Application of the complex scaling method for few-body scattering problems including the breakup

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Abstract. A formalism based on the complex-scaling method is used to solve a few-particle scattering problem in configuration space. This method allows to use trivial boundary conditions and is compatible with most of the bound state techniques. In this contribution calculations of neutron scattering on triton is presented using realistic nuclear Hamiltonians for neutron energies above four-nucleon breakup threshold.

1. Introduction
Rigorous description of the quantum-mechanical collisions is one of the most complex problems in theoretical physics. During the last two decades exact numerical solutions for bound states containing dozens of particles became available, however the full solution of the scattering problem (containing elastic, rearrangement and breakup channels) remained limited to the three-body case. Therefore there is a natural interest in adapting bound-state techniques to solve the scattering problems. In particular, some recent efforts have been successful [1, 2, 3, 4, 5, 6].

The main difficulty to solve the scattering problem in configuration space is related to the fact that, unlike the bound state wave functions, scattering wave functions are not localized. One is therefore obliged to find solutions for multidimensional differential equations, which satisfy extremely complex boundary conditions. Number of the open channels increases rapidly with number of particles and/or total energy of the system, strongly complicating asymptotic structure of the wave function of the system. In particular the asymptotic structure of the systems wave function becomes complex if breakup channels in three or more particle clusters are open. Notably breakup asymptotic for charged clusters are not known analytically. Therefore it is rather obvious that one will not be able to handle such a complicate boundary behavior directly for the systems containing more than three or four particles¹.

Therefore, finding a method which enables us to solve the scattering problem without an explicit use of the asymptotic form (or singularities in momentum space) of the wave function is of great importance. In this contribution I will present a formalism based on the complex-scaling method [7, 6]. Several applications have been already provided proving efficiency of the method in describing elastic and three-body breakup reactions for Hamiltonians which may combine short-range, Coulomb as well as optical potentials [8, 10]. In this presentation this formalism

¹ One should notice that the scattering wave functions are localized in momentum space, however they contain complex structure of singularities which are as difficult to treat numerically as a boundary conditions in configuration space [2, 4]
is applied to solve four-nucleon scattering problem above the breakup threshold using realistic interactions.

2. Guidelines of the formalism
In our recently published review article [8] we have explained in detail how to implement the complex scaling method to solve the general scattering problem for a few-particle systems. Here, without losing generality, we will briefly summarize the main ideas of this formalism and in particular its application in conjunction with the Faddeev-Yakubovski (FY) for a system of four identical particles.

The method of complex scaling (or coordinates) for two- and three-particle scattering was proposed by Nuttall and Cohen [7]. The main idea of the method is that, the configuration is composed of only single incoming wave Ψ\textsubscript{in}, determined by the incident state and thus known \textit{a priori}, and as many outgoing waves as there are open channels. Regardless their complexity the outgoing wave functions are some analytic functions of the coordinates which will fall off exponentially for rotated \( r = |r| e^{i\theta} \), where \( 0 < \theta < \pi \). Thus one may set \( \Psi\textsubscript{out} = \Psi - \Psi\textsubscript{in} \) with \( \Psi\textsubscript{out} \) representing the difference between the complete scattering wave function \( \Psi \) and the wave function \( \Psi\textsubscript{in} \) describing the incident state. \( \Psi\textsubscript{out} \) should contain only outgoing waves and thus fall off exponentially for the complex scaled coordinates. The physical observables are straightforwardly related with the scattering amplitudes, which on their turn might be expressed as integrals involving \( \Psi\textsubscript{out} \), regardless the fact that only transform of this function is available for the complex scaled coordinates. Therefore the whole calculation can be performed using a wave functions part \( \Psi\textsubscript{out} \) which decreases exponentially and thus using standard bound-state techniques to approximate it.

