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Analytic Structure and Power-Series Expansion of the Jost Matrix

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Abstract For the Jost-matrix that describes the multi-channel scattering, the momentum dependencies at all the branching points on the Riemann surface are factorized analytically. The remaining single-valued matrix functions of the energy are expanded in the power-series near an arbitrary point in the complex energy plane. A systematic and accurate procedure has been developed for calculating the expansion coefficients. This makes it possible to obtain an analytic expression for the Jost-matrix (and therefore for the S -matrix) near an arbitrary point on the Riemann surface (within the domain of its analyticity) and thus to locate the resonant states as the S -matrix poles. This approach generalizes the standard effective-range expansion that now can be done not only near the threshold, but practically near an arbitrary point on the Riemann surface of the energy. Alternatively, The semi-analytic (power-series) expression of the Jost matrix can be used for extracting the resonance parameters from experimental data. In doing this, the expansion coefficients can be treated as fitting parameters to reproduce experimental data on the real axis (near a chosen center of expansion E_0) and then the resulting semi-analytic matrix $S(E)$ can be used at the nearby complex energies for locating the resonances. Similarly to the expansion procedure in the three-dimensional space, we obtain the expansion for the Jost function describing a quantum system in the space of two dimensions (motion on a plane), where the logarithmic branching point is present.

1 Introduction

Power-series expansions are used in physics very often. An expansion of this kind that is most frequently used in quantum scattering theory, is known as the effective-range expansion. For a short-range potential, it reads

$$k^{2\ell+1} \cot \delta_\ell(k) = \sum_{n=0}^{\infty} c_{\ell n} k^{2n}, \quad (1)$$

where $\delta_\ell(k)$ is the scattering phase shift and the right-hand side is a sum of terms proportional to even powers of the collision momentum k , i.e. to the powers of the energy $E \sim k^2$. The $c_{\ell n}$ are energy independent expansion coefficients.

This expansion was suggested long ago in nuclear physics for the S -wave nucleon-nucleon scattering in the form

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$$k \cot \delta_0(k) = -\frac{1}{a} + \frac{1}{2}r_0k^2 - Pr_0^3k^4 + Qr_0^5k^6 + \dots, \quad (2)$$

where the first two parameters on the right-hand side, namely, a and r_0 , were called the scattering length and the effective radius.

The traditional approach has one significant limitation, namely, the effective-range expansion is only applicable near the point $k = 0$, i.e. when the energy is close to the threshold. Another limitation of the expansion (1) consists in the fact that it is written for a single-channel problem.

In the present work, we suggest a more general power-series expansions (for the Jost matrix and thus for S -matrix) which are done not only near the threshold, like $\sum_n d_n E^n$, but around an arbitrary point E_0 on the complex energy surface, i.e. $\sum_n q_n (E - E_0)^n$. We also generalize it for multichannel problems, and for two-dimensional problems, where the Riemann surface of the energy has logarithmic singularity.

2 Single-Channel Case

In order to make the basic idea clear, let us begin with the simplest single-channel problem for a spherically symmetric short-range (exponentially decaying) potential,

$$V(r) \xrightarrow{r \rightarrow \infty} \sim e^{-\eta r}, \quad \eta > 0. \quad (3)$$

At large distances ($r \rightarrow \infty$) the radial Schrödinger equation

$$\left[\partial_r^2 + k^2 - \frac{\ell(\ell+1)}{r^2} \right] u_\ell(k, r) = V(r)u_\ell(k, r) \quad (4)$$

becomes the Riccati-Bessel equation,

$$\left[\partial_r^2 + k^2 - \frac{\ell(\ell+1)}{r^2} \right] u_\ell(k, r) \simeq 0, \quad (5)$$

whose two independent solutions are any pair of the Riccati-Bessel, Riccati-Neumann, and the Riccati-Hankel functions [1]: $j_\ell(kr)$, $y_\ell(kr)$, $h_\ell^{(+)}(kr)$, $h_\ell^{(-)}(kr)$. If we choose the pair $h_\ell^{(\pm)}$ then any other solution is their linear combination, and thus

$$u_\ell(k, r) \xrightarrow{r \rightarrow \infty} C_1 h_\ell^{(-)}(kr) + C_2 h_\ell^{(+)}(kr). \quad (6)$$

Since the Riccati-Hankel functions describe the incoming and outgoing spherical waves,

$$h_\ell^{(\pm)}(kr) \xrightarrow{|kr| \rightarrow \infty} \mp i \exp\left(\pm ikr + i\frac{\ell\pi}{2}\right), \quad (7)$$

the combination coefficients in Eq. (6) are the corresponding amplitudes,

$$u_\ell(k, r) \xrightarrow{r \rightarrow \infty} f_\ell^{(\text{in})}(k)h_\ell^{(-)}(kr) + f_\ell^{(\text{out})}(k)h_\ell^{(+)}(kr). \quad (8)$$

These amplitudes $f_\ell^{(\text{in/out})}(k)$ depend on the momentum k and are called the Jost functions. Formally, we consider them as the functions of complex variable k . Of course the Jost functions $f_\ell^{(\text{in})}(k)$ and $f_\ell^{(\text{out})}(k)$ are not independent from each other. Indeed, the incoming and outgoing spherical waves swap their roles under complex conjugation as well as when the momentum changes its sign. It is not difficult to show that these functions have the symmetry properties summarized in Fig. 1, where the dashed lines connect the points at which the values indicated next to them are identical.

