Explicit Representations for the T-Matrix on Unphysical Energy Sheets and Resonances in Two- and Three-Body Systems

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Abstract. We describe basic structure of the two- and three-body T-matrices, scattering matrices, and resolvents continued to the unphysical energy sheets. The description is based on the explicit representations that have been found for analytically continued kernels of the T-operators.

1 Introduction

Resonance is one of the most interesting and intriguing phenomena in quantum scattering. With a resonance one usually associates an unstable state that only exists during a certain time. The original idea of interpreting resonances in quantum mechanics as complex poles of the scattering amplitude (and hence, as those of the scattering matrix) goes back to G. Gamov (1928). For radially symmetric potentials, the interpretation of two-body resonances as poles of the analytic continuation of the scattering matrix has been entirely elaborated in terms of the Jost functions. Beginning with E. C. Titchmarsh (1946) it was also realized that the s-matrix resonances may show up as poles of the analytic continuation of the Green functions.

Another, somewhat distinct approach to resonances is known as the complex scaling (or complex rotation) method. The complex scaling makes it possible to rotate the continuous spectrum of the N-body Hamiltonian in such a way that resonances in certain sectors of the complex energy plane turn into usual eigenvalues of the scaled Hamiltonian. In physics literature the origins of such an approach are traced back at least to C. Lovelace (1964). A rigorous approval of the complex scaling method has been done by E. Balslev and J. M. Combes (1971). A link between the s-matrix interpretation of resonances and its complex

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rotation counterpart was established by G. A. Hagedorn (1979) who has proven that for a wide class of potentials the scaling resonances are also the scattering matrix resonances.

If support of the interaction is compact, the resonances of a two-body system can be treated within the approach created by P. Lax and R. Phillips (1967). An advantage of the Lax-Phillips approach is in the opportunity of giving an elegant operator interpretation of resonances. The resonances show up as the discrete spectrum of a dissipative operator which is the generator of the compressed evolution semigroup.

For more details on the history of the subject and other approaches to resonances, as well as for a bibliography we refer to paper [1]. Here we only notice that, in contrast to the “normal” bound and scattering states, the resonant ones are still a mysterious object and many questions related to resonances remain unanswered. In particular, it is still unknown how to describe (in an indisputable way) the scattering of a particle on a resonant state of two other particles. To say the truth, there is a problem even with definition of resonance since resonances are not a unitary invariant of a self-adjoint (Hermitian) operator. Moreover, following to B. Simon [2], one may conclude that no satisfactory definition can rely on a single Hamiltonian and always an extra structure is necessary. Say, an unperturbed dynamics (in quantum scattering theory) or geometric setup (in acoustical or optical problems). Resonances are always relative as the scattering matrix itself.

In our approach we follow the typical setup where the resonances arising due to an interaction \( V \) are considered relative to the unperturbed dynamics described by the kinetic energy operator \( H_0 \). The resolvent \( G(z) = (H - z)^{-1} \) of the total Hamiltonian \( H = H_0 + V \) is an analytic operator-valued function of \( z \in \mathbb{C} \setminus \sigma(H) \). The spectrum \( \sigma(H) \) of \( H \) is a natural boundary for holomorphy domain of \( G(z) \) considered as an operator-valued function. However the kernel \( G(\cdot,z) \) may admit analytic continuation through the continuous spectrum of \( H \). Or the form \( \langle G(z)\varphi,\psi \rangle \) may do this for any \( \varphi,\psi \) of a dense subset of the Hilbert space \( \mathcal{H} \). Or the “compressed” resolvent \( PG(z)P \) admits such a continuation for \( P \) the orthogonal projection onto a subspace of \( \mathcal{H} \). In any of these cases one deals with the Riemann surface of an analytical function.

In the simplest example with \( H = H_0 = -\Delta \), the two-body kinetic energy operator in coordinate representation, we have

\[
G(x,x',z) = \frac{1}{4\pi} \frac{e^{i\frac{1}{2}|z|}|x-x'|}{|x-x'|},
\]

where \( x,x' \) are three-dimensional vectors. Clearly, \( G(x,x',z) \) as a function of the energy \( z \) has a two-sheeted Riemann surface which simply coincides with that of the function \( z^{1/2} \).

