Multi-channel inverse scattering problem in the J-matrix approach

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Abstract

Using the analytical properties of the S-matrix as the base a set of the inverse scattering problem equations has been obtained within the J-matrix approach. This method is appropriate in the case of a multi-channel scattering with the different channel threshold energies.

1 Introduction

In this work a method for constructing separable potential with the Laguerre form factors from a given multi-channel S-matrix is considered. The desired potential is written as

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

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

$$V^{\alpha\,\beta} = \frac{\hbar^2}{2\mu}\sum_{n=0}^{N_\alpha-1}\sum_{n'=0}^{N_\beta-1}\left|\overline{\phi}_n^{(\alpha)}\right\rangle V_{n,\,n'}^{\alpha\,\beta}\left\langle\overline{\phi}_{n'}^{(\beta)}\right|. \tag{2}$$

Here, the α and β denote sets of quantum numbers including the values of the orbital momenta ℓ_α and ℓ_β, and

$$\left|\overline{\phi}_n^{(\alpha)}\right\rangle = \frac{n!}{r\,(n+2\ell_\alpha+1)!}(2br)^{\ell_\alpha+1}\,e^{-br}\,L_n^{2\ell_\alpha+1}(2br), \tag{3}$$

are the functions bi-orthogonal to the Laguerre basis functions $\left|\phi_n^{(\alpha)}\right\rangle$ [2] in the channel α

$$\left|\phi_n^{(\alpha)}\right\rangle = (2br)^{\ell_\alpha+1}\,e^{-br}\,L_n^{2\ell_\alpha+1}(2br), \tag{4}$$

i. e. $\left\langle\phi_n^{(\alpha)}\middle|\overline{\phi}_{n'}^{(\alpha)}\right\rangle = \delta_{n\,n'}$. Here, b is a scale parameter, μ is the (common) channel reduced mass. Conservation of energy $\hbar^2k_1^2/2\mu$ of the system requires that

$$k_1^2 = k_\alpha^2 + t_\alpha^2, \qquad \alpha = 1,\ldots,\,N_c, \tag{5}$$

where k_α is the channel wave number and $\hbar^2k_1^2/2\mu$, $t_\alpha \geq 0$ is the threshold energy of the α-th channel.

It is easy to verify that the potential (1), (2) matrix is given by the following expression:

$$\mathbf{V} = \mathbf{D}^{-1}(\mathbf{Z}\boldsymbol{\Lambda}\widetilde{\mathbf{Z}} - \mathbf{T})\widetilde{\mathbf{D}}^{-1} - \mathbf{h}_0, \tag{6}$$

where the tilde denotes transposition. In Eq. (6) $\mathbf{h}_0$ is the matrix of the operator $\sum\limits_{\alpha} |\alpha\rangle\, \widehat{h}_0^{(\alpha)}\, \langle\alpha|$, where

$$\widehat{h}_0^{(\alpha)} = -\frac{d^2}{dr^2} + \frac{\ell_\alpha(\ell_\alpha+1)}{r^2} \tag{7}$$

is free Hamiltonian, calculated in the basis $\left\{|\alpha\rangle \left|\phi_n^{(\alpha)}\right\rangle,\ n=\overline{0,\ N_\alpha-1},\ \alpha=\overline{1,\ N_c}\right\}$. $\mathbf{Z}$ is the orthogonal matrix of eigenvectors, and $\mathbf{\Lambda}$ is the diagonal matrix of the eigenvalues $\{\lambda_j\}$ of the matrix of the operator $\sum\limits_{\alpha} |\alpha\rangle\, (\widehat{h}_0^{(\alpha)} + t_\alpha^2)\, \langle\alpha| + \frac{2\mu}{\hbar^2}\widehat{V}$, $\mathbf{T}$ is the matrix of the operator $\sum\limits_{\alpha} |\alpha\rangle\, t_\alpha^2\, \langle\alpha|$. The last two operators matrices are calculated in the orthonormalized basis $\left\{|\alpha\rangle \left|\psi_n^{(\alpha)}\right\rangle,\ n=\overline{0,\ N_\alpha-1},\ \alpha=\overline{1,\ N_c}\right\}$. $\mathbf{D}$ is the block-diagonal matrix involving the $N_\alpha \times N_\alpha$ submatrices $\mathbf{D}^{(\alpha)}$, $\alpha = 1,\, N_c$ of the transformation to the orthonormal basis $\left\{\left|\psi_n^{(\alpha)}\right\rangle,\ n=\overline{0,\ N_\alpha-1}\right\}$, i. e.

