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Tools for Assigning Resonance Structures in Collisions of Few-Body Quantum Systems*

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Abstract. The complex dilated Mittag-Leffler, the *T*-matrix, and the Siegert pseudostate methods are briefly reviewed. Their respective strengths and weaknesses and some recent results are discussed.

1 Introduction

Recent experimental development in atomic and molecular physics allows better energy resolution at relatively low collision energies. The atom-diatom experiments on the F + HD of Liu et al. [1] gave, for the first time, evidence for an isolated resonance as a triatomic reaction complex. The double electrostatic storage ring DESIREÉ [2], currently being constructed at Stockholm University, is expected to produce data on a variety of collisions between atomic and molecular systems. For example, it should be able to collide positive and negative ions, or ions and neutral atoms, or molecules with a very small relative kinetic energy ($\sim 10\,\mathrm{K}$). The corresponding cross sections will most likely have peaks which

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may be the signature of resonances. Theoreticians therefore need to design tools that will be able to analyze these data.

Below we discuss the results of some recent model potential studies [3–8], which may be instrumental in analyzing structures in a cross section and decide if a certain peak is the result of one or several resonances.

2 Three Theoretical Tools

All discussions below relate to the Schrödinger equation written as

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + V(x) - E \right] \phi(x) = 0, \tag{1}$$

where $V(x)$ is a potential describing a single channel radial problem on a semiaxis $x \in [0, +\infty)$, or a barrier transmission problem on an entire axis $x \in (-\infty, +\infty)$.

The complex dilation method applied to the radial problem defines the coordinate transformation $x \to g(x)$ such that $|g(x) - [x_0 + (x - x_0)\exp(i\theta)]| \to 0$ when $x \to +\infty$ for real $\theta < \theta_{\text{crit}}$ and real $x_0 \geq 0$. This transforms a purely outgoing wave into a square integrable one. A similar transformation can be applied to the barrier transmission problem. Using these transformations we obtain a complex dilated Schrödinger equation, which, with similarly dilated boundary conditions, leads to a complex eigenvalue problem [3, 12].

2.1 Mittag-Leffler Expansion and Complex Scaling – The CML Method

The partial-wave S-matrix is normally defined by the two Jost solutions $f_l^{\pm}(k, x)$, which in turn are expressed in terms of the Wronskian [9]. The standard Green's formula for a second-order differential operator H can now be generalized [3, 10] to the analytically continued Hamiltonian. This enables us to show that the Wronskians defining the Jost functions and therefore the partial-wave S-matrix $S_l(z)$ can be continued analytically using the complex dilation technique. Thus S_l becomes a meromorphic function in a sector of the fourth quadrant of the complex momentum $k = \sqrt{2E}$ plane (see refs. [3, 10]). Now, let $S_l(z)$ be analytic at the origin and meromorphic within the interior region bounded by a closed contour C. Assuming that there are poles at $k = k_j$ and using Cauchy's integral theorem, we can express $S_l(k)$ as

$$S_l(k) = S_l(a) + \sum_j \text{Res}[S_l(k_j)] \left\{ \frac{1}{k - k_j} + \frac{1}{k_j - a} \right\} + \frac{k - a}{2\pi i} \oint_C \frac{S_l(z)\, dz}{(z - k)(z - a)}. \tag{2}$$

This so-called Mittag-Leffler expansion of the partial-wave S-matrix $S_l(z)$ focuses our attention on the poles k_i and their residues $\text{Res}[S_l(k_j)]$. We have shown [3] that the residues can be calculated from the resonant wave function $\varphi(k_j, \eta x)$ and the Jost solutions $f^-(k, x)$ as

$$\text{Res}[S_l(k_j)] = \frac{i[W[f_l^-(k_j, x), \varphi_l(k_j, x)]]^2}{4\eta k_j \int_0^\infty dx\, \varphi^2(k_j, \eta x)},$$

which can be shown to be independent of the complex dilation. A generalization of Eq. (2) to a *two-channel problem* was recently studied in ref. [7], where it was used together with the Argand plot technique for analyzing the role played by individual poles.