The ratio of the amplitudes of the outgoing and incoming spherical waves,

$$s_\ell(k) = \frac{f_\ell^{(\text{out})}(k)}{f_\ell^{(\text{in})}(k)}, \quad (9)$$

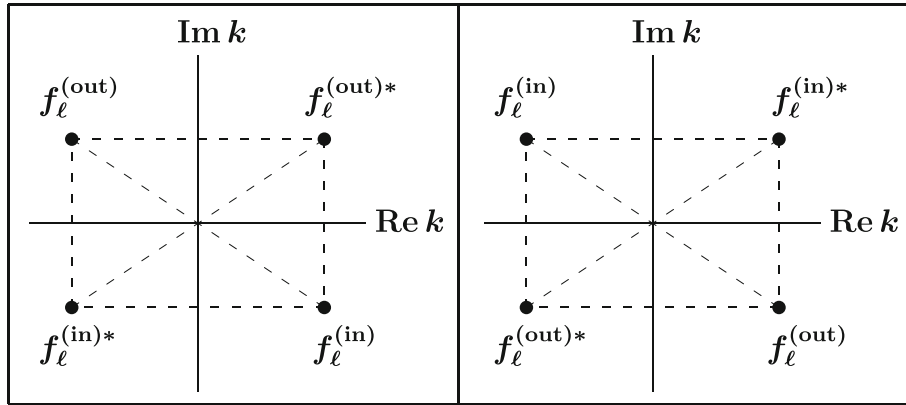


Fig. 1 The Jost functions or their complex conjugate values are equal at the points connected with the *dashed lines*

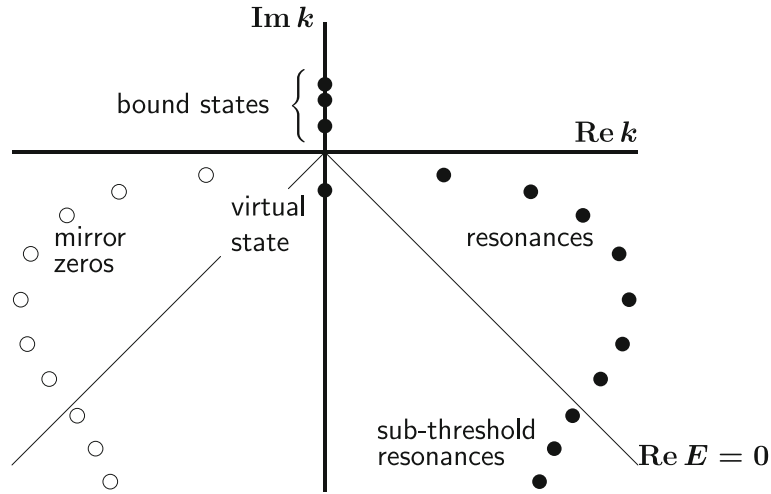


Fig. 2 Typical distribution of the spectral points in the complex momentum plane. Each resonance spectral point has a partner which is symmetric relative to the imaginary axis (*open circles*)

gives the S -matrix that determines all the scattering observables. The zeros of the Jost function at complex momenta k_n ($n = 1, 2, 3, \dots$),

$$f_\ell^{(\text{in})}(k_n) = 0, \quad (10)$$

correspond to the spectral points shown in Fig. 2. This simple picture with the Jost function defined on a single complex plane, is only possible in the case of a single-channel problem. When we have more than one channel, there are several channel momenta, but still only one total energy. Therefore it is more logical and consistent to consider (even for the single-channel case) the Jost function as a function of the energy, i.e.

$$f_\ell^{(\text{in/out})}(k) \rightarrow f_\ell^{(\text{in/out})}(E)$$

This, however, reveals a complication: $f_\ell^{(\text{in/out})}(E)$ are not single-valued functions. Indeed, for each value of the energy, we have two values of the momentum,

$$k = \pm \sqrt{\frac{2\mu E}{\hbar^2}}. \quad (11)$$

Therefore, as a function of E , the Jost function is defined on a Riemann surface. For a single-channel problem this surface consists of two layers and has one branching point at $E = 0$. The bound states are represented

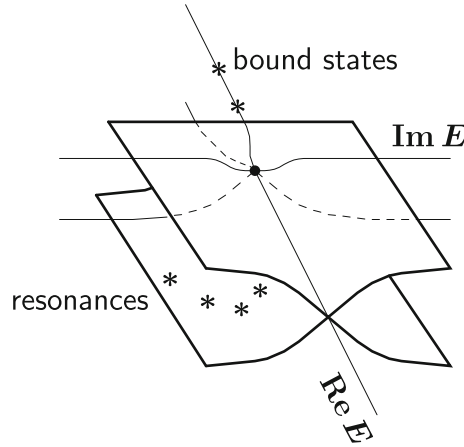


Fig. 3 Typical distribution of bound and resonant states on the Riemann surface of the energy for a single-channel problem

here by zeros of the Jost function on the negative real axis of the physical sheet and resonances by zeros on the non-physical sheet.