$$\left|\psi_n^{(\alpha)}\right\rangle = \sum_{j=1}^{N_\alpha} D_{n+1,j}^{(\alpha)} \left|\phi_{j-1}^{(\alpha)}\right\rangle. \tag{8}$$

In our case

$$\left|\psi_n^{(\alpha)}\right\rangle = \left(\frac{2bn!}{(n+2\ell_\alpha+2)!}\right)^{1/2} (2br)^{\ell_\alpha+1}\, e^{-br} L_n^{2\ell_\alpha+2}(2br), \tag{9}$$

i. e. the matrices $\mathbf{D}^{(\alpha)}$ are defined by the expressions

$$D_{i,j}^{(\alpha)} = \begin{cases} d_{i-1}^{(\alpha)}, & i \geq j, \\ 0, & i < j, \end{cases} \tag{10}$$

where

$$d_n^{(\alpha)} = \left(\frac{2bn!}{(n+2\ell_\alpha+2)!}\right)^{1/2}. \tag{11}$$

2 Description of the method

The S-matrix $\mathcal{S}_{\alpha,\beta}^{(\mathcal{N})}$ corresponding to the potential (1), (2) is of the form [1]

$$\overline{\mathcal{S}}^{(\mathcal{N})} = \left[\mathcal{C}_{N-1}^{(+)} - \mathcal{P}\mathcal{J}\mathcal{C}_N^{(+)}\right]^{-1} \left[\mathcal{C}_{N-1}^{(-)} - \mathcal{P}\mathcal{J}\mathcal{C}_N^{(-)}\right], \quad \mathcal{S}_{\alpha,\beta}^{(\mathcal{N})} = \sqrt{\frac{k_\alpha}{k_\beta}}\, \overline{\mathcal{S}}_{\alpha,\beta}^{(\mathcal{N})}, \tag{12}$$

where diagonal $N_c \times N_c$ matrices $\mathcal{C}_{N-1}^{(\pm)}$, $\mathcal{C}_N^{(\pm)}$ and $\mathcal{J}$ are defined by [2]

$$\begin{gathered} \left[\mathcal{C}_{N-1}^{(\pm)}\right]_{\alpha,\beta} = \delta_{\alpha,\beta}\, C_{N_\alpha-1}^{(\pm)(\alpha)}(k_\alpha), \quad \left[\mathcal{C}_N^{(\pm)}\right]_{\alpha,\beta} = \delta_{\alpha,\beta}\, C_{N_\alpha}^{(\pm)(\alpha)}(k_\alpha), \\ C_n^{(\pm)(\alpha)}(k_\alpha) = \frac{1}{(2\sin\zeta_\alpha)^{\ell_\alpha}}\, q_n^{\ell_\alpha(\pm)}(k_\alpha), \\ q_n^{\ell(\pm)}(k) = -\frac{\Gamma(n+1)}{\Gamma(n+\ell+2)}(-\xi)^{\pm(n+1)}{}_2F_1(-\ell,\, n+1;\, n+\ell+2;\, \xi^{\pm 2}), \\ \xi = e^{\mathrm{i}\zeta} = \frac{\mathrm{i}b-k}{\mathrm{i}b+k}, \\ [\mathcal{J}]_{\alpha,\beta} = \delta_{\alpha,\beta}\frac{(N_\alpha+2\ell_\alpha+1)!}{2\,b\,(N_\alpha-1)!}(b^2+k_\alpha^2). \end{gathered} \tag{13}$$