2.2 The T-Matrix, Green Function Complex-Scaling Approach – The CT Method

The S-operator $\hat{S}$ can be expressed in terms of the transition operator $\hat{T}$, which in turn can be expressed via the interaction potential $\hat{V}$ and Green operator $\hat{G}$,

$$\hat{S} = 1 - 2\pi i\hat{T}, \qquad \text{with} \quad \hat{T} = \hat{V} + \hat{V}\hat{G}\hat{V}. \tag{3}$$

This technique has been studied by Rescingo et al. [11] and Moiseyev [12]. All quantities in Eq. (3) can be expanded into partial waves. The partial-wave Green function can further be expanded in its eigenfunctions to obtain

$$T_l^{if} = \langle \Phi_f | V | \Phi_i \rangle + \sum_j \frac{\langle \Phi_f | V | \varphi_l(k_j, x) \rangle \langle \varphi_l(k_j, x) | V | \Phi_i \rangle}{E - E_j}. \tag{4}$$

Now we can perform complex scaling and use Eq. (4) to obtain an expression for the S-matrix in the explicit form. In particular, for the orbital momentum $l = 0$, using $\Phi_f = \Phi_i = \sqrt{2/(\pi k)} \sin kx$, we obtain

$$S_0(k) = 1 - \frac{4i}{k} \int dx \sin^2(kx)\, V(x) - \frac{2i}{k} \sum_{n=1} \frac{1}{E - E_n} \left(\int dx\, g'(x) \sin[kg(x)]\, V[g(x)]\, \varphi_0[k_n, g(x)] \right)^2. \tag{5}$$

Also here we are able to express the partial-wave S-matrix in terms of a background and its poles. In particular, we can study the influence of a single pole by omitting it in the sum in Eq. (5) and computing the remaining cross section.

2.3 Siegert's Pseudostate Method – The SPS Method

In recent papers [4, 6] we demonstrated the common features of barrier scattering on the interval $x \in (-\infty, +\infty)$ and the two-channel radial problem $[x \in [0, +\infty)]$ using the Siegert pseudostate method. A Siegert state $\phi(x)$ for a barrier potential $V(x)$ is defined as the solution of Eq. (1) with the boundary conditions

$$\left(\frac{d}{dx} + ik_1 \right) \Big|_{x=a_1} \phi(x) = 0 \qquad \text{and} \qquad \left(\frac{d}{dx} - ik_2 \right) \Big|_{x=a_2} \phi(x) = 0.$$

It is presumed that $V(x) = v_1$ for $x < a_1$ and $V(x) = v_2$ for $x > a_2$ with $v_2 > v_1$. The momenta are defined by $k_1 = \sqrt{2(E - v_1)}$ and $k_2 = \sqrt{2(E - v_2)}$. The solutions of this boundary problem exist only for discrete values of the energy E_n; these eigenenergies are generally complex-valued and correspond to the poles of the S-matrix or the Green function.

Using this method we can express the S-matrix elements in terms of product functions containing the eigenmomenta $k_1^{(n)}$ and $k_2^{(n)}$. The explicit expressions for

Table 1. Comparison of $\mathrm{Res}[S_{12}(E_j)]$ with $\mathcal{M}_j \equiv \sqrt{\mathrm{Res}[S_{11}(E_j)]\,\mathrm{Res}[S_{22}(E_j)]}$, using S-matrix element residues calculated numerically (Rakityansky and Elander [7]); $\zeta = 10^{-4}$

Resonance energy E_j	Res $S_{12}(E_j)$	$\mathcal{M}_j$
$4.768197 - i0.000710$	$(0.26429 - i0.02943) \times \zeta$	$(0.26288 - i0.029206) \times \zeta$
$7.241200 - i0.755956$	$0.90478 + i0.25589$	$0.901791 + i0.254717$
$8.171217 - i3.254166$	$-7.30357 - i0.80750$	$-7.2852 - i0.797861$
$8.440526 - i6.281492$	$10.99059 - i17.56517$	$10.9451 - i17.5472$
$8.072634 - i9.572815$	$30.61007 + i17.10104$	$30.5965 + i17.0329$
$7.123813 - i13.012669$	$-5.46659 + i44.46505$	$5.39717 - i44.437$