How can we calculate the Jost functions for a given potential? In order to find a method, we look at the asymptotic behaviour (8) of the radial wave function, which is valid at large distances where the potential is zero. Let us look for the solution of radial Schrödinger equation in a similar form at all r ,

$$u_\ell(E, r) = F_\ell^{(\text{in})}(E, r)h_\ell^{(-)}(kr) + F_\ell^{(\text{out})}(E, r)h_\ell^{(+)}(kr), \tag{12}$$

where the coefficients of the Riccati-Hankel functions are not constants anymore, but are some unknown functions depending on the radius. Apparently, if we cut off the potential at a point $r = R$, then these functions should coincide with the Jost functions,

$$V(r > R) \equiv 0 \Rightarrow F_\ell^{(\text{in/out})}(E, R) = f_\ell^{(\text{in/out})}(E). \tag{13}$$

If we do not cut the potential off, then these functions must approach the Jost functions asymptotically at large distances

$$\lim_{r \rightarrow \infty} F_\ell^{(\text{in/out})}(E, r) = f_\ell^{(\text{in/out})}(E). \tag{14}$$

Substituting the ansatz (12) for $u_\ell(E, r)$ into the Schrödinger equation, we obtain (the details can be found in Refs. [2–13]) the following system of first-order differential equations for the new unknown functions

$$\partial_r F_\ell^{(\text{in})} = -\frac{1}{2ik} h_\ell^{(+)} V \left[F_\ell^{(\text{in})} h_\ell^{(-)} + F_\ell^{(\text{out})} h_\ell^{(+)} \right], \tag{15}$$

$$\partial_r F_\ell^{(\text{out})} = \frac{1}{2ik} h_\ell^{(-)} V \left[F_\ell^{(\text{in})} h_\ell^{(-)} + F_\ell^{(\text{out})} h_\ell^{(+)} \right], \tag{16}$$

with simple boundary conditions at $r = 0$

$$F_\ell^{(\text{in})}(E, 0) = F_\ell^{(\text{out})}(E, 0) = 1/2, \tag{17}$$

which follow from the fact that physical wave function is regular at the origin.

Therefore the recipe for calculating the Jost functions is very simple. For a given complex value of the momentum k , We start at $r = 0$ with the boundary values (17) and numerically integrate the differential Eqs. (15, 16) to a sufficiently large distance R where the potential is negligibly small. The values obtained in such a way should coincide with the Jost functions in accordance with Eq. (14).

If the energy is real, this method works perfectly well. For complex energies, there is one technical complication here. The problem is that according to the asymptotics (7) with complex $k = k_r \pm i\kappa$, one of the functions $h_\ell^{(\pm)}(kr)$ is always divergent at large r ,

$$h_\ell^{(-)}(kr) \sim e^{\pm\kappa r}, \quad h_\ell^{(+)}(kr) \sim e^{\mp\kappa r}. \tag{18}$$

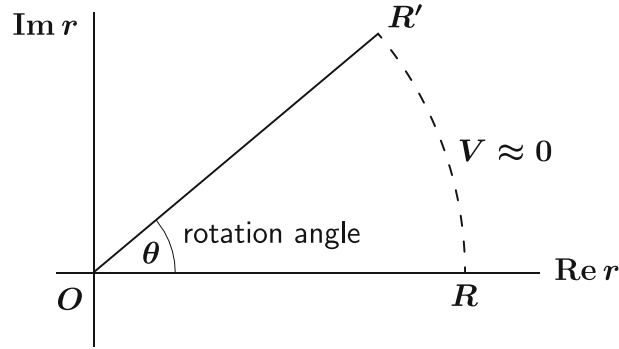


Fig. 4 The complex path $OR'R$ for integrating Eqs. (15, 16) with $k = |k| \exp(-i\theta)$

As a result, we cannot reach the limits of $F_\ell^{(\text{in/out})}$ by numerically integrating Eqs. (15, 16) along the real axis. We can circumvent this difficulty, if make a detour via complex r -plane ($OR'R$ as is shown in Fig. 4) in such a way that the product kr remains real on the integration path OR' ,

$$kr = |k|e^{-i\theta} \cdot |r|e^{+i\theta} \Rightarrow \text{Im}(kr) = 0, \quad (19)$$

where θ is the polar angle of the complex number k . On the arc $R'R$, the potential is zero and thus this segment can be ignored.