The elements of $N_c \times N_c$ matrix $\mathcal{P}$ (so-called $\mathcal{P}$-matrix) are defined as following [1, 3]

$$\mathcal{P}_{\alpha,\beta}(\epsilon) = d^{(\alpha)}_{N_\alpha-1}\, d^{(\beta)}_{N_\beta-1} \sum_{j=1}^{\mathcal{N}} \frac{Z_{K_\alpha,j}\, Z_{K_\beta,j}}{\epsilon-\lambda_j}, \quad K_\alpha = \sum_{\beta\le\alpha} N_\beta, \quad \epsilon = k^2, \quad k \equiv k_1. \tag{14}$$

Open channels

Let us fix some values of b, N_α and define matrix

$$\widetilde{\mathcal{P}} = \mathcal{J}^{-1}\left[\mathcal{C}^{(-)}_{N-1} - \mathcal{C}^{(+)}_{N-1}\overline{\mathcal{S}}\right]\left[\mathcal{C}^{(-)}_{N} - \mathcal{C}^{(+)}_{N}\overline{\mathcal{S}}\right]^{-1}, \tag{15}$$

by inverting expression (12) relative to the $\mathcal{P}$-matrix. In Eq. (15) $\overline{\mathcal{S}}$ is the "experimental" S-matrix. If the "theory" S-matrix $\overline{\mathcal{S}}^{(N)}$ coincides with the "experimental" one, the same will be true for matrices $\mathcal{P}$ and $\widetilde{\mathcal{P}}$. Consequently, in view of Eq. (14), the parameters $\{\lambda_j\}$ and $\{Z_{K_\alpha,j}\}$ can be obtained from Eqs [3]

$$\det\left[\mathcal{C}^{(-)}_{N}(\sqrt{\lambda_j}) - \mathcal{C}^{(+)}_{N}(\sqrt{\lambda_j})\overline{\mathcal{S}}(\sqrt{\lambda_j})\right] = 0 \tag{16}$$

and

$$Z_{K_\alpha,j}\, Z_{K_\beta,j} = \left(d^{(\alpha)}_{N_\alpha-1}\, d^{(\beta)}_{N_\beta-1}\right)^{-1} \underset{\epsilon=\lambda_j}{Res}\, \widetilde{\mathcal{P}}_{\alpha,\beta}(\epsilon). \tag{17}$$

respectively.

Notice that eigenvalues $\{\lambda_j\}$ and rows $\left\{Z_{K_\alpha,j}, \alpha = \overline{1,\, N_c}\right\}$ of the eigenvectors matrix $\mathbf{Z}$ specify the set of the phase-equivalent potentials (1), (2) to within the orthogonal matrix $\mathbf{Z}$ construction method from given K_α-th rows [3, 4].

Bound states

The Fredholm determinant $\mathcal{D}^{(+)} \equiv \det(\mathcal{I} - \widehat{G}^{(+)}\widehat{V})$ corresponding to the potential (1), (2) is of the form

$$\mathcal{D}^{(+)} = \det\left[\mathcal{Q}^{(+)}_{N-1} - P\mathcal{J}\mathcal{Q}^{(+)}_{N}\right] \prod_{j=1}^{\mathcal{N}}(k^2-\lambda_j) \prod_{\alpha=1}^{N_c} \frac{-(N_\alpha+2\ell_\alpha+1)!}{(N_\alpha-1)!(2\ell_\alpha+1)!(k_\alpha^2+b^2)^{N_\alpha}}. \tag{18}$$

