like \( \tilde{C}(r)J \)-matrix solution
\[ \tilde{C}(r) = \sum_{n=0}^{\infty} C_{n,\ell}(q) \phi_{\ell}^n(x) \]
construction has been detailed in [7] (see also [13]). \( S_{n,\ell} \) are formally given by the Fourier projection (see, e.g., [14, 13])
\[ S_{n,\ell}(q) = \int_0^\infty \sqrt{\pi qx/2} J_{\ell+1/2}(qx) \phi_{\ell}^n(x) \, dx, \]
i.e.
\[ \tilde{S}(r) = \sum_{n=0}^{\infty} S_{n,\ell}(q) \phi_{\ell}^n(x) = \sqrt{\pi kr/2} J_{\ell+1/2}(kr). \]

Note that the sine-like \( \tilde{S}(r) \) and cosine-like \( \tilde{C}(r) \) \( J \)-matrix solutions subject to the asymptotic conditions [7]
\[ \tilde{S}(r) \sim r \to \infty \sin(kr - \ell \pi/2), \quad \tilde{C}(r) \sim r \to \infty \cos(kr - \ell \pi/2). \]
(16)

As for the coefficients of the expansion
\[ \psi_\nu(r) = \sum_{n=0}^{\infty} c_n(ik_\nu) \phi_{\ell}^n(x) \]
(17)
of the normalized bound-state wavefunction \( \psi_\nu \) with the energy \( -\kappa_\nu^2/2 \),
\[ c_n(ik_\nu) = f_n(ik_\nu) = M_{n,\ell} e^{i(\epsilon_{n,\ell}(ik_\nu))} \]
holds as \( n \to \infty \). Here, \( M_{n,\ell} \) is the bound-state normalization constant which is related to the residue of the \( S \)-matrix [15]:
\[ i \text{ Res } S(k) = (-1)^\ell M_{n,\ell}. \]
(19)

It can be easily verified that from the completeness relation for the solutions \( \psi(k, r) \), \( \psi_\nu(r) \) [16]
\[ \frac{2}{\pi} \int_0^\infty dk \overline{\psi(k, x)} \psi(k, y) + \sum_\nu \psi_\nu(x) \overline{\psi_\nu(y)} = \delta(x - y) \]
(20)
it follows that
\[ \frac{2}{\pi} \int_0^\infty dk e_n(k) \overline{e_m(k)} + \sum_\nu c_n(ik_\nu) \overline{c_m(ik_\nu)} = \delta_{n,m}. \]
(21)
3. The inverse problem

To take advantage of the algebraic analogue of the Marchenko method it is essential that there exist coefficients $K_{n,m}$ (independent of $k$) such that

$$c_n(k) = \sum_{m=n}^{\infty} K_{n,m} f_m(k).$$

By analogy with [11] assume that

$$c_n(k) = f_n(k), \quad n \geq N$$

($N$ specifies the order of a potential matrix). If $f_N$ and $f_{N+1}$ are inserted (instead of respectively $c_N$ and $c_{N+1}$) into equation (10) for $n = N$, we obtain, in view of equation (13),

$$c_{N-1}(k) = \left( T_{N,N-1} f_{N-1}(k) + \left[ T_{N,N} - a_N \right] f_N(k) + \left[ T_{N,N+1} - b_{N+1} f_{N+1}(k) \right] \right) / b_N.$$

Then, using the three-term recursion relation (13) with every $n = N - 1, \ldots, 1$, we obtain

$$c_n(k) = \sum_{m=n}^{2N-n-1} K_{n,m} f_m(k), \quad n = 0, 1, \ldots, N - 1$$

(which in the limit $N \to \infty$ gives (22)).

The coefficients $K_{n,m}$ are found from the completeness relation (21). From the condition of the orthogonality of $c_n$ and every $c_m, m > n$ follows the condition of the orthogonality of $c_n$ and every $f_m, m > n$, i.e.

$$2 \pi \int_0^{\infty} dk c_n(k) f_m(k) + \sum_{\nu} c_n(i\kappa_{\nu}) f_m(i\kappa_{\nu}) = 0, \quad m > n.$$  

Inserting the expansion of (25) in (26) gives the system of linear equations in $K_{n,m}$

$$K_{n,m} Q_{n,m} + \sum_{p=n+1}^{2N-n-1} K_{n,p} Q_{p,m} = 0, \quad m > n.$$  

Then, inserting equation (25) into (21) and putting $n = m$, we obtain, in view of equation (26), the equation in $K_{n,m}$

$$K_{n,m} \left( K_{n,n} + \sum_{p=n+1}^{2N-n-1} K_{n,p} Q_{p,n} \right) = 1.$$  

Note that from equation (27) it follows that $K_{n,m}, m > n$ are proportional to $K_{n,n}$. In equations (27) and (28), $Q_{n,m}$ are defined from the scattering data by

$$Q_{n,m} = 2 \pi \int_0^{\infty} dk f_n(k) f_m(k) + \sum_{\nu} f_n(i\kappa_{\nu}) f_m(i\kappa_{\nu}).$$  