the residues in terms of Siegert poles are as follows,

$$\mathrm{Res}[S_{11}(E_j)] = \exp\left[i2k_1^{(j)}a_1\right]\frac{1}{q}\left(k_1^{(j)}\right)^2 k_2^{(j)}\prod_{n\neq j}\frac{1}{2q}\,\frac{k_1^{(j)}k_2^{(n)} + k_1^{(n)}k_2^{(j)}}{k_1^{(j)} - k_1^{(n)}},$$

$$\mathrm{Res}[S_{22}(E_j)] = \exp\left[-i2k_2^{(j)}a_2\right]\frac{1}{q}\,k_1^{(j)}\left(k_2^{(j)}\right)^2\prod_{n\neq j}\frac{1}{2q}\,\frac{k_1^{(j)}k_2^{(n)} + k_1^{(n)}k_2^{(j)}}{k_2^{(j)} - k_2^{(n)}},$$

$$\mathrm{Res}[S_{12}(E_j)] = \exp\left[ik_1^{(j)}a_1 - ik_2^{(j)}a_2\right]\frac{1}{q}\left(k_1^{(j)}k_2^{(j)}\right)^{3/2} \times \prod_{n\neq j}\frac{1}{2q}\,\frac{k_1^{(j)}k_2^{(n)} + k_1^{(n)}k_2^{(j)}}{\left(k_1^{(j)} - k_1^{(n)}\right)^{1/2}\left(k_2^{(j)} - k_2^{(n)}\right)^{1/2}}, \tag{6}$$

where $q = \sqrt{(v_2 - v_1)/2}$. These formulae are equivalent to the expressions presented in ref. [6] in terms of the uniformization variable u. Basing on the Breit-Wigner formula for isolated resonances

$$S_{\alpha\beta}(E) \approx \exp[2i\delta_\alpha]\,\delta_{\alpha\beta} - i\exp[i(\delta_\alpha + \delta_\beta)]\,\frac{\sqrt{\Gamma_\alpha\Gamma_\beta}}{E - E_0 + i\Gamma/2},$$

we find the relation between the S-matrix residues and partial widths Γ_α,

$$\sqrt{\Gamma_\alpha\Gamma_\beta} = |\mathrm{Res}[S_{\alpha\beta}(E_m)]|.$$

A *universal relation* exists between the residues, as seen from formula (6): $\mathrm{Res}[S_{12}(E_m)]$ equals a geometric mean of $\mathrm{Res}[S_{11}(E_m)]$ and $\mathrm{Res}[S_{22}(E_m)]$,

$$\mathrm{Res}[S_{12}(E_m)] = \sqrt{\mathrm{Res}[S_{11}(E_m)]\,\mathrm{Res}[S_{22}(E_m)]}. \tag{7}$$

Applying Eq. (7) to the two-channel problem studied in ref. [7], we find, as seen in Table 1, a close agreement especially for the lower resonances, which implies that they were computed with a better accuracy than the higher ones.

3 Discussion

3.1 Formal Aspects

The aim of the present contribution is to discuss various ways to assign quantum numbers and understand the origin of resonant structures in few-body collisions. In

practice we need formally stable and computationally efficient methods. As discussed above, it is meaningful to characterize a resonance through two complex quantities–its energy and its residue[1].

When the three methods are applied to one-dimensional problems, we find a particular difference. The CML and the SPS methods describe the contributions to the partial-wave *S*-matrix in terms of its residues at the corresponding poles. These contributions, apart from the $(k - k_n)$ in the denominator, are independent of the scattering energy. The CT methods, on the other hand, contain resonance contributions in terms of matrix elements which are dependent on the scattering energy [5]. A comparison of the results obtained from Eqs. (2) and (5), reported in ref. [8], shows that the results are numerically identical. We can compare the CML and the CT methods by removing one and the same resonance from the two sums in Eqs. (2) and (5). When doing so, we still get good agreement between the cross sections obtained by these two techniques.