2.1 Factorization of the Branching Dependence

Functions $f_\ell^{(\text{in})}(E)$ and $f_\ell^{(\text{out})}(E)$ are double-valued because they involve the dependence on odd powers of k . To explicitly separate such a dependence, we construct the following linear combinations of the functions $F_\ell^{(\text{in/out})}(E, r)$

$$A_\ell = F_\ell^{(\text{in})} + F_\ell^{(\text{out})}, \quad B_\ell = i \left[F_\ell^{(\text{in})} - F_\ell^{(\text{out})} \right]. \quad (20)$$

The corresponding combinations of Eqs. (15, 16) give an equivalent set of equations,

$$\partial_r A_\ell = -\frac{1}{k} y_\ell V [A_\ell j_\ell - B_\ell y_\ell], \quad (21)$$

$$\partial_r B_\ell = -\frac{1}{k} j_\ell V [A_\ell j_\ell - B_\ell y_\ell], \quad (22)$$

with the boundary conditions

$$A_\ell(E, 0) = 1, \quad B_\ell(E, 0) = 0. \quad (23)$$

Now, we use the fact that the Riccati-Bessel and Riccati-Neumann functions can be represented by absolutely convergent series,

$$j_\ell(kr) = k^{\ell+1} \tilde{j}_\ell(E, r), \quad y_\ell(kr) = k^{-\ell} \tilde{y}_\ell(E, r), \quad (24)$$

where we factorized the “tilded” functions

$$\tilde{j}_\ell(E, r) = \left(\frac{r}{2}\right)^{\ell+1} \sum_{n=0}^{\infty} \frac{(-1)^n \sqrt{\pi}}{\Gamma(\ell + 3/2 + n)n!} \left(\frac{kr}{2}\right)^{2n}, \quad (25)$$

$$\tilde{y}_\ell(E, r) = \left(\frac{2}{r}\right)^\ell \sum_{n=0}^{\infty} \frac{(-1)^{n+\ell+1}}{\Gamma(-\ell + 1/2 + n)n!} \left(\frac{kr}{2}\right)^{2n} \quad (26)$$

that do not depend on odd powers of k and thus are single-valued holomorphic functions of the energy E .

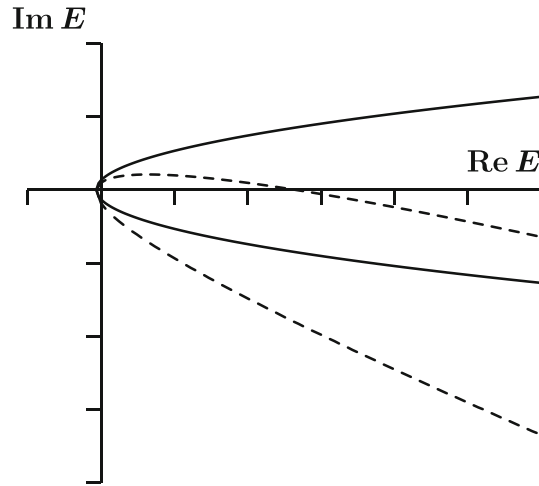


Fig. 5 Typical domain \mathcal{D} within which the functions $\tilde{a}_\ell(E)$ and $\tilde{b}_\ell(E)$ are holomorphic. The *dashed curve* shows \mathcal{D} for the rotation angle $\theta = 0.05\pi$

Introducing the tilded functions

$$\tilde{A}_\ell(E, r) = A_\ell(E, r) \text{ and } \tilde{B}_\ell(E, r) = k^{-(2\ell+1)} B_\ell(E, r), \quad (27)$$

and substituting them in Eqs. (21, 22), we obtain the following differential equations that do not involve any odd powers of k

$$\partial_r \tilde{A}_\ell = -\tilde{y}_\ell V \left[\tilde{A}_\ell \tilde{j}_\ell - \tilde{B}_\ell \tilde{y}_\ell \right], \quad (28)$$

$$\partial_r \tilde{B}_\ell = -\tilde{j}_\ell V \left[\tilde{A}_\ell \tilde{j}_\ell - \tilde{B}_\ell \tilde{y}_\ell \right]. \quad (29)$$

At any finite r , all the coefficients of these equations are holomorphic functions of E . The boundary conditions,

$$\tilde{A}_\ell(E, 0) = 1, \quad \tilde{B}_\ell(E, 0) = 0, \quad (30)$$

do not depend on E . According to the Poincaré theorem [14], See also [15], this means that $\tilde{A}_\ell(E, r)$ and $\tilde{B}_\ell(E, r)$ are also holomorphic functions of the energy parameter E at any finite r . It can be proved [13] that for the short-range potentials of the type (3), their limits

$$\tilde{a}_\ell(E) = \lim_{r \rightarrow \infty} \tilde{A}_\ell(E, r), \quad \tilde{b}_\ell(E) = \lim_{r \rightarrow \infty} \tilde{B}_\ell(E, r) \quad (31)$$

remain holomorphic within certain domain \mathcal{D} along the real energy-axis and this domain can be extended using complex rotation of the coordinate, as is shown in Fig. 5.