When considering four-nucleon scattering problem we start with Faddeev-Yakubovski (FY) equations for a system of four identical particles \(^2\). In this particular case, we start by separating the incoming plane wave from the FY components (see figure 1):

\[
\begin{align*}
K(x, y, z) &= K\textsubscript{out}(x, y, z) + K\textsubscript{in}(x, y, z) \\
H(x, y, z) &= H\textsubscript{out}(x, y, z) + H\textsubscript{in}(x, y, z).
\end{align*}
\]

Note, that the four-body FY equations involve components of two types, \( K \) and \( H \). These components in their \( z \to \infty \) asymptotes separate respectively elastic 3+1 and 2+2 particle channels. Therefore, in the last equation, one has \( H\textsubscript{in} \equiv 0 \) when considering collision of 3+1 particle clusters, whereas \( K\textsubscript{in} \equiv 0 \) when considering 2+2 particle collisions. Asymptotes of the FY components \( K\textsubscript{out} \) and \( H\textsubscript{out} \) will contain only various combinations of the outgoing waves. These components are solutions of the driven FY equations, which have the form:

\[
\begin{align*}
(E - H_0 - V_{12}) K\textsubscript{out} &- V_{12}(P^+ + P^-) \left[ (1 + Q) K\textsubscript{out} + H\textsubscript{out} \right] \\
&= V_{12}(P^+ + P^-) \left[ (1 + Q) H\textsubscript{in} + Q K\textsubscript{in} \right], \\
(E - H_0 - V_{12}) H\textsubscript{out} &- V_{12}\tilde{P} \left[ (1 + Q) K\textsubscript{out} + H\textsubscript{out} \right] = V_{12}\tilde{P} \left[ (1 + Q) K\textsubscript{in} \right],
\end{align*}
\]

where \( P^- = P_{23}P_{12}, \ P^+ = P_{12}P_{23}, \ Q = P_{34} \) and \( \tilde{P} = P_{13}P_{24} \) are particle permutation operators.

It is practical to use smooth complex scaling operator (CSO), which acts only on hyperradial variable \( r^2 = x^2 + y^2 + z^2 \) and thus does not affect coordinate transformation operators. The smooth CSO is expressed as

\[
\hat{S} = e^{i\theta r \frac{\partial}{\partial r}} = e^{i\theta (x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} + z \frac{\partial}{\partial z})},
\]

\(^2\) Equivalent formulation is possible for the Schrödinger equation. We prefer to use FY equations simply because we dispose some earlier developed tools, which are proper to these equations.
Figure 1. The FY components $K_{12,3}^4$ and $H_{12}^{34}$ for a given particle ordering. As $z \to \infty$, the $K$ components describe 3+1 particle channels, while the $H$ components contain asymptotic states of 2+2 channels.

where $\theta$ is the complex scaling angle. The action of the complex scaling operator on outgoing wave gives

$$\tilde{S}\exp(ikr) = \exp(-kr \sin \theta) \exp(ikr \cos \theta).$$

(6)

As aforementioned one may get exponentially decreasing functions $K^{\text{out}}$ (or $H^{\text{out}}$) by acting on them with the complex scaling operator (5). On contrary through the same operation functions $K^{\text{in}}$ (or $H^{\text{in}}$) gets exponentially divergent. Nevertheless these functions appear in the FY equations (3-4) only together with potential energy operator terms, and thus if interactions are exponentially bound the kernel of the complex scaled equations becomes compact.

The scattering amplitudes are extracted from the solutions of eqs. (3-4) by using integral relations, obtained through the Green’s theorem [6, 8]. In particular, scattering amplitude for 3+1 particle channels is provided by:

$$A_{31}(\vec{k}) = \frac{m}{\hbar^2} \int \int \int dV_{xyz} \left\{ 6K^4_K(H_0 - E)(K^{\text{out}} + K^{\text{in}}) + 3K^1_H(H_0 - E)(H^{\text{out}} + H^{\text{in}}) \right\}$$

(7)

with $K_K = \frac{1}{2}(P^+ + P^-)Q(1 + P^+ + P^-)K^{\text{in}}$ and $K_H = \tilde{P}(1 + P^+ + P^-)K^{\text{in}}$. The scattering amplitudes are scalars and do not depend on $r$, therefore they are not affected by the complex scaling operator $\tilde{S}A(\vec{k}) = A(\vec{k})$.