The elements $a_n$ and $b_n$ of the sought-for Hamiltonian matrix (6) are related to $K_{n,m}$ by the equations

$$a_n = T_{n,n} + \frac{K_{n,n+1}}{K_{n,n}} T_{n+1,n}, \quad b_n = -\frac{K_{n-1,n} K_{n,n}}{K_{n-1,n-1}} T_{n,n-1}.$$  

$a_0$ is specified by the solutions $c_0$ and $c_1$ to equation (10).
4. A numerical realization

To this point, the assumption has been made that the phase shift $\delta_\ell(k)$ is a continuous function of the wave number $k$ that meets the conditions [16]

$$\delta_\ell(\infty) = 0, \quad \int_0^\infty k^{-1}\left|\delta_\ell(k)\right|\,dk < \infty.$$  

In this case, $\delta_\ell$ must satisfy stringent requirements. Indeed, the integrated function on the rhs of equation (29) can be expressed in the form of a product $g_nS_m$ of (real) functions

$$g_n(q) = S_m(q) \cos \delta_\ell + C_m(q) \sin \delta_\ell.$$  

(31)

It is obvious that a sufficient condition to the convergence of the integrals in (29) is that $g_n$ are square integrable. Note that from (12) it follows that

$$S_n(q) \sim (-1)^n \frac{\pi \rho}{n! \Gamma(n + \frac{1}{2})} q^{2n+1} e^{-q^2/2},$$  

(32)

i.e., the first term in (31) decays exponentially at asymptotically large $q$. However, $C_m$ grows exponentially with increasing $q$:

$$C_m(q) \sim (-1)^m \frac{\pi \rho n! \Gamma(n + \frac{1}{2})}{\pi} q^{-(2n+2)} e^{q^2/2}.$$  

(33)

This suggests that the phase shift $\delta_\ell$ must decay rapidly enough to provide the convergence of the integral on the rhs of equation (29).

Actually the phase shift $\delta_\ell^N$ corresponding to the potential (1) of rank $N$ [7]

$$\tan \delta_\ell^N = -\frac{S_{N-1,\ell}(q) - P_N(\ell)Tr_{N-1,\ell}S_{N,\ell}(q)}{c_{N-1,\ell}(q) - P_N(\ell)Tr_{N-1,\ell}C_{N,\ell}(q)},$$  

(34)

as seen in equations (32), (33), fulfills the even more strict requirement

$$\delta_\ell^N \sim \frac{\pi}{(N-1)! \Gamma(N + \frac{1}{2})} q^{4N+2\ell-1} e^{-q^2}.$$  

(35)

Because of the restriction (35) on the phase shift $\delta_\ell^N$ the potential (1) of finite rank $N$ generally is incapable of describing the scattering data on the infinite interval $k \in [0, \infty)$. At most, we can set ourselves the task of constructing the potential (1) that describes the experimental phase shift $\delta_\ell$ on some finite interval $[0, k_0]$, since generally $\delta_\ell$ needs to be modified in the region $k > k_0$ to provide at least the convergence of the integrals in equation (29).

As an example, we consider the s-wave scattering case. The ‘experimental’ phase shift $\delta_\ell$ (dotted curve in figure 1) is that of the scattering on the potential given by straight well with the depth $V_0$: $\sqrt{\frac{2\mu}{\hbar^2}} V_0 R = 1.5$. The potential (1) is sought that describes the phase shift on the interval $[0, k_0]$, $k_0 R = 6$ (in figure 1 crosses represent a modified phase shift). The phase shift $\delta_\ell^N$ corresponding to the resulting potential (1) of rank $N = 6$ and $\rho = \frac{1}{2} R$ is shown in figure 1 (solid curve). Note that $C_m$ explodes exponentially with increasing $q$. Thus, the contribution from the region $q > q_0 = \rho k_0 = 3$ to the integral in equation (29) may become overwhelming (see figure 2 where $g_n^2(q)/\rho$ is plotted), with the result that the method fails. Matters can be improved by a transition to lesser $\rho$ that shifts $q_0$ to a region where $C_m$ is not that large, or replacing $\delta_\ell$ at $q > q_0$ with a function that decays rapidly enough.