Here, $\mathcal{Q}^{(+)}_{N-1}$, $\mathcal{Q}^{(+)}_{N}$ are the diagonal matrices with the elements:

$$\left[\mathcal{Q}^{(+)}_{N-1}\right]_{\alpha,\alpha} = q^{\ell_\alpha(+)}_{N_\alpha-1}(k_\alpha), \qquad \left[\mathcal{Q}^{(+)}_{N}\right]_{\alpha,\alpha} = q^{\ell_\alpha(+)}_{N_\alpha}(k_\alpha). \tag{19}$$

Notice that the bound state with the energy $E_b = -\kappa^2$ corresponds to the zero of the Fredholm determinant

$$\det\left[\mathcal{Q}^{(+)}_{N-1} - P\mathcal{J}\mathcal{Q}^{(+)}_{N}\right]\Big|_{k=\mathrm{i}\kappa} = 0 \tag{20}$$

and the asymptotic normalization constants vector $\mathcal{M}$ of length N_c that obeys equation

$$\mathrm{i}\underset{k=\mathrm{i}\kappa}{Res}\,[S(k)]_{\alpha,\beta} = e^{\mathrm{i}\frac{\pi}{2}(\ell_\alpha+\ell_\beta)}\mathcal{M}_\alpha\mathcal{M}_\beta. \tag{21}$$

Closed channels

Unfortunately, direct use of equations (16) in order to obtain all λ_j is impossible, because only the open-channel sub-matrix of the S-matrix is accessible to experimental determination. However reference to Eqs (13), (18) shows that $\mathcal{D}^{(+)}$ (as a function of $k \equiv k_1$) has the pole at the point $k = -ib$ of multiplicity $2(N_1+\ell_1)$. In consequence of this the element $\mathcal{S}^{(\mathcal{N})}_{1,1}$ of the S-matrix (12) has the pole at the point $k_0 = ib$ of multiplicity $2(N_1 + \ell_1)$ in addition to the simple poles corresponding to the bound states. From this property of the S-matrix $\mathcal{S}^{(\mathcal{N})}$ (12) it follows that

$$\begin{gathered}
\frac{b}{\pi}\int\limits_0^\infty \frac{dk}{k^2+b^2}\left[C_m^{(1)(-)}(k) - C_m^{(1)(+)}(k)\overline{\mathcal{S}}^{(\mathcal{N})}_{1,1}(k)\right]\left[C_n^{(1)(-)}(k) - C_n^{(1)(+)}(k)\overline{\mathcal{S}}^{(\mathcal{N})}_{1,1}(k)\right]^* + \\
+\sum_{\nu=1}^{N_b}\frac{1}{2\kappa_\nu}\left(\frac{b^2-\kappa_\nu^2}{4b\kappa_\nu}\right)^{2\ell_1-1}\left(\mathcal{M}_1^{(\nu)}\right)^2 q_m^{\ell_1(+)}(\mathrm{i}\kappa_\nu)q_n^{\ell_1(+)}(\mathrm{i}\kappa_\nu)- \\
-\delta_{m,n}\frac{n!}{(n+2\ell_1+1)!(n+\ell_1+1)} = \\
= \mathrm{i}\,\underset{k=\mathrm{i}b}{Res}\,\frac{2b}{(k^2+b^2)}\left(1-\overline{\mathcal{S}}^{(\mathcal{N})}_{1,1}(k)\right)C_m^{(1)(+)}(k)C_n^{(1)(+)}(k), \\
m+n < 2N_1 - 1.
\end{gathered} \tag{22}$$

Inserting in the left hand side of (22) the "experimental" $\overline{\mathcal{S}}_{1,1}$ and setting $m+n < 2N_1-1$, we obtain in addition to (16), (17) 0 the equations in the parameters $\{\lambda_j,\ Z_{K_\alpha,j},\ \lambda_j < t_2^2\}$. Eqs (22) combined with the orthonormalization condition

$$\sum_{j=1}^{\mathcal{N}} Z_{K_\alpha,j}\, Z_{K_\beta,j} = \delta_{\alpha\beta} \tag{23}$$

gives the set of equations.