Combining all the definitions, we have

$$f_\ell^{(\text{in})}(E) = \frac{1}{2} \left[\tilde{a}_\ell(E) - ik^{2\ell+1} \tilde{b}_\ell(E) \right], \quad (32)$$

$$f_\ell^{(\text{out})}(E) = \frac{1}{2} \left[\tilde{a}_\ell(E) + ik^{2\ell+1} \tilde{b}_\ell(E) \right]. \quad (33)$$

These representations give us the analytic structure of the Jost functions that we were looking for. Indeed, all the “trouble” with the fact that they are double-valued, is caused by the factor $k^{2\ell+1}$ while $\tilde{a}_\ell(E)$ and $\tilde{b}_\ell(E)$ are “nice” single-valued functions defined in the domain \mathcal{D} of a single energy-plane.

2.2 Power-Series Expansion

Since the functions $\tilde{a}_\ell(E)$ and $\tilde{b}_\ell(E)$ are analytic, they can be expanded in Taylor series,

$$\tilde{a}_\ell(E) = \sum_{n=0}^{\infty} \alpha_n (E - E_0)^n, \quad \tilde{b}_\ell(E) = \sum_{n=0}^{\infty} \beta_n (E - E_0)^n, \quad (34)$$

near an arbitrary point E_0 within the domain \mathcal{D} of their analyticity. Apparently, everything what is said about the functions $\tilde{a}_\ell(E)$ and $\tilde{b}_\ell(E)$, is also valid for the functions $\tilde{A}_\ell(E, r)$ and $\tilde{B}_\ell(E, r)$ because they have the same meaning for a potential cut off at the distance r . Therefore

$$\tilde{A}_\ell(E, r) = \sum_{n=0}^{\infty} \mathcal{A}_n(r) (E - E_0)^n, \quad \tilde{B}_\ell(E, r) = \sum_{n=0}^{\infty} \mathcal{B}_n(r) (E - E_0)^n, \quad (35)$$

where

$$\alpha_n = \lim_{r \rightarrow \infty} \mathcal{A}_n(r), \quad \beta_n = \lim_{r \rightarrow \infty} \mathcal{B}_n(r). \quad (36)$$

The expansion coefficients $\mathcal{A}_n(r)$, $\mathcal{B}_n(r)$ can be obtained by substituting the series (35) together with

$$\tilde{j}_\ell(E, r) = \sum_{n=0}^{\infty} \mathcal{J}_n(r) (E - E_0)^n, \quad \tilde{y}_\ell(E, r) = \sum_{n=0}^{\infty} \mathcal{Y}_n(r) (E - E_0)^n \quad (37)$$

(a procedure for finding the coefficients \mathcal{J}_n and \mathcal{Y}_n is given in Ref. [12]) into the differential Eqs. (28, 29). Then, equalizing the terms of the same powers of $(E - E_0)$, we obtain

$$\partial_r \mathcal{A}_n = - \sum_{i+j+k=n} \mathcal{Y}_i V (\mathcal{A}_j \mathcal{J}_k - \mathcal{B}_j \mathcal{Y}_k), \quad (38)$$

$$\partial_r \mathcal{B}_n = - \sum_{i+j+k=n} \mathcal{J}_i V (\mathcal{A}_j \mathcal{J}_k - \mathcal{B}_j \mathcal{Y}_k), \quad (39)$$

with the boundary conditions $\mathcal{A}_n(0) = \delta_{n0}$, $\mathcal{B}_n(0) = 0$, $n = 0, 1, 2, \dots$

Thanks to the condition $i + j + k = n$, not all equations are coupled to each other,

$$\begin{aligned} \partial_r \mathcal{A}_0 &= -\mathcal{Y}_0 V (\mathcal{A}_0 \mathcal{J}_0 - \mathcal{B}_0 \mathcal{Y}_0), \\ \partial_r \mathcal{B}_0 &= -\mathcal{J}_0 V (\mathcal{A}_0 \mathcal{J}_0 - \mathcal{B}_0 \mathcal{Y}_0), \\ \partial_r \mathcal{A}_1 &= -\mathcal{Y}_1 V (\mathcal{A}_0 \mathcal{J}_0 - \mathcal{B}_0 \mathcal{Y}_0) - \mathcal{Y}_0 V (\mathcal{A}_1 \mathcal{J}_0 - \mathcal{B}_1 \mathcal{Y}_0) - \mathcal{Y}_0 V (\mathcal{A}_0 \mathcal{J}_1 - \mathcal{B}_0 \mathcal{Y}_1), \\ \partial_r \mathcal{B}_1 &= -\mathcal{J}_1 V (\mathcal{A}_0 \mathcal{J}_0 - \mathcal{B}_0 \mathcal{Y}_0) - \mathcal{J}_0 V (\mathcal{A}_1 \mathcal{J}_0 - \mathcal{B}_1 \mathcal{Y}_0) - \mathcal{J}_0 V (\mathcal{A}_0 \mathcal{J}_1 - \mathcal{B}_0 \mathcal{Y}_1), \\ &\text{etc} \quad \dots \end{aligned}$$

