# Efficient numerical solution of coupled radial differential equations in multichannel scattering problems

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**Abstract.** Numerical solution of coupled radial differential equations which are encountered in multichannel scattering problems is presented. Numerical approach is based on the combination of the exterior complex scaling method and the finite-elements method with the discrete variable representation. This method can be used not only to solve multichannel scattering problem but also to find bound states and resonance positions and widths directly by diagonalization of the corresponding complex scaled Hamiltonian. Efficiency and accuracy of this method is demonstrated on an analytically solvable two-channel problem.

**Keywords:** multichannel scattering, exterior complex scaling, discrete variable representaion
**PACS:** 02.60.Lj, 02.70.-c, 34.10.+x, 34.80.-i

## INTRODUCTION

In atomic, molecular, and nuclear physics the quantum-mechanical scattering problems are very important. If at least one of colliding particles cannot be considered as an elementary one and can be found in different excited states then we have to deal with multichannel scattering. Electron collisions with atoms and molecules are basic examples of such multichannel processes.

In a certain range of energies (typically below a threshold of ionization or dissociation) the general multichannel scattering theory [1] leads, after the partial wave analysis, to a system of coupled radial differential equations which have to be solved with appropriate boundary conditions to obtain the cross sections of processes of interest.

Several numerical methods were proposed to solve these kinds of problems, for example the *R*-matrix method [2]. In this paper we discuss an application of the exterior complex scaling method combined with the finite-element method and the discrete variable representation [3] to the multichannel problem.

## MATHEMATICAL FORMULATION OF THE PROBLEM

We consider the following system of coupled linear differential equations given in a concise form as

$$(E-H)\Psi_{sc} = V\Psi_i \tag{1}$$

which describes a system of the total energy $E$ and the multichannel Hamiltonian

$$H_{\alpha\beta} = \delta_{\alpha\beta}\left(\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{l_\alpha(l_\alpha+1)}{2\mu r^2} + \varepsilon_\alpha\right) + V_{\alpha\beta}(r) \tag{2}$$

depends on the reduced mass $\mu$, channel angular momenta $l_\alpha$, and channel threshold energies $\varepsilon_\alpha$. For simplicity of our discussion, we suppose that channel potentials $V_{\alpha\alpha}(r)$ and couplings $V_{\alpha\beta}(r)$ are of short-range, i.e. they fall faster than $1/r^2$ as $r \to \infty$.

In the multichannel scattering problems the initial state $\Psi_i$ on the right-hand-side of (1) is given as an energy-normalized free-particle wave function in the channel $\alpha_i$

$$\Psi_{i,\alpha}(r) = \delta_{\alpha\alpha_i}\sqrt{\frac{2\mu}{\pi k_\alpha}}k_\alpha r\, j_{l_\alpha}(k_\alpha r) \tag{3}$$

where $k_\alpha$ are channel wave numbers $k_\alpha = \sqrt{2\mu(E-\varepsilon_\alpha)}$ and $j_l(z)$ is the spherical Bessel function of the first kind [4]. The scattered wave function $\Psi_{sc}$ satisfies the outgoing boundary condition in the open channels and is bound in the closed channels. Once $\Psi_{sc}$ is determined one can calculate the physical wave function $\Psi^+ = \Psi_i + \Psi_{sc}$ and the cross sections

$$\sigma_{\alpha_i \to \alpha_f}(E) = \frac{4\pi^3}{k^2_{\alpha_i}} |\Psi_f^T V \Psi^+|^2 \tag{4}$$

where the final state $\Psi_f$ is of the form (3) with $\alpha_i$ replaced with $\alpha_f$.

## NUMERICAL METHOD

To solve the system of coupled differential equations (1) with the outgoing (open channels) or exponentially decaying (closed channels) boundary conditions we have made use of the method of the exterior complex scaling (ECS) implemented using a combination of the finite-element method (FEM) and the discrete variable representation (DVR). This method was proposed by [3] as an efficient numerical grid method to solve Schrödinger equation (to find both bound states and scattering states) and reviewed recently in [5] where applications of this method for three particle Coulombic break-up problem can be found.