Equations (3-4) are solved by expanding spin, isospin and angular dependence of the FY components in partial-waves. The radial dependence of the FY components, on variables $(x, y, z)$, is expanded by using Lagrange-Laguerre mesh technique [9].

3. Results

Already in early seventies McDonald and Nuttall applied the complex scaling method to solve neutron-deuteron scattering problem above the breakup threshold [7]. At that time very primitive nucleon-nucleon interaction model was used, which has not been compatible with two-nucleon scattering data, therefore their pioneering results has been difficult to analyze. Lately interest in complex scaling method have been revived by Japanese scientists in relation with various nuclear reactions due to external probe/perturbation [11, 12, 13, 14, 15, 16]. During the few last years I have also pursued the pioneering studies of Nuttall in applying complex scaling method to solve different 3-body scattering problems. In particular accurate and reliable results for phaseshifts and inelasticity parameters in 3 and 4-nucleon systems using phenomenological Malfliet and Tjon potential have been obtained [6, 17]. Also it has been demonstrated that it is possible to extract accurately the breakup amplitudes for neutron-deuteron scattering [6]. Validity of the complex scaling method have been also demonstrated for three-body Hamiltonians which may include optical potentials in conjunction with one repulsive Coulomb interaction [10].
Lately we have developed computer code which is capable to handle four-nucleon problems for the realistic Hamiltonians. In particular we have considered $E_{lab} = 22.1$ MeV neutron’s scattering on triton, i.e. energy above the four-nucleon breakup threshold. Calculations have been performed for total angular momenta $J \leq 4$ (but excluding $J = 4^+$ case). To reach the convergence one had to add all the partial waves with partial angular momenta satisfying $\max(l_x, l_y, l_z) \leq 4$ condition. In table 1 we compare our calculated phaseshifts $\delta$ and inelasticity parameters $\eta$ using INOY04 potential. Results of this work are compared with ones of Deltuva et al. [4] obtained using momentum space calculations based on complex energy method. All the phaseshifts and inelasticity parameters agree within three significant digits. Single exception is for inelasticity parameter of $^1S_0$ wave; this inelasticity is very close to unity (demonstrating that this channel is strongly dominated by the elastic scattering) and is very difficult to determine accurately. In figure 2 different model predictions for the elastic differential cross section and neutron analyzing power $A_y$ are presented. Once again we should remark very nice agreement for INOY04 model with results of Ref. [4]. One may remark small model dependence for the elastic cross section, which is probably related with the fact that AV.18 model is not able to reproduce properly three and four-nucleon breakup thresholds. There is also small discrepancy with respect to experimental data, which might be also due to the underestimated experimental error bars near the cross section minima. On the other hand agreement for the calculated neutron analyzing power $A_y$ is quite nice.

Finally, in the figure 3 total elastic and breakup cross section dependence on the binding energy of the triton, provided by three different realistic nucleon-nucleon interaction models (namely INOY04, CD-Bonn and AV18), is presented. One may observe rather simple linear correlation pattern for both cross sections. Thus suggesting that at this energy proper reproduction of the breakup thresholds is very important, whereas sensibility to the short-range details of the nuclear Hamiltonian is rather weak.

### Table 1. Some calculated phaseshifts $\delta$ and inelasticity parameters $\eta$ for 22.1 MeV neutron scattering on triton using INOY04 potential. This work results are compared with the ones of [4].

| $l$ | PW This work | Ref. [4] | $\delta$ (deg.) |
|-----|--------------|----------|-----------------|
| $^1S_0$ | 0.985 | 0.990 | 62.74 | 62.63 |
| $^3P_0$ | 0.959 | 0.959 | 43.07 | 43.04 |
| $^3P_2$ | 0.949 | 0.950 | 65.25 | 65.27 |

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Figure 2. Calculated $n^{-3}H$ elastic differential cross sections (left panel) and neutron analyzing power $A_y$ (right panel) for neutrons of laboratory energy 22.1 MeV and 22.1 MeV compared with experimental results of Seagrave et al. [18].

Figure 3. Dependence of the calculated $n^{-3}H$ total elastic and inelastic (breakup) cross sections on the triton binding energy.

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