In this way one also arrives with the concept of the unphysical energy sheet(s). The copy of the complex energy plane where the resolvent \( G(z) \) is considered initially as an operator-valued function is called the physical sheet. The remainder of the Riemann surface is assumed to consist of the unphysical sheets (in general, an unphysical sheet may only be a small part of the complex plane).
Analytic function is uniquely defined by its values on an infinite set in \( C \) having limiting point(s). Thus, if one knows the resolvent (\( T \)-matrix, \( S \)-matrix) on the physical sheet then one may, in principle, to express it on unphysical sheets through its values in the physical sheet. In this case all the study of resonances would reduce to a work completely on the physical sheet.

In [1, 3] we have found just such expressions. More precisely, we have derived explicit representations for the two- and three-body \( G(z) \), \( T(z) \), and \( S(z) \) on unphysical energy sheets in terms of these quantities themselves only taken on the physical sheet. In particular, the representations obtained show which blocks of the scattering matrix are “responsible” for resonances on a certain unphysical sheet.

2 Two-body problem

In general, we assume that the interaction potential \( v \) falls off in coordinate space not slower than exponentially. When studying resonances of a two–body system with such an interaction one can employ equally well both coordinate and momentum representations. However in the three-body case it is much easier for us to work in the momentum space (for an explanation see [1], p. 149). This is one of the reasons why we proceed in the same way in the two-body case. Thus, for the two-body kinetic energy operator \( h_0 \) we set \((h_0f)(k) = k^2f(k)\) where \( k \in \mathbb{R}^3 \) stands for the reduced relative momentum. In case of a local potential we have \( v(k, k') = v(k - k') \) and \( v(k) = v(-k) \). For simplicity we assume that the function \( v(k) \) is holomorphic in \( k \) on the whole three-dimensional complex space \( \mathbb{C}^3 \).

The transition operator (t-matrix) reads
\[
t(z) = v - vg(z)v,
\]
where \( g(z) = (h - z)^{-1} \) denotes the resolvent of the perturbed Hamiltonian \( h = h_0 + v \). The operator \( t \) is the solution of the Lippmann-Schwinger equation
\[
t(z) = v - vg_0(z)t(z),
\]
that is,
\[
t(k, k', z) = v(k, k') - \int_{\mathbb{R}^3} dq \frac{v(k, q)t(q, k', z)}{q^2 - z}
\]
taking into account that \( g_0(k, k', z) = \delta(k - k')/(k^2 - z) \).

Clearly, all dependence of \( t \) on \( z \) is determined by the integral term on the r.h.s. part of (3) that looks like a particular case of the Cauchy type integral
\[
\Phi(\lambda) = \int_{\mathbb{R}^N} dq \frac{f(q)}{\lambda + q^2 - z}
\]
for \( N = 3 \). Cauchy integrals of the same form but for both \( N = 3 \) and \( N = 6 \) we will also have below in three-body equations of Sec. 3.

Let \( \Re_\lambda, \lambda \in \mathbb{C} \), be the Riemann surface of the function
\[
\zeta(z) = \begin{cases} 
(z - \lambda)^{1/2}, & N \text{ odd}, \\
\log(z - \lambda), & N \text{ even}.
\end{cases}
\]
If \( N \) is odd, \( \mathcal{R}_\lambda \) is formed of two sheets of the complex plane. One of them, where \( (z - \lambda)^{1/2} \) coincides with the arithmetic square root \( \sqrt{z - \lambda} \), we denote by \( \Pi_0 \). The other one, where \( (z - \lambda)^{1/2} = -\sqrt{z - \lambda} \), is denoted by \( \Pi_1 \).

If \( N \) is even, the number of sheets of \( \mathcal{R}_\lambda \) is infinite. In this case as the index \( \ell \) of a sheet \( \Pi_\ell \) we take the branch number of the function \( \log(z - \lambda) \) picked up from the representation \( \log(z - \lambda) = \log |z - \lambda| + i 2\pi \ell + i \phi \) with \( \phi \in [0, 2\pi) \).

The following statement can be easily proven by applying the residue theorem (if necessary, see [11] for a proof).

**Lemma 1.** For a holomorphic \( f(q) \), \( q \in \mathbb{C}^N \), the function \( \Phi(z) \) given by (11) is holomorphic on \( \mathbb{C} \setminus [\lambda, +\infty) \) and admits the analytic continuation onto \( \mathcal{R}_\lambda \) as follows

\[
\Phi(z)|_{\Pi_\ell} = \Phi(z) - \ell \pi i (\sqrt{z - \lambda})^{N-2} \int_{S^{N-1}} d\tilde{q} f(\sqrt{z - \lambda} \tilde{q}),
\]

where \( S^{N-1} \) denotes the unit sphere in \( \mathbb{R}^N \) centered at the origin. (Position of the argument \( z \) in the sheet \( \Pi_0 \) on the r.h.s. part of (10) is the same as that of the argument of \( \Phi|_{\Pi_\ell} \) on the sheet \( \Pi_\ell \).)