3.2 Numerical Aspects

The numerical realization of the CML theory is computationally heavy, this is especially true for the contour integral in Eq. (2). For this reason numerical applications of this theory are limited to a few channels [7].

Our numerical realization of the CT and SPS methods is based on a one-dimensional finite element code [14] which is rather efficient. In particular, the SPS *S*-matrix is created from the Siegert pseudostates, which thus makes the present SPS *S*-matrix numerically stable. The CT method seems to be able to only converge for small complex dilation angles, θ, and will therefore only reveal explicitly the influence of the more narrow resonances. This disadvantage may be compensated by the advantage that is easily extended from two channels to a realistic set of several (5–10) channels.

4 Conclusions

We have here reviewed methods which show how the technique of analytic continuation can be used to compute the contributions of resonances and background to the cross sections. The idea behind this approach is based on a model-potential study [15], where it was shown how the spectral density can be decomposed into components from its poles, which are the same as the *S*-matrix poles, and a free-particle background (see also ref. [16]). The results obtained so far show that the residues of the CML and CT methods are numerically identical. The cross sections obtained with the two methods are also in close numerical agreement. The CML method allows us to separate the contributions of narrow as well as wide resonances from the background, which is set by the choice of the integration contour. The convergence of the contributions from the complex dilated continuum does on the other hand limit the applicability of the CT method to only separate narrow resonances from a background.

[1] Generally, the entire *S*-matrix, including its residues, is expressible in terms of Siegert pseudostates [13], albeit this requires a *complete set*.

Since the SPS method is likely to be a stable method it can be expected to be able to describe the influence of wider resonances, as does the CML method. While the complex-dilation-based Mittag-Leffler expansion (CML) and the Siegert pseudostate (SPS) methods are applicable only to one-dimensional problems, the complex-dilated *T*-matrix approach (CT) is originally formulated for three-dimensional systems. The need to describe wide resonances in realistic problems will finally influence the choice among the three techniques.

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References

1. Liu, K., Skodje, R. T., Manolopoulos, D. E.: Phys. Chem. Comm. **5**, 27 (2002)
2. Rensfelt, K. G., et al.: Proceedings of the 9th European Particle Accelerator Conference. Lucern, Switzerland: EPAC 2004
3. Alferova, T., Elander, N.: Int. J. Quant. Chem. **97**, 922 (2004)
4. Ostrovsky, V. N., Elander, N.: Phys. Rev. **A71**, 052707 (2005)
5. Alferova, T., Ostrovsky, V. N., Elander, N.: Few-Body Systems **34**, 185 (2004)
6. Ostrovsky, V. N., Elander, N.: Chem. Phys. Lett. **411**, 155 (2005)
7. Rakityanski, S., Elander, N.: Int. J. Quant. Chem. (in press) (published online 2005.11.04)
8. Shilyaeva, K., Yarevsky, E., Elander, N.: Int. J. Quant. Chem. (in press)
9. Newton, R. G.: Scattering of Waves and Particles. New York: McGraw-Hill 1996
10. Rittby, M., Elander, N., Brändas, E.: In: Lecture Notes in Physics, Vol. 325 (Brändas, E., Elander, N., eds.), p. 129. Berlin Heidelberg New York: Springer 1989
11. Rescigno, T., McCurdy, C. W.: Phys. Rev. **A37**, 624 (1985)
12. Moiseyev, N.: Phys. Rep. **302**, 211 (1998)
13. Tolstikhin, O. I., Ostrovsky, V. N., Nakamura, H.: Phys. Rev. **A58**, 2077 (1998)
14. Scrinzi, A., Elander, N.: J. Chem. Phys. **98**, 3866 (1993)
15. Engdahl, E., Brändas, E., Rittby, M., Elander, N.: Phys. Rev. **A37**, 3777 (1988)
16. Brack, M., Kaidel, J., Winkler, P., Fedotkin, S. N.: Few-Body Systems **38**, 147 (2006); Kaidel, J., Winkler, P., Brack, M.: Phys. Rev. **E70**, 066208 (2004)