The exterior complex scaling method is a generalization of the well-known complex scaling method which was found to be an efficient way to determine resonance positions and widths in quantum-mechanical problems (see e.g. [6]). By rotating the radial coordinate by the angle $\eta$ to the complex plane at a sufficiently large distance $r_\eta$

$$R(r) = \begin{cases} r, & r < r_\eta, \\ r_\eta + (r - r_\eta)e^{i\eta}, & r > r_\eta. \end{cases} \tag{5}$$

one effectively changes the wave functions describing resonance and scattering states to bound ones. Therefore we can look for them in a quadratically integrable basis. Furthermore, if we apply the transformation (5) to the Hamiltonian (2) and calculate the inversion of $(E-H)$ in Eq. (1) then we obtain the scattered wave function $\Psi_{sc}$ with the correct outgoing boundary condition on the interval $\langle 0, r_\eta \rangle$. For details see e.g. [5].

A choice of the square-integrable basis constructed using finite elements with the DVR basis in each element proved to be one of the most efficient ways to implement the exterior complex scaling method. Details on how to construct such a basis using Lagrange interpolating polynomials and Gauss-Lobatto quadrature can be found in [3] and [5]. The main advantages of this basis are that the potential energy operator is diagonal and the kinetic energy operator is band and represented with high accuracy owing to the use of the Gauss-Lobatto quadrature. Thus this method results in very sparse matrices for systems like (1) and efficient algorithms for solving sparse linear systems can be applied.

## RESULTS FOR TWO-CHANNEL PROBLEM

As a testing model on which the efficiency of the numerical method described above will be demonstrated was chosen an analytically solvable *s*-wave ($J_\alpha$) two-channel problem [1] where channel potentials and couplings have a form of potential wells

$$V_{\alpha\beta}(r) = \begin{cases} v_{\alpha\beta}, & r < r_0, \\ 0, & r > r_0. \end{cases} \tag{6}$$

The analytical solution of this problem and detailed discussion of its properties can be found in [1] or [7]. Here we only compare our results with the exact ones for numerical values $v_{11} = v_{22} = -2$, $v_{12} = v_{21} = -1/2$, $r_0 = 1$, $\varepsilon_1 = 0$, and $\varepsilon_2 = 2$ (all values are given in atomic units) which were also used in [7].

Because of the discontinuity at $r = r_0$ one has to choose the numerical grid carefully. By employing finite elements we can handle such a point of discontinuity easily by placing one endpoint of two neighboring elements to it and evaluating the potential at it as a weighted mean of the left and right limits where weights are the quadrature weights at this point taken from the left and right element resp. The basic numerical grid which we used in our calculations is

$$\begin{aligned} &\eta = 40^\circ,\ N_{DVR} = 15, N_b = 83, N_{el} = 6, \\ &\text{endpoints of elements} = \{r_{min} = 0, 1, r_\eta = 2, 3, 6, 14, r_{max} = 30\} \end{aligned} \tag{7}$$