3 Example

As an example we consider the two coupled channels case. The "experimental" S-matrix corresponds to the (s-wave) interactions where the potential in each channel is given by straight well with the radius R and the depth V_0: $V_{11} = -V_0$ and $V_{22} = -V_0$. The off-diagonal part of the interaction is given by straight well with the radius R and the height $4V_0$, i. e. $V_{12} = V_{21} = 4V_0$. The threshold value of the second channel is given by $\hbar^2/2\mu T$. The interaction is specified by the set of the parameters:

$$\begin{gathered}
\mathcal{K}_{11}R = \frac{R}{\hbar}\sqrt{-2mV_0} = 1, \quad \mathcal{K}_{22}R = \frac{R}{\hbar}\sqrt{-2mV_0} = 1, \\
\mathcal{K}_{12}R = \frac{R}{\hbar}\sqrt{-8mV_0} = 1, \quad TR^2 = 2.25
\end{gathered} \tag{24}$$

Setting bR=3 and $N_1 = N_2 = 6$, we are able to describe the "experimental" S-matrix [5] behaviour on the interval $kR \in [0, 6]$. In this case only 10 in 12 parameters $\{\lambda_j\}$ and corresponding pairs $\{Z_{6,j},\ Z_{12,j}\}$, $j = \overline{3,\,12}$ can be obtained from Eqs (16), (17), since a bound state with the energy $E_b = -(\kappa R)^2$, $\kappa = .4658816565$ and asymptotic normalization constants $\mathcal{M}_1^2 = 1.1517792615$, $\mathcal{M}_1\mathcal{M}_2 = -3.4125588474$ exists in the system and is associated with the negative eigenvalue λ_1. Moreover, eigenvalue λ_2 belongs to the interval $[0,\ TR^2]$ where the second channel is closed (see Table). To fulfill the condition (23), we add to the unknown parameter list $\{\lambda_1,\ \lambda_2,\ Z_{6,1},\ Z_{6,2},\ Z_{12,1},\ Z_{12,2}\}$ the parameters $Z_{6,12}$ and $Z_{12,12}$. In our case the set of eight equations involved three conditions (23), Eqs (20), (21) and two Eqs (22) with combinations $m = 0$, $n = 7$ and $m = 0$, $n = 8$. Notice that all equations (20)-(23) are polynomial in the parameters $\{\lambda_j,\ Z_{K_\alpha,j}\}$. The results are presented in Table.

Table

$\ell_1 = \ell_2 = 0,\ bR = 3,\ N_1 = N_2 = 6,\ TR^2 = 2.25$

j	$Z_{6,j}$	$Z_{12,j}$	$\lambda_j R^2$
1	−.0374006646	−.0015223313	−.2019362768
2	−.1988751868	.0372809163	1.0446566297
3	.1139678173	.1332656469	2.8020660248
4	.2603833979	−.1532370931	3.7342907744
5	.2121413196	.2610086689	5.4540250659
6	.2260936623	−.2978434124	8.4744474489
7	.3650138463	.2484083127	12.838694393
8	.2289207539	−.3765434277	17.1376543674
9	.4285368721	.3437298697	34.3468296010
10	.3011079853	−.3998635888	43.6111561066
11	.4812119562	−.280391759	171.9167526468
12	.3010394551	.4902835493	176.3809094262

For comparison, the parameters $\widetilde{\lambda}_2$, $\widetilde{Z}_{6,2}$ and $\widetilde{Z}_{12,2}$ obtained from Eqs (16), (17) using the analytical continuation of the "experimental" S-matrix:

$$\widetilde{\lambda}_2 R = 1.0245524447, \quad \widetilde{Z}_{6,2} = .0391899547, \quad \widetilde{Z}_{12,2} = .0000099119. \tag{25}$$

The element $\mathcal{S}_{11}^{\mathcal{N}}$ of the "theory" S-matrix (solid line) and the element $\mathcal{S}_{11}$ of the "experimental" one (diamonds) are presented in Fig.1.