In the second example, scattering data on the potential with a bound state have been used as input. The phase shift $\delta_\ell$ (dotted curve in figure 3) corresponds to the s-wave scattering on a spherically symmetric potential in the form of straight well. The well parameter $\sqrt{\frac{2\mu}{\hbar^2}} V_0 R = 2$...
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Figure 1. Phase shift: $\delta_\ell$ (dotted curve) for the straight wall potential which does not sustain bound states; the modified phase shift (crosses) that is employed as input in the JME; $\delta_N^\ell$ (solid curve) for the resulting potential (1).

Figure 2. The integrated function on the rhs of (29) (with $n = m = 0$) that corresponds to the modified phase shift plotted in figure 1.

determines the bound state with the energy $E = -\kappa^2$, $\kappa R = 0.638\,045$ and the asymptotic normalization constant $\mathcal{M}R^{1/2} = 1.583\,324$. $k_0$ and $\rho$ have been taken the same as in the first example (the modified phase shift is represented by crosses in figure 3). It is well known that a phase shift does not depend on energy positions and asymptotic normalization constants of bound states. Thus, the inverse scattering problem in the presence of a bound state can be split into two steps.

In the first step, we focus on describing the phase shift and, in spite of all of scattering data being used (see equation (29)), do not seek to describe the bound state with a high degree of accuracy. The phase shift $\delta_N^\ell$ corresponding to the potential (1) parameters, which together with $\kappa R$ and $\mathcal{M}R^{1/2}$ are presented in the left half of table 1, is shown in figure 3 (solid curve).

In the second step, to improve the description of the bound states we use the relationship (19) between the poles and residues of the $S$-matrix and the characteristics of the bound states (see, e.g., [5]). Here, the smallest eigenvalue $\lambda_0$ and the corresponding eigenvector component $Z_{N-1,0}$ associated with the bound state are found from the system
Figure 3. Same as in figure 1, but for potentials with a bound state.

Table 1. The parameter values of the resulting potential (1) which supports the bound state.

\[ N = 7, \rho = \frac{\kappa R}{\pi} \]

| j | \( Z_{N-1,j} \) | \( \lambda_j \) | \( Z_{N-1,j} \) | \( \lambda_j \) |
|---|---|---|---|---|
| 0 | 0.035 651 451 7 | -0.038 126 017 8 | 0.036 207 525 9 | -0.035 327 957 5 |
| 1 | 0.210 721 214 7 | 0.300 065 278 1 | 0.314 094 528 1 | 0.320 980 153 9 |
| 2 | 1.324 064 527 8 | 2.504 469 600 0 | 1.349 271 214 7 | 2.504 469 600 0 |
| 3 | 2.300 064 527 8 | 4.108 938 428 2 | 2.300 064 527 8 | 4.108 938 428 2 |
| 4 | 3.000 064 527 8 | 5.618 424 946 5 | 3.000 064 527 8 | 5.618 424 946 5 |
| 5 | 3.500 064 527 8 | 7.138 938 428 2 | 3.500 064 527 8 | 7.138 938 428 2 |
| 6 | 3.900 064 527 8 | 8.658 424 946 5 | 3.900 064 527 8 | 8.658 424 946 5 |

Equations (37), (38) are derived from the S-matrix formula for the potential (1) [7]

\[ \mathcal{S}_\ell^N \left( \frac{\kappa R}{\pi} \right) = \mathcal{S}_\ell^N \left( \frac{\kappa R}{\pi} \right) = \frac{1}{T_{N-1,N}} \frac{C_{N-1,\ell}^{(+)}(\kappa \rho)}{C_{N-1,\ell}^{(-)}(\kappa \rho)}, \quad (37) \]

\[ \frac{d}{dq} \left[ C_{N-1,\ell}^{(+)}(q) - \mathcal{P}_N(q)(q^2/2)T_{N-1,N}^{(\ell)}(q) \right] \bigg|_{q = \imath(k \rho)} = i(-1)^{\ell+1} \rho \mathcal{M}^2. \quad (38) \]

and equation (19). Note that the component \( Z_{N-1,N-1} \) corresponding to the leading eigenvalue \( \lambda_{N-1} \) is involved to meet the normalization condition (36). The phase shift is scarcely affected by changing the parameters \( \{\lambda_0, Z_{N-1,0}, Z_{N-1,N-1}\} \) from the initial values obtained in the first step to the ones that are evaluated from equations (36)–(38). The potential parameters, which provide the correct values of \( \kappa R \) and \( \mathcal{M} R^{1/2} \), are presented in the right half of table 1.
5. The Laguerre basis

5.1. Preliminaries

For the sake of simplicity, we restrict our consideration to the scattering of neutral particles. However, the resulting equations still stand in the presence of the repulsive Coulomb interaction. The potential sought is given by the expression

$$V_l(r, r') = \frac{\hbar^2}{2\mu} \sum_{n,m=0}^{N-1} \overline{\phi_n^\ell}(x)V_{n,m}\phi_m^\ell(x')$$

(40)

where the functions

$$\overline{\phi_n^\ell}(x) = \frac{n!}{r(n + 2\ell + 1)!}\phi_n^\ell(x)$$

(41)

are bi-orthogonal to the base Laguerre functions \(\phi_n^\ell\):

$$\int_0^\infty dr \overline{\phi_n^\ell}(x)\phi_m^\ell(x) = \delta_{n,m}.$$  

(43)

Here, \(b\) is the scale parameter: \(x = br\).