Therefore, the procedure of expanding the Jost functions near an arbitrary point E_0 consists in solving a finite number $n = 0, 1, 2, \dots, M$ of equations of this system up to a sufficiently large distance $R \rightarrow \infty$ (along the path shown in Fig. 4). Then the expansion coefficients are $\alpha_n = \mathcal{A}_n(R)$, $\beta_n = \mathcal{B}_n(R)$. As a result, we obtain the semi-analytic expressions

$$f_\ell^{(\text{in/out})}(E) \approx \frac{1}{2} \sum_{n=0}^M (\alpha_n \mp ik^{2\ell+1} \beta_n) (E - E_0)^n \quad (40)$$

that are valid around the point E_0 (which can be far away from the threshold).

2.3 Standard Effective-Range Expansion

Standard effective-range expansion (1) is the particular case of our expansion with $E_0 = 0$. In such a case, we have

$$f_\ell^{(\text{in/out})} \approx \frac{1}{2} \sum_{n=0}^M (\alpha_n \mp ik^{2\ell+1} \beta_n) E^n. \quad (41)$$

Since $f_\ell^{(\text{in/out})} = e^{\mp i\delta_\ell}$ and thus $f_\ell^{(\text{out})} + f_\ell^{(\text{in})} = 2 \cos \delta_\ell$, $f_\ell^{(\text{out})} - f_\ell^{(\text{in})} = 2i \sin \delta_\ell$, we obtain

$$k^{2\ell+1} \cot \delta_\ell = \frac{\alpha_0 + \alpha_1 E + \alpha_2 E^2 + \dots}{\beta_0 + \beta_1 E + \beta_2 E^2 + \dots} = \frac{\alpha_0}{\beta_0} + \left(\frac{\alpha_1}{\beta_0} - \frac{\alpha_0 \beta_1}{\beta_0^2} \right) E + \dots, \quad (42)$$

where the quantities α_n, β_n can be calculated by solving Eqs. (38, 39), as described in Sect. 2.2.

3 Multi-Channel Jost Matrix

Everything that was described in previous sections, can be generalized for the case of an N -channel problem. We start with the radial Schrödinger equation,

$$\left[\partial_r^2 + k_n^2 - \frac{\ell_n(\ell_n + 1)}{r^2} \right] u_n(E, r) = \sum_{n'=1}^N V_{nn'}(r) u_{n'}(E, r), \quad (43)$$

where the channel momentum $k_n = \pm \sqrt{\frac{2\mu_n}{\hbar^2} (E - E_n)}$ is expressed via the channel reduced mass μ_n and the threshold energy E_n . It is well known (see, for example, Ref. [16]) that Eq. (43) has $2N$ linearly independent column-solutions and only half of them are regular at $r = 0$. Combining the regular columns in a square matrix, we obtain the fundamental matrix of regular solutions,

$$\Phi(E, r) = \begin{pmatrix} \phi_{11}(E, r) & \phi_{12}(E, r) & \dots & \phi_{1N}(E, r) \\ \phi_{21}(E, r) & \phi_{22}(E, r) & \dots & \phi_{2N}(E, r) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{N1}(E, r) & \phi_{N2}(E, r) & \dots & \phi_{NN}(E, r) \end{pmatrix}. \quad (44)$$

Any physical solution is regular and therefore can be written as a linear combination of the columns (44),

$$\begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix} = C_1 \begin{pmatrix} \phi_{11} \\ \phi_{21} \\ \vdots \\ \phi_{N1} \end{pmatrix} + C_2 \begin{pmatrix} \phi_{12} \\ \phi_{22} \\ \vdots \\ \phi_{N2} \end{pmatrix} + \dots + C_N \begin{pmatrix} \phi_{1N} \\ \phi_{2N} \\ \vdots \\ \phi_{NN} \end{pmatrix}, \quad (45)$$

where the combination coefficients C_n are determined by the boundary conditions. When $r \rightarrow \infty$, the potential vanishes and the equations of the system (43) become the Riccati-Bessel equations. The $2N$ linearly independent column-solutions of this simplified system can be combined in two square matrices,

$$W^{(\text{in/out})} = \begin{pmatrix} h_{\ell_1}^{(\mp)}(k_1 r) & 0 & \dots & 0 \\ 0 & h_{\ell_2}^{(\mp)}(k_2 r) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \vdots & h_{\ell_N}^{(\mp)}(k_N r) \end{pmatrix}, \quad (46)$$

describing the incoming ($W^{(\text{in})}$) and outgoing ($W^{(\text{out})}$) waves. These $2N$ columns form a basis in the space of solutions when $r \rightarrow \infty$. Therefore at large distances each column of matrix (44) is a linear combination of the $2N$ columns (46). This can be written as

$$\Phi(E, r) \xrightarrow{r \rightarrow \infty} W^{(\text{in})}(E, r) f^{(\text{in})}(E) + W^{(\text{out})}(E, r) f^{(\text{out})}(E), \quad (47)$$

where the energy-dependent matrices $f^{(\text{in/out})}(E)$ are called Jost matrices. It is not difficult to show that they determine the S -matrix,

$$S(E) = f^{(\text{out})}(E) \left[f^{(\text{in})}(E) \right]^{-1}, \quad (48)$$

and thus give complete description of the underlying physical system. The spectral points $E = \mathcal{E}_n$ (bound states and resonances) are those where the inverse matrix $[F^{(\text{in})}(E)]^{-1}$ does not exist, i.e. the points where $\det f^{(\text{in})}(\mathcal{E}_n) = 0$.