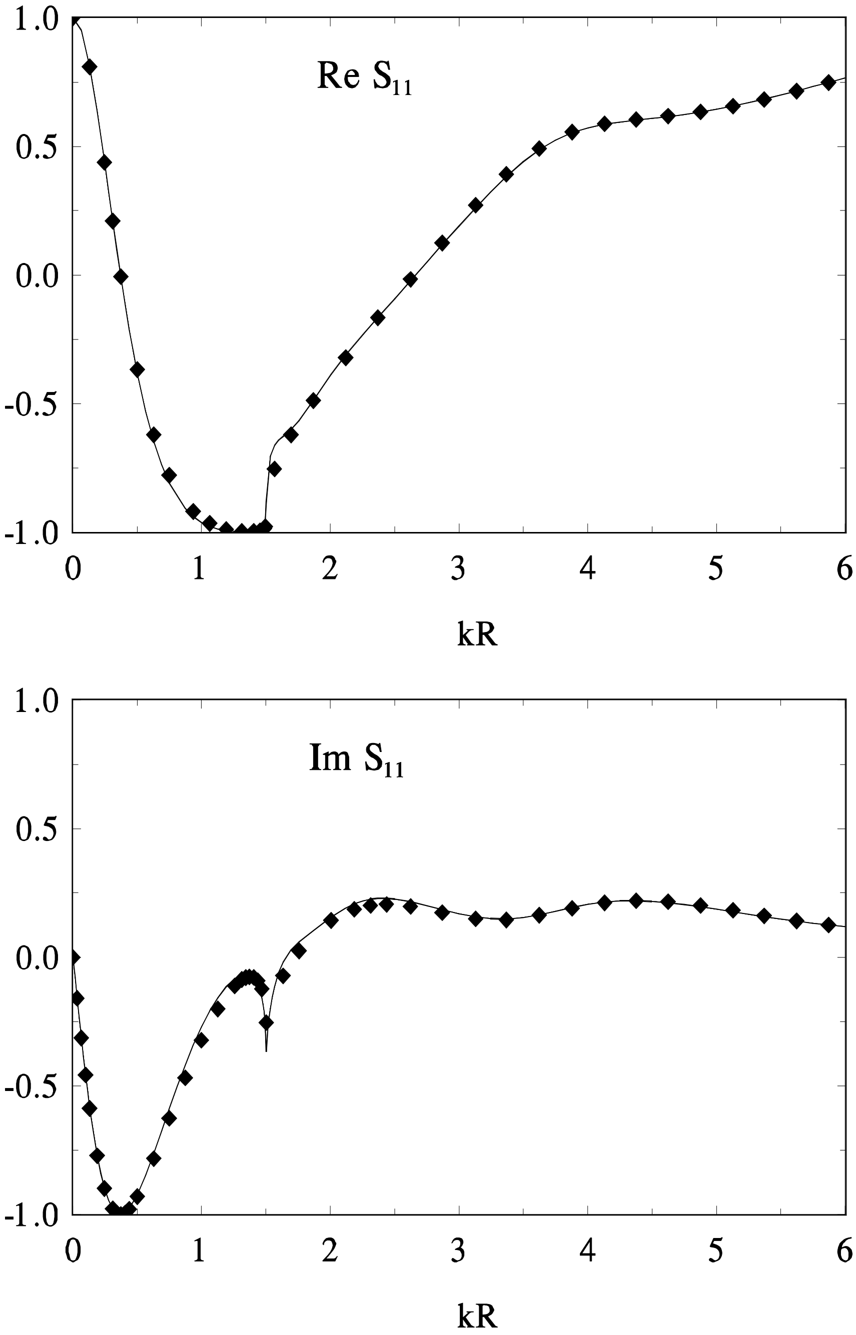

Figure 1: The element $\mathcal{S}_{11}$ of the S-matrix

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