The coefficients \(u_n\) of the expansion

$$\psi(k, r) = \sum_{n=0}^{\infty} u_n(k)\phi_n^\ell(x)$$

(44)

of the Schrödinger equation regular solution \(\psi(k, r)\) satisfy the system of equations

$$\left(\hbar^0_{n,m} + V_{n,m}\right)u_m(k) = k^2A_{n,m}^\ell u_m(k), \quad n = 0, 1, \ldots$$

(45)

Here, \(\|h^0_{n,m}\|\) is the symmetric tridiagonal matrix of the reference Hamiltonian \(\frac{\hbar^2}{\mu}H^0\) calculated in the basis (42) [1]:

$$h^0_{n,n} = b\frac{(n + 2\ell + 1)!}{n!}(n + \ell + 1),$$

$$h^0_{n,n+1} = h^0_{n+1,n} = b\frac{(n + 2\ell + 2)!}{2n!}, \quad n = 0, 1, \ldots$$

(46)

\(\|A_{n,m}^\ell\|\) signifies the basis-overlap matrix

$$A_{n,m}^\ell = \int_0^\infty dr \overline{\phi_n^\ell}(x)\phi_m^\ell(x)$$

(47)

which is also of Jacobi form:

$$A_{n,n}^\ell = \frac{(n + 2\ell + 1)!}{bn!}(n + \ell + 1),$$

$$A_{n,n+1}^\ell = A_{n+1,n}^\ell = -\frac{(n + 2\ell + 2)!}{2bn!}, \quad n = 0, 1, \ldots$$

(48)

The asymptotic behaviour of the coefficients \(u_n(k), k > 0\), as \(n \to \infty\) is given by the following expression:

$$u_n(k) = w_n(k) \equiv \frac{1}{2}[C_{n,n}^{(\ell)}(k) - S(k)C_{n,n}^{(\ell)}(k)]$$

(49)

where the functions [7]

$$C_{n,n}^{(\ell)}(k) = -\frac{n!}{(n + \ell + 1)!}\left(-\xi\right)^{\ell(n+1)}2F_1(-\ell, n + 1; n + \ell + 2; \xi),$$

$$\xi = e^{i\ell} = \frac{ib - k}{ib + k}$$

(50)
obey the inhomogeneous ‘free’ equation

\[ J^{\ell}_{n,m}(k)C^{(b)}_{m,\ell}(k) = \delta_{n,0} \frac{k}{S_{\ell,\ell}(k)}, \quad n = 0, 1, \ldots \]

(51)

Here, \( \|J^{\ell}_{n,m}(k)\| = \|H^0_{n,m} - k^2 A^\ell_{n,m}\| \) is the so-called \( J \)-matrix. \( S_{\ell,\ell} \) are the solutions of the system of equations

\[
J^{\ell}_{n,m}(k)S_{m,\ell}(k) = 0, \quad n = 0, 1, \ldots.
\]

(52)

\[
S_{\ell,\ell}(k) = \ell! (2 \sin \xi)^{\ell+1} \frac{(-\xi)^n}{2(2\ell + 1)!} F_1(-n, \ell + 1; 2\ell + 2; 1 - \xi^{-2}).
\]

(53)

It can easily be shown that the completeness relation for the functions \( S_{\ell,\ell} \) of [17] can be rewritten as

\[
2 \int_0^\infty dk S_{\ell,\ell}(k) A^\ell_{n,m} S_{m,\ell}(k) = \delta_{n,n'}.
\]

(54)

The coefficients \( u_n(ik\nu) \) of the expansion of the bound-state normalized wavefunction \( \psi_n(r) \) with the energy \(-\kappa^2\) have the following asymptotic behaviour:

\[
u_n(ik\nu) = w_n(ik\nu) \equiv \mathcal{M}_n \gamma C_{n\ell}(ik\nu)
\]

(55)

as \( n \to \infty \).