Using the same approach as in the single-channel case, it can be shown (see Ref. [13]) that the elements of the Jost matrices have the following analytic structure

$$f_{mn}^{(\text{in/out})}(E) = \frac{k_n^{\ell_n+1}}{2k_m^{\ell_m+1}} \tilde{a}_{mn}(E) \mp i \frac{k_m^{\ell_m} k_n^{\ell_n+1}}{2} \tilde{b}_{mn}(E), \quad (49)$$

where matrix functions $\tilde{a}(E)$ and $\tilde{b}(E)$ are holomorphic. Within their analyticity domain (see the same Fig. 5), they can be expanded in the power series,

$$\tilde{a}(E) = \sum_{n=0}^{\infty} \alpha_n (E - E_0)^n, \quad \tilde{b}(E) = \sum_{n=0}^{\infty} \beta_n (E - E_0)^n, \quad (50)$$

where the matrices α_n and β_n are determined in the same manner as in the single-channel case. Actually, the corresponding equations formally remain exactly the same as Eqs. (35, 36, 37, 38, 39). The only difference is that now all the quantities in these equation are matrices.

4 Two-Dimensional Problem

The two-dimension motion of a quantum particle requires special treatment. When the particle is restricted to move on a plane, its angular momentum ℓ can only be directed either up or down, i.e. $m = \pm\ell$. In such a case the partial-wave analysis (see, for example, Ref. [17]) gives the following radial Schrödinger equation

$$\left[\partial_r^2 + k^2 - \frac{\lambda(\lambda+1)}{r^2} - V(r) \right] u_\ell(E, r) = 0, \quad (51)$$

where $\lambda = \ell - 1/2$. Formally, this equation looks the same as Eq. (4). However, the simple fact that $\lambda = -1/2, 1/2, 3/2, \dots$ is half-integer, significantly changes the analytic properties of the Jost functions $f_\ell^{(\text{in/out})}(E)$ defined as the amplitudes of the incoming and outgoing circular waves,

$$u_\ell(E, r) \xrightarrow{r \rightarrow \infty} f_\ell^{(\text{in})}(E) h_{\ell-1/2}^{(-)}(kr) + f_\ell^{(\text{out})}(E) h_{\ell-1/2}^{(+)}(kr). \quad (52)$$

The power-series expansions of these circular waves $h_\lambda^{(\pm)}(z) = j_\lambda(z) \pm i y_\lambda(z)$ obtained from

$$j_\lambda(kr) = k^{\lambda+1} \sum_{n=0}^{\infty} k^{2n} t_n^{(\lambda)}(r) \text{ and } y_\lambda(kr) = k^{-\lambda} \sum_{n=0}^{\infty} k^{2n} g_n^{(\lambda)}(r) + h(k) j_\lambda(kr), \quad (53)$$

involve the logarithmic factor $h(k) = (2/\pi) \ln(k\rho/2)$, where ρ is the unit of length. The coefficients of the series (53) can be obtained using formulae 9.1.2, 9.1.10 and 9.1.11 of Ref. [1].

Following the same method as in Sec. 2.1, we can explicitly factorize the logarithmic dependence of the Jost functions,

$$f_\ell^{(\text{in/out})}(E) = \frac{1}{2} \left\{ \tilde{a}_\ell(E) + k^{2\lambda+1} [h(k) \mp i] \tilde{b}_\ell(E) \right\}, \quad (54)$$

where $\tilde{a}_\ell(E)$ and $\tilde{b}_\ell(E)$ are single-valued analytic functions in the domain \mathcal{D} that looks like it is shown in Fig. 5. These functions are determined by the same Eqs. (28, 29, 30, 31) where the holomorphic parts \tilde{j}_ℓ and \tilde{y}_ℓ of the Riccati functions are defined as

$$j_\lambda(kr) = k^{\lambda+1} \tilde{j}_\ell(E, r), \quad y_\lambda(kr) = k^{-\lambda} \tilde{y}_\lambda(E, r) + k^{\lambda+1} h(k) \tilde{j}_\ell(E, r). \quad (55)$$