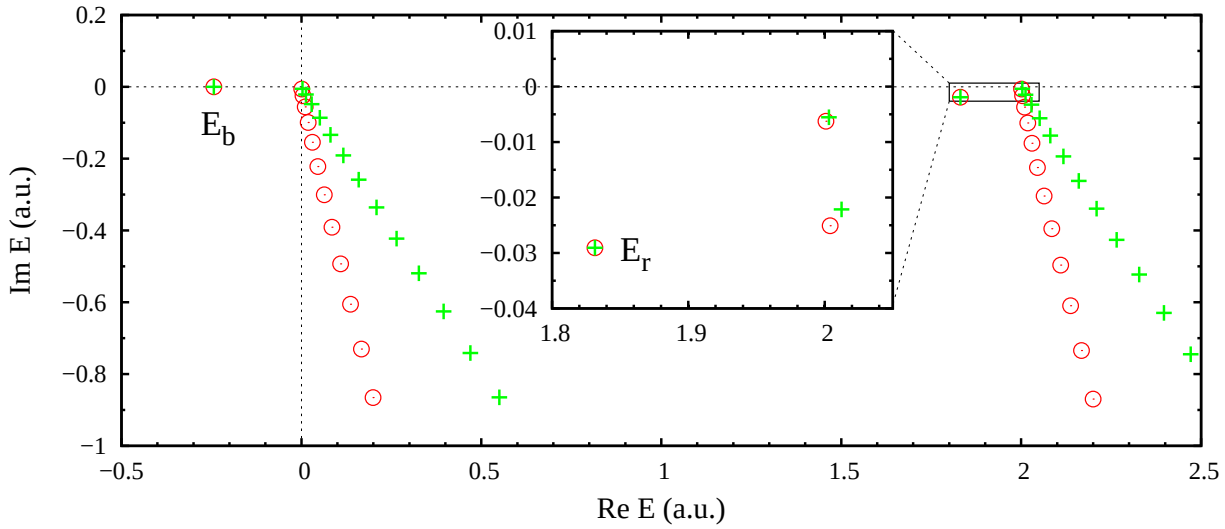


**FIGURE 1.** Spectrum of the complex scaled Hamiltonian for the two-channel problem (6) using the numerical grid (7) with $\eta = 40^\circ$ (circles) and $\eta = 30^\circ$ (crosses).

where $N_{DVR}$ denotes the number of the DVR basis functions (the same in each element), $N_{el}$ is the number of elements and $N_b = (N_{DVR} - 1)N_{el} - 1$ is the total number of basis functions (see [3] for details). The complex part of the grid must start at the radius where all the potentials and couplings are negligible (here we have chosen $r_\eta = 2 > r_0$) and must be sufficiently large to allow the wave functions to fall to zero.

In Fig. 1, the spectrum of the complex scaled Hamiltonian (2) with the potential matrix (6) is shown for the numerical grid (7) with two different scaling angles $\eta = 40^\circ$ (circles) and $30^\circ$ (crosses). Energies of bound states and resonances (for sufficiently large scaling angles) should be independent of the scaling angle in contrast to the continuum states which are rotated by the angle $2\eta$. The energy of the bound state in the first channel ($E_b = -2.4309650981$) and of the resonance in the second channel ($E_r = 1.8315168862 - 0.0290733625i$) were determined with the relative error less than $10^{-10}$.

When solving the scattering problem one can expect to find a resonance in the elastic cross section $\sigma_{1\to1}$ at energy $\mathrm{Re}\,E_r$. We can see such a resonant structure in Fig. 2, upper panel, where the exact cross sections (lines) are compared with the cross sections obtained using the numerical grid (7). In the lower panel of Fig. 2 we plotted the relative error of the cross section $\sigma_{1\to1}$ for the grid (7) and for three other grids. We can see that the used method gives very accurate results even for quite small number of basis functions $N_b$ (relative error of order $10^{-8}$ for $N_b = 53$ for energies not too close to thresholds). Inaccuracy at very small energies and in the vicinity of the thresholds where a new channel opens is due to very slow decrease of the wave functions on the complex contour (5) as $r \to r_{max}$ (wave functions on the complex part of the grid are proportional to $\exp(-k_\alpha r)$, thus the smaller the channel wave number is, the slower is the decrease of the wave function and the more inaccurate is the calculation because in our approach we set a boundary condition $\Psi(r_{max}) = 0$). As $r_{max}$ is increased (the number of basis functions must also be increased correspondingly to obtain high accuracy) we can get very accurate results even for very small energies and energies close to thresholds (see results for last two grids in Fig. 2, lower panel).

## CONCLUSIONS

The numerical grid method which employs the exterior complex scaling technique and the finite elements with the DVR basis was used to solve the system of coupled radial differential equations. This method proved to be an efficient tool to solve both the eigenvalue problem (when one needs to look for positions and widths of resonances) and the scattering problem for even with a relatively small number of basis functions one can get highly accurate results.