Note that the sine-like \( J \)-matrix solutions \( \tilde{S}(r) = \sum_{n=0}^{\infty} S_{n,\ell}(k)\phi_n(x) \) and the cosine-like one \( \tilde{C}(r) = \sum_{n=0}^{\infty} C_{n,\ell}(k)\phi_n(x) \), where \( C_{n,\ell}(k) = \frac{1}{2} (C^\ell_{n,\ell}(k) + C^\ell_{n,-\ell}(k)) \), have the asymptotic behaviour (16).

The completeness relation (20) is transformed into

\[
2 \int_0^\infty u_n(k) A^\ell_{n,m} u_m(k) + \sum_{\nu} u_n(ik\nu) A^\ell_{n,m} u_m(ik\nu) = \delta_{n,n'}.
\]

(56)

5.2. Inverse problem

In the framework of the \( J \)-matrix version [4] of the inverse scattering problem, the spectral parameter set \( \{\lambda_j, Z_{N-1,j}\}_{j=0}^{N-1} \) is obtained from the scattering data of the truncated Hamiltonian matrix of order \( N \) in the orthogonal basis \( \psi_n^\ell = \sum_{m=0}^{N-1} D_{n,m}^\ell \phi_m^\ell \), where

\[
D_{n,m}^\ell = \begin{cases} d_n^\ell, & n \geq m, \\ 0, & n < m, \\ d_n^\ell = \sqrt{\frac{2bn!}{(n + 2\ell + 2)!}}. \end{cases}
\]

(57)

i.e.,

\[
\psi_n^\ell(x) = d_n^\ell (2br)^{\ell+1} e^{-br} L_n^{2\ell+2}(2br).
\]

(58)

Clearly the set \( \{\lambda_j, Z_{N-1,j}\}_{j=0}^{N-1} \) determines a tridiagonal Hamiltonian matrix of order \( N \) in any orthogonal basis \( \chi_n^\ell = \sum_{m=0}^{N-1} P_{n,m}^\ell \psi_m^\ell \) where \( \|P_{n,m}^\ell\| \) is an arbitrary orthogonal \((N \times N)\)-matrix of the form

\[
\|P_{n,m}^\ell\| = \begin{pmatrix} p_{0,0}^\ell & \cdots & p_{0,N-2}^\ell & 0 \\ \vdots & \ddots & \vdots & \vdots \\ p_{N-2,0}^\ell & \cdots & p_{N-2,N-2}^\ell & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}.
\]

(59)

Let us assume that \( \|P_{n,m}^\ell\| \) is the orthogonal transformation matrix that performs the change from \( \{\psi_n^\ell\}_{n=0}^{N-1} \) to the new basis \( \{\chi_n^\ell\}_{n=0}^{N-1} \) in which the kinetic energy operator truncated matrix is tridiagonal. To perfect the analogy with the oscillator basis case, let us denote the kinetic
energy operator \( \frac{2}{\hbar^2} \hat{H} \) (7) tridiagonal matrix in the basis \( \{ \phi_n^\ell \}_{n=0}^{N-1} \) by \( \| T_{n,m}^\ell \| \). The sought Hamiltonian \( \frac{2}{\hbar^2} \hat{H} \) matrix \( \| h_{n,m} \| \) of order \( N \) is presumed to be of a Jacobi form (6) in the basis \( \{ \chi_n \}_{n=0}^{N-1} \).

Thus, the first \( N - 1 \) of the wavefunction \( \psi(k, r) \) expansion coefficients in the combined basis set \( \{ \chi_n \}_{n=0}^{N-1}, \{ \phi_n^\infty \}_{n=N} \) obey the equations

\[
(a_0 c_0(k) + b_1 c_1(k)) = k^2 c_0(k),
\]

\[
b_n c_{n-1}(k) + a_n c_n(k) + b_{n+1} c_{n+1}(k) = k^2 c_n(k), \quad n = 1, \ldots, N - 2.
\]

It is easy to check that a sufficient condition that the algebraic version of the Marchenko method be applicable for the construction of the tridiagonal Hamiltonian matrix (6) is that

\[
a_{n+1} = T_{n+1,n+1}^\ell, \quad b_{n+1} = T_{n,n+1}^\ell, \quad \text{for} \quad n = M, \ldots, N - 2, \quad M = \left\lfloor \frac{N}{2} \right\rfloor.
\]

If \( N \) is odd, to (61) must be added the constraint that \( a_M = T_{M,M}^\ell \). In this case, \( c_{M+1} = f_{M+1}, c_M = f_M \), where \( f_s \) satisfy the ‘free’ equations

\[
T_{n,n-1}^\ell f_{n-1}(k) + T_{n,n}^\ell f_n(k) + T_{n,n+1}^\ell f_{n+1}(k) = k^2 f_n(k), \quad n = 1, \ldots, N - 2,
\]

and we obtain for \( n \leq M - 1 \)

\[
c_n(k) = \sum_{m=0}^{N-n-1} K_{n,m} f_m(k).
\]