Now set \( (g_0(z)f_1, f_2) = \int_{\mathbb{R}^3} d\tilde{q} \frac{f_1(q)f_2(q)}{q^2 - z} \) where \( f_1 \) and \( f_2 \) are holomorphic. Then by Lemma 1

\[
(g_0(z)f_1, f_2)|_{\Pi_1} = (g_0(z)f_1, f_2)|_{\Pi_0} - \pi i \sqrt{z} \int_{S^2} d\tilde{q} f_1(\sqrt{z} \tilde{q}) f_2(\sqrt{z} \tilde{q}).
\]

which means that the continuation of the free Green function \( g_0(z) \) onto the unphysical sheet \( \Pi_1 \) can be written in short form as

\[
g_0(z)|_{\Pi_1} = g_0(z) + a_0(z) j^\dagger j(z),
\]

where \( a_0(z) = -\pi i \sqrt{z} \) and \( j(z) \) is the operator forcing a (holomorphic) function \( f \) to set onto the energy shell, i.e. \( (j(z)f)(k) = f(\sqrt{z}^2 k) \).

Taking into account (10), on the unphysical sheet \( \Pi_1 \) the Lippmann-Schwinger equation (2) turns into

\[
t' = v - v g_0 a_0 j^\dagger j t', \quad t'|_{\Pi_1} = t.
\]

Hence \( (I + v g_0) t' = v - v a_0 j^\dagger j t' \). Invert \( I + v g_0 \) by using the fact that \( t(z) = v - v g_0 t \) and, hence, \( (I + v g_0)^{-1} v = t \):

\[
t' = t - a_0 j^\dagger j t',
\]

(7)

Apply \( j(z) \) to both parts of (7) and obtain \( j t' = j t - a_0 j t^\dagger j t' \), which means

\[
(I + a_0 j t^\dagger j) j t' = j t.
\]

(8)

Observe that \( I + a_0 j t^\dagger j \) is nothing but the scattering matrix \( s(z) \) since the kernel of \( s(z) \) reads

\[
s(\tilde{k}, \tilde{k}', z) = \delta(\tilde{k}, \tilde{k}') - \pi i \sqrt{z} t(\sqrt{z} \tilde{k}, \sqrt{z} \tilde{k}', z).
\]

Hence \( j t' = [s(z)]^{-1} j t \). Now go back to (7) and get \( t' = t - a_0 j t^\dagger [s(z)]^{-1} j t \), that is,

\[
t(z)|_{\Pi_1} = t(z) - a_0(z) t(z) j^\dagger(z) [s(z)]^{-1} j(z) t(z).
\]

(9)
All entries on the r.h.s. part of (9) are on the physical sheet. This is just the representation for the t-matrix on the unphysical sheet we looked for.

From (9) one immediately derives representations for the continued resolvent,

\[ g(z)|H_1 = g + a_0 (I - gv)j^\dagger [s(z)]^{-1}j(I - vg), \] (10)

and continued scattering matrix,

\[ s(z)|H_1 = \mathcal{E} [s(z)]^{-1} \mathcal{E}, \] (11)

where \( \mathcal{E} \) is the inversion, \( (\mathcal{E} f)(\hat{k}) = f(-\hat{k}) \). Hence, the resonances are nothing but zeros of the scattering matrix \( s(z) \) in the physical sheet. That is, the energy \( z \) on the unphysical sheet \( \Pi_1 \) is a resonance if and only if there is a non-zero vector \( A \) of \( L^2(S^2) \) such that \( s(z)A = 0 \) for the same \( z \) on the physical sheet.

The function \( \mathcal{A}(\hat{k}) \) is the breakup amplitude of the resonance state. This means that in coordinate space the corresponding “Gamov vector” (the resonance solution to the Schrödinger equation) has the following asymptotics

\[ \psi_{\text{res}}(x) \sim x \to \infty A(-\hat{x})e^{-i\sqrt{z}|x|}. \]

3 Three-body problem

Let \( H_0 \) be the three-body kinetic energy operator in the center-of-mass system. Assume for simplicity that there are no three-body forces and thus the total interaction reads \( V = v_1 + v_2 + v_3 \) where \( v_\alpha, \alpha = 1, 2, 3 \), are the corresponding two-body potentials having just the same properties as in the previous section.