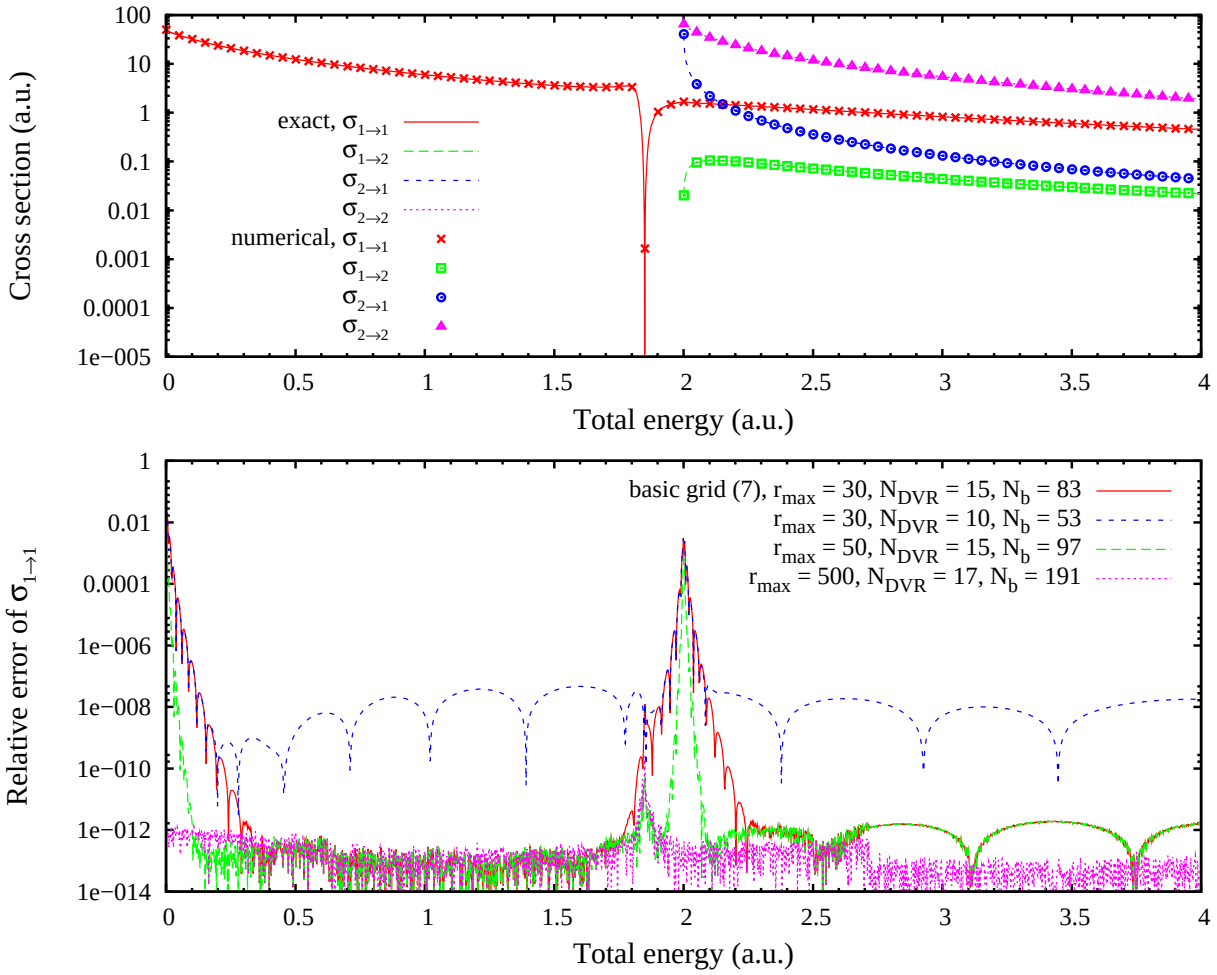


**FIGURE 2.** Upper panel: dependence of the cross sections for all transitions on the total energy (lines – exact results, points – numerical results). Lower panel: the relative error of the numerical values of the cross section $\sigma_{1\to1}$ for four different grids.

## ACKNOWLEDGMENTS

Support from the Czech Science Foundation by Grant No. 202/07/0833 and by Zamer MSM0021620860 is gratefully acknowledged.

## REFERENCES

1. R. G. Newton, *Scattering Theory of Waves and Particles, 2nd Ed*, Springer-Verlag, New York, 1982, chap. 16 and 17.
2. P. G. Burke and K. A. Berrington, *Atomic and molecular processes: an R-matrix approach*, Institute of Physics Publishing, Bristol and Philadelphia, 1993.
3. T. N. Rescigno and C. W. McCurdy, *Phys. Rev. A* **62**, 032706 (2000).
4. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Dover Publications, New York 1972
5. C. W. McCurdy, M. Baertschy, and T. N. Rescigno, *J. Phys. B* **37**, R137–R187 (2004).
6. N. Moiseyev, *Phys. Rep.* **302**, 211 (1998).
7. T. P. Grozdanov and R. McCarroll, *J. Chem. Phys.* **126**, 034310 (2007).