Note that in going from the initial Laguerre basis \( \{ \phi_n^\ell \}_{n=0}^{\infty} \) to the combined basis set \( \{ \chi_n \}_{n=0}^{N-1}, \{ \phi_n^\infty \}_{n=N} \), the submatrices \( \| h_{n,m}^0 \|_{n,m=0}^{N-1} \) and \( \| A_{n,m}^\ell \|_{n,m=0}^{N-1} \) are transformed into \( \| T_{n,m}^\ell \|_{n,m=0}^{N-1} \) and the identity matrix of order \( N \), respectively. In addition, the elements \( h_{0,N-1}^0, A_{N-1,N}^\ell \) and \( h_{N,N-1}^0, A_{N,N-1}^\ell \) are multiplied by \( d_{N-1}^\ell \). The rest of the (infinite) matrices \( \| h_{n,m}^0 \| \) and \( \| A_{n,m}^\ell \| \) are unaltered. It thus follows that \( f_n \) must satisfy (in addition to (62)) the equations

\[
T_{N-1,N-2}^\ell f_{N-2}(k) + T_{N-1,N-1}^\ell f_{N-1}(k) + d_{N-1}^\ell J_{N-1,N}^\ell f_N(k) = k^2 f_{N-1}(k),
\]

\[
d_{N-1}^\ell J_{N,N}^\ell f_{N-1}(k) + J_{N,N}^\ell f_{N}(k) = 0,
\]

\[
J_{N,n-1}^\ell f_m(k) = 0, \quad n = N + 1, \ldots.
\]

Putting \( f_n = S_{n,\ell} \) for \( n \geq N \) and \( f_{n-1} = S_{N-1,\ell} \) in (view of equations (64) and (65), respectively), from equation (64) by using the tree-term recursion relation (62) we obtain the coefficients \( \tilde{S}_{n,\ell} \) with \( n = 0, \ldots, N - 2 \). Similarly, setting \( f_0 = C_{n,\ell}^{(\pm)} \) for \( n \geq N \) and \( f_{n-1} = C_{N-1,\ell}^{(\pm)} \) in (65), we obtain the coefficients \( \tilde{C}_{n,\ell}^{(\pm)} \) with \( n = 0, \ldots, N - 2 \). From the Wronskian-like relation (see, e.g., [18])

\[
J_{n+1,n}^\ell (C_{n+1,\ell}^{(\pm)}(k)S_{n,\ell}(k) - C_{n,\ell}^{(\pm)}(k)S_{n+1,\ell}(k)) = k,
\]

it follows that

\[
T_{n+1,n}^\ell (C_{n+1,\ell}^{(\pm)}(k)S_{n,\ell}(k) - C_{n,\ell}^{(\pm)}(k)S_{n+1,\ell}(k)) = k, \quad 0 \leq n \leq N - 2.
\]

Besides, since the system of equations (52) in \( S_{n,\ell} \) is homogeneous, the sets \( \{ S_{n,\ell} \}_{n=0}^{\infty} \) and \( \{ \tilde{S}_{n,\ell} \}_{n=0}^{\infty} \) are connected by a linear transformation and therefore \( \tilde{S}_{n,\ell} \) also satisfy the homogeneous equation

\[
T_{0,0}^\ell \tilde{S}_{0,\ell}(k) + T_{0,1}^\ell \tilde{S}_{1,\ell}(k) = k^2 \tilde{S}_{0,\ell}(k),
\]
whereas $C_{n,\ell}^{(\pm)}$ obey the inhomogeneous one
\[
T_{0,0}^{\ell} \tilde{S}_{0,0}^{(k)}(k) + T_{0,1}^{\ell} \tilde{S}_{1,0}^{(k)}(k) = k^2 C_{0,\ell}^{(\pm)}(k) + \frac{k}{\tilde{S}_{0,\ell}^{(k)}}. \tag{70}
\]
Thus, the two sets, $\{\tilde{S}_{n,\ell}\}_{n=0}^{\infty}$ and $\{\tilde{C}_{n,\ell}\}_{n=0}^{\infty}, \tilde{C}_{n,\ell} = \frac{1}{2}(\tilde{C}_{n,\ell}^{(-)} + \tilde{C}_{n,\ell}^{(+)}), \text{ are ‘free’ independent,}
respectively, sine-like $\{\tilde{S}_{n,\ell} = S_{n,\ell}, n \geq N\} \text{ and cosine-like } \{\tilde{C}_{n,\ell} = C_{n,\ell}, n \geq N\}$ solutions to equations (62)–(66) (see, e.g., [7]).