Within the domain \mathcal{D} , the holomorphic functions $\tilde{a}_\ell(E)$ and $\tilde{b}_\ell(E)$ can be expanded in the Taylor series around an arbitrary point E_0 in the same way as it is done in Sect. 2.2. As a result, we obtain the corresponding expansions of the Jost functions,

$$f_\ell^{(\text{in/out})}(E) = \frac{1}{2} \sum_{n=0}^{\infty} \left\{ \alpha_n^{(\ell)}(E_0) + k^{2\lambda+1} [h(k) \mp i] \beta_n^{(\ell)}(E_0) \right\} (E - E_0)^n. \quad (56)$$

In the particular case $E_0 = 0$, these series give the two-dimensional effective-range expansion,

$$\begin{aligned} k^{2\lambda+1} [\cot \delta_\ell(E) - h(k)] &= \frac{\sum_{n=0}^{\infty} \alpha_n^{(\ell)}(0) E^n}{\sum_{n=0}^{\infty} \beta_n^{(\ell)}(0) E^n} \\ &= \frac{\alpha_0^{(\ell)}}{\beta_0^{(\ell)}} \left[1 + \left(\frac{\alpha_1^{(\ell)}}{\alpha_0^{(\ell)}} - \frac{\beta_1^{(\ell)}}{\beta_0^{(\ell)}} \right) E + \dots \right]. \end{aligned} \quad (57)$$

5 Conclusion

We consider three- and two-dimensional problems with short-range potentials. In all the cases, we show that the Jost function (or each element of the Jost matrix) can be written as a sum of terms that involve holomorphic functions of the energy E and certain functions of the momentum having branching points. For the holomorphic energy-dependent functions, we obtain a system of differential equations. Then we expand these functions in the power series around an arbitrary point E_0 within certain domain \mathcal{D} and obtain differential equations that determine the expansion coefficients.

The suggested method makes it possible to obtain semi-analytic expressions for the Jost functions around an arbitrary point on the Riemann surface. The resonant states thus can be located as the S -matrix poles. Alternatively, if the unknown expansion coefficients are treated as fitting parameters, the scattering data can be parametrized. Such a parametrization has the correct analytic structure. When the parameters are found by fitting the data given at real energies, the semi-analytic Jost function can be used to explore the nearby complex energies in search for possible resonances. In this way the resonance parameters can be extracted directly from experimental data.

References

1. Abramowitz, M., Stegun, A. (eds.): Handbook of mathematical functions. National Bureau of Standards, Washington, DC (1964)
2. Rakityansky, S.A., Sofianos, S.A., Amos, K.: A method of calculating the Jost function for analytic potentials. *Nuovo Cimento B* **111**, 363–378 (1996)
3. Sofianos, S.A., Rakityansky, S.A.: Exact method for locating potential resonances and Regge trajectories. *J. Phys. A: Math. Gen.* **30**, 3725 (1997)
4. Sofianos, S.A., Rakityansky, S.A., Vermaak, G.P.: Sub-threshold resonances in few-neutron systems. *J. Phys. G: Nucl. Part. Phys.* **23**, 1619–1629 (1997)
5. Rakityansky, S.A., Sofianos, S.A.: Jost function for coupled partial waves. *J. Phys. A: Math. Gen.* **31**, 514975 (1998)
6. Sofianos, S.A., Rakityansky, S.A., Massen, S.E.: Jost function for singular potentials. *Phys. Rev. A* **60**, 33743 (1999)
7. Rakityansky, S.A., Sofianos, S.A.: Jost function for coupled channels. *Few-Body Syst. Suppl.* **10**, 93–96 (1999)
8. Massen, S.E., Sofianos, S.A., Rakityansky, S.A., Oryu, S.: Resonances and off-shell characteristics of effective interactions. *Nucl. Phys. A* **654**, 597–611 (1999)
9. Rakityansky, S.A.: Unified treatment of bound, scattering, and resonant states in one-dimensional semiconductor nanostructures. *Phys. Rev. B* **68**, 195320 (2003)

10. Rakityansky, S.A.: Modified transfer matrix for nanostructures with arbitrary potential profile. *Phys. Rev. B* **70**, 205323 (2004)
11. Rakityansky, S.A., Sofianos, S.A., Elander, N.: Pade approximation of the S -matrix as a way of locating quantum resonances and bound states. *J. Phys. A: Math. Theor.* **40**, 14857–14869 (2007)
12. Rakityansky, S.A., Elander, N.: Generalized effective-range expansion. *J. Phys. A: Math. Theor.* **42**, 225302 (2009)
13. Rakityansky, S.A., Elander, N.: Multi-channel analog of the effective-range expansion. *J. Phys. A: Math. Theor.* **44**, 115303 (2011)
14. Poincaré, H.: Sur les groupes des équations linéaires. *Acta Math.* **4**, 201–311 (1884)
15. Lefschetz, S.: *Differential equations: geometric theory*. Interscience, New York (1957)
16. Brand, L.: *Differential and difference equations*. John Wiley & Sons Inc., New York (1966)
17. Rakityansky, S.A., Elander, N.: Analytic structure and power-series expansion of the Jost function for the two-dimensional problem. arXiv:1201.0172v1 [quant-ph] (2012)