The best way to proceed in the three-body case is to work with the Faddeev components \[ M_{\alpha\beta} = \delta_{\alpha\beta}v_\alpha - v_\alpha G(z)v_\beta \quad (\alpha, \beta = 1, 2, 3) \]
of the T-operator \( T(z) = V - VG(z)V \) where, as usually, \( G(z) \) denotes the resolvent of the total Hamiltonian \( H = H_0 + V \). The components \( M_{\alpha\beta} \) satisfy the Faddeev equations

\[ M_{\alpha\beta}(z) = \delta_{\alpha\beta}t_\alpha(z) - t_\alpha(z)G_0(z)\sum_{\gamma \neq \alpha} M_{\gamma\beta}(z) \] (12)

with \( G_0(z) = (H_0 - z)^{-1} \) and \( t_\alpha(P, P', z) = t_\alpha(k_\alpha, k'_\alpha, z - p_\alpha^2)\delta(p_\alpha - p'_\alpha) \) where \( k_\alpha, p_\alpha \) denote the corresponding reduced Jacobi momenta (see [1] for the precise definition we use) and \( P = (k_\alpha, p_\alpha) \in \mathbb{R}^6 \) is the total momentum.

Assume that any of the two-body subsystems has only one bound state with the corresponding energy \( \varepsilon_\alpha < 0, \alpha = 1, 2, 3 \). Assume in addition that all of these three binding energies are different. It is easy to see that the thresholds \( \varepsilon_1, \varepsilon_2, \varepsilon_3, \) and 0 are associated with particular Cauchy type integrals in the integral equations (12). By Lemma 1 the two-body thresholds \( \varepsilon_\alpha \) appear to be square-root branching points while the three-body threshold 0 is the logarithmic one. In order to enumerate the unphysical sheets we introduce the multi-index
\( \ell = (\ell_0, \ell_1, \ell_2, \ell_3) \) with \( \ell_0 = \ldots, -1, 0, 1, \ldots \) and \( \ell_\alpha = 0, 1 \) if \( \alpha = 1, 2, 3 \). Clearly, only encircling the two-body thresholds one arrives at seven unphysical sheets. The three-body threshold generates infinitely many unphysical sheets. (There might also be additional branching points on the unphysical sheets, in particular due to two-body resonances.)

It turns out that the analytically continued equations \( \{12\} \) can be explicitly (!) solved in terms of the matrix \( M = \{M_\alpha\beta\} \) itself taken only on the physical sheet, just like in the case of the two-body t-matrix. But, of course, now the result depends on the unphysical sheet \( \Pi_\ell \) concerned. More precisely, the resulting representation reads as follows

\[
M|_{\Pi_\ell} = M + Q_M L S_\ell^{-1} \tilde{L} \tilde{Q}_M.
\]

In the particular case we deal with, \( L \) and \( \tilde{L} \) are \( 4 \times 4 \) scalar matrices of the form \( L = \text{diag}(\ell_0, \ell_1, \ell_2, \ell_3) \) and \( \tilde{L} = \text{diag}(|\ell_0|, \ell_1, \ell_2, \ell_3) \), respectively; \( S_\ell(z) = I + L(S(z) - I)\tilde{L} \) is a truncation of the total scattering matrix \( S(z) \) and the entries \( Q_M, \tilde{Q}_M \) are explicitly written in terms of the half-on-shell kernels of \( M \) (see formula (7.34) of \( \{1\} \)). From \( \{13\} \) one also derives explicit representations for \( G(z)|_{\Pi_\ell} \) and \( S(z)|_{\Pi_\ell} \) similar to those of \( \{10\} \) and \( \{11\} \), respectively.

Thus, to find resonances on the sheet \( \Pi_\ell \) one should simply look for the zeros of the truncated scattering matrix \( S_\ell(z) \), that is, for the points \( z \) in the physical sheet where equation \( S_\ell(z)A = 0 \) has a non-trivial solution \( A \). The vector \( A \) will consist of breakup amplitudes of the resonance state into the various possible channels. Within such an approach one can also find the virtual states.

In order to find the amplitudes involved in \( S_\ell \), one may employ any suitable method, for example the one of Refs. \( \{5, 6, 7\} \) based on the Faddeev differential equations. In these works the approach we discuss has been successfully applied to several three-body systems. In particular, the mechanism of emerging the Efimov states in the \( ^4\text{He} \) trimer has been studied \( \{5, 6\} \).

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