From the above discussion, it follows that to obtain $f_n$ with $0 \leq n \leq N - 1$, which are
involved in equation (63), we can place $f_N = w_N, f_{N-1} = w_{N-1}/d_{N-1}, \text{ where } w_n \text{ are defined by (49).}$
Then, inserting this $f_N$ and $f_{N-1}$ in equation (64) gives $f_{N-2}$. Once $f_{N-2}$ and $f_{N-1}$
are known, $f_n$ for $n = N - 3, \ldots, 0$ are obtained by using the tree-term recursion relation
(62). $K_{n,m}$ are determined by equations (27) and (28) (in which the upper limit in the sums is
equal to $N - n - 1$). The expressions for $\{a_n\}, \{b_n\}$ are the same as (30).

$Q_{n,n'}$ with $n \leq N - 1$ in equations (27) and (28) are defined (in view of the overlap matrix form in the combined basis) by
\[
Q_{n,n'} = \frac{1}{\pi} \int_0^\infty f_n(k) f_{n'}(k) \sum_v f_v(ik_v) f_v(ik_v), \quad n' \leq N - 2, \tag{71}
\]
\[
Q_{n,N-1} = \frac{1}{\pi} \int_0^\infty f_n(k) \left[ \frac{w_{N-1}(k)}{d_{N-1}} + \frac{d_{N-1}^\ell A_{n,N-1}^\ell(k)}{w_{N}(k)} \right] \sum_v f_v(ik_v) \left[ \frac{w_{N-1}(ik_v)}{d_{N-1}} + \frac{d_{N-1}^\ell A_{n,N-1}^\ell(ik_v)}{w_{N}(ik_v)} \right], \tag{72}
\]
\[
Q_{n,n'} = \frac{1}{\pi} \int_0^\infty f_n(k) A_{n,m}^\ell w_m(k) + \sum_v f_v(ik_v) A_{v,m}^\ell w_m(ik_v), \quad n' \geq N. \tag{73}
\]

Note that at large $k$, as seen in equation (50), $C_{n,\ell}^{(\pm)}(k) \sim k^\ell$. Thus, as in the case of the oscillator basis, we should restrict ourselves to the description of the scattering data on a finite energy interval, beyond the boundary of which the phase shift needs generally to be modified to provide the convergence of the integrals in equations (71)–(73).

6. Conclusion

In the potential scattering case, the finite-difference approach and $J$-matrix method share
the tridiagonal representation of the Hamiltonian. The analogy can be carried over to
the inverse scattering problem formalism. Here, the $J$-matrix version of the Marchenko
equation algebraic analogue is formulated and its numerical realization features are considered.
The merit of JME is that it is free from a parameter fit inherent in the previous $J$-matrix inverse
scattering approach [2–5]. We also construct a tridiagonal Hamiltonian matrix of some order
$M$ in an orthogonalized Laguerre basis; in doing so it is sufficient to tridiagonalize the
matrix representation of the reference Hamiltonian in the finite orthogonal basis subset of size
$N = 2M$. As has been shown in [5], in the two coupled-channel case without threshold, the
sought interaction matrix may be of a ‘quasi-tridiagonal’ form. With this assumption, JME
can be easily expanded to multichannel scattering.

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Appendix. The spectral function in the oscillator basis case

As a preliminary, note that the polynomials \( p_n(\epsilon) \) defined by

\[
p_n(\epsilon) = \frac{S_{n,\ell}(q)}{S_{0,\ell}(q)} \tag{A.1}
\]
satisfy the three-term recursion relations

\[
T_{n,n-1}^{\ell} p_{n-1}(\epsilon) + T_{n,n}^{\ell} p_n(\epsilon) + T_{n,n+1}^{\ell} p_{n+1}(\epsilon) = \epsilon p_n(\epsilon), \quad n = 1, \ldots \tag{A.2}
\]

and the boundary conditions

\[
p_0(\epsilon) = 1; \quad T_{0,0}^{\ell} p_0(\epsilon) + T_{0,1}^{\ell} p_1(\epsilon) = \epsilon p_0(\epsilon) \tag{A.3}
\]

(see (13), (14)). \( p_n(\epsilon) \) are orthogonal with respect to the weight \( \tau(\epsilon) \)

\[
\int_{-\infty}^{\infty} p_n(\epsilon) p_m(\epsilon) d\tau(\epsilon) = \delta_{nm} \tag{A.4}
\]

where

\[
\frac{d\tau(\epsilon)}{d\epsilon} = \frac{2}{\Gamma(\ell + 3/2)} q^{2\ell+1} e^{-q^2} \tag{A.5}
\]

(see (15)). The second solution \( y_{\pm n}(\epsilon) \) of the three-term recursion relation (A.2) obeys the boundary condition [13, 14]

\[
T_{0,0}^{\ell} y_{\pm 0}(\epsilon) + T_{0,1}^{\ell} y_{\pm 1}(\epsilon) = \epsilon y_{\pm 0}(\epsilon) + 1, \quad \epsilon > 0 \tag{A.7}
\]

i.e., \( p_n(\epsilon) \) and \( y_{n}(\epsilon) \) satisfy the Wronskian-like relation

\[
T_{n,n+1}^{\ell} (y_{n+1}(\epsilon) p_n(\epsilon) - y_{n}(\epsilon) p_{n+1}(\epsilon)) = 1. \tag{A.8}
\]

The Green’s function has the matrix representation [14]

\[
G_{nn'}^{(\pm)} = -p_n y_{n'}^{(\pm)}, \tag{A.9}
\]

with \( n_+ = \min(n, n') \), \( n_- = \max(n, n') \).

The first \( N \) equations (A.2), (A.3) are altered by the potential (1) with the tridiagonal matrix \( V \) of order \( N \):

\[
b_n \tilde{p}_{n-1}(\epsilon) + a_n \tilde{p}_n(\epsilon) + b_{n+1} \tilde{p}_{n+1}(\epsilon) = \epsilon \tilde{p}_n(\epsilon), \quad n = 1, 2, \ldots N - 1, \tag{A.10}
\]

\[
\tilde{p}_0(\epsilon) = 1; \quad a_0 \tilde{p}_0(\epsilon) + b_1 \tilde{p}_1(\epsilon) = \epsilon \tilde{p}_0(\epsilon) \tag{A.11}
\]

(see (10)). It is desired to obtain the spectral function with respect to which the polynomials \( \tilde{p}_n(\epsilon) \) are orthonormal

\[
\int_{-\infty}^{\infty} \tilde{p}_n(\epsilon) \tilde{p}_m(\epsilon) d\sigma(\epsilon) = \delta_{nm}. \tag{A.12}
\]

Having found \( \sigma(\epsilon) \), one constructs the potential by the Gel’fand–Levitan procedure. It was demonstrated by Broad in [14] that \( \sigma(\epsilon) \) and \( \tau(\epsilon) \) are related by the equation

\[
\frac{d\sigma(\epsilon)}{d\epsilon} = \begin{cases} \frac{d\tau(\epsilon)}{d\epsilon} \frac{1}{|B^{(\epsilon)}(\epsilon)|^2}, & \epsilon \geq 0, \\ \frac{d\tau(\epsilon)}{d\epsilon} \left( -2\pi i \text{Res}_{\epsilon \to \epsilon_0} \frac{1}{B^{(\epsilon)}(\epsilon)B^{(-\epsilon)}(\epsilon)} \right) \delta(\epsilon - \epsilon_0), & \epsilon < 0, \end{cases} \tag{A.13}
\]
where
\[ B^{(\pm)}(\epsilon) = T_{N-1}^{\ell} \left( y^{(\pm)}_N \tilde{p}_N - y^{(\pm)}_{N-1} \tilde{p}_{N-1} \right). \] (A.14)

Employing equations (A.2), (A.3) and (A.7)–(A.11), it can be shown that \( B^{(\pm)} \) and the Fredholm determinant (the Jost function),
\[ F(\pm k) = \det(1 - G^{(\pm)} V), \] (A.15)
differ only by a factor:
\[ B^{(\pm)} = F^{(\pm)} k / A, \quad A = \prod_{n=1}^{N-1} \frac{b_n}{\tilde{p}_{n-1}}. \] (A.16)

Using the normalization constants formula [16]
\[ C^{-1}_{\nu} = (-1)^{\ell} \frac{\tilde{F}(ik_{\nu}) \tilde{F}(-ik_{\nu})}{4ik^{2\ell+2}_{\nu}}, \] (A.17)
(A.13) can be rewritten in the form
\[ \frac{d\sigma}{d\epsilon} = \begin{cases} A^2 \frac{2}{\Gamma(\ell + 3/2)} e^{-q^2} \epsilon^{-q} \left| F(k) \right|^2, & \epsilon \geq 0, \\ A^2 \frac{\pi}{\Gamma(\ell + 3/2)} C_{\nu} \rho^{2\ell+3} e^{\xi^2/\rho^2} \delta(\epsilon - \epsilon_{\nu}), & \epsilon < 0, \end{cases} \] (A.18)
where \( A \) is determined by the normalization condition (see, e.g., [19])
\[ \int_{-\infty}^{\infty} d\sigma(\epsilon) = 1. \] (A.19)

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