Complex scaling method for three- and four-body scattering above the break-up thresholds

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(Dated: May 5, 2014)

Abstract

A formalism based on the complex-scaling method is presented to solve the few particle scattering problem in configuration space using bound state techniques with trivial boundary conditions. Several applications to A=3,4 systems are presented to demonstrate the efficiency of the method in computing elastic as well as break-up reactions with Hamiltonians including both short and long-range interaction.

PACS numbers:

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I. INTRODUCTION

The theoretical description of the quantum-mechanical collisions is one of the most complex problems in theoretical physics. The main difficulty to solve the scattering problem in configuration space is related to the fact that, unlike the bound state case, the scattering wave functions are not localized. One is therefore obliged to solve multidimensional integro-differential equations with extremely complex boundary conditions. Therefore, finding a method which could enable us to solve the scattering problem without an explicit use of the asymptotic form of the wave function is of great importance. Recently, the research in this field has been intensified very much [1–7].

One of the pioneering works in this direction is the development of the Lorentz integral transform [1], which allows to calculate the integral cross section of a scattering process using bound state like techniques. Still its application to compute differential observables becomes rather involved. Few years later, the complex energy method has been applied to the four-nucleon problem with separable potential [2], providing full information on the scattering process. Lately, after some technical improvements, this method was successfully applied to describe realistic four-nucleon break-up process [7]. Other recent developments include momentum lattice technique [3] and a method based on discretized continuum solutions [6], although they are no yet tested in the four-body sector and to the break-up case respectively.

On the other hand, already in the late sixties, Nuttal and Cohen [8] proposed a very handy method to treat the scattering problem for short range potentials using coordinate space variational bound state techniques, namely the complex scaling method. However application of this method to the scattering problem has lingered. Only recently a variant of the complex scaling method to calculate scattering observables above the break-up threshold has been proposed and applied by Giraud et al. [9]. Still this variant relies on the spectral function formalism and requires a diagonalization of the full N-body matrices to get converged results, which makes it difficult to extend beyond the N=3 case.

In [5] we have demonstrated that only a slightly modified original version of the complex scaling method by Nuttal and Cohen [8], if combined with Fadddeev equations, turns to be very efficient in describing three-nucleon scattering, including break-up reactions. We have shown that this method may treat strong interaction of almost any complexity: realistic local and non-local potentials, optical potentials, all of them in conjunction with repulsive
Coulomb force. The method allows to calculate both elastic as well as break-up amplitudes, thus providing a full description of the three-body collisions. There are no formal obstacles in extending this method to treat collisions involving any number of particles, as long as one is able to handle the eventual large scale numerical problem. In this contribution we will summarize this current effort and present some new results concerning the solution of the 4-nucleon scattering problem above the breakup thresholds.

II. FORMALISM

In our previous paper [5] we have presented the basic ideas of the complex scaling method used to solve the scattering problem for 2- and 3-particle systems. Here, without losing generality, we will briefly summarize the formalism for solving the Faddeev-Yakubovski (FY) equations for a system of four identical particles. In this particular case, we start by separating the incoming plane wave from the FY components (see figure 1):

\[ K(\vec{x}, \vec{y}, \vec{z}) = K^{\text{out}}(\vec{x}, \vec{y}, \vec{z}) + K^{\text{in}}(\vec{x}, \vec{y}, \vec{z}) \]  
\[ H(\vec{x}, \vec{y}, \vec{z}) = H^{\text{out}}(\vec{x}, \vec{y}, \vec{z}) + H^{\text{in}}(\vec{x}, \vec{y}, \vec{z}). \]

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

\[ (E - H_0 - V_{12}) K^{\text{out}} - V_{12}(P^+ + P^-) \left[ (1 + Q)K^{\text{out}} + H^{\text{out}} \right] \]
\[ = V_{12}(P^+ + P^-) \left[ (1 + Q)H^{\text{in}} + QK^{\text{in}} \right], \]
\[ (E - H_0 - V_{12}) H^{\text{out}} - V_{12} \tilde{P} \left[ (1 + Q)K^{\text{out}} + H^{\text{out}} \right] = V_{12} \tilde{P} \left[ (1 + Q)K^{\text{in}} \right], \]

It is interesting to introduce the complex scaling operator (CSO)

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

where \( r^2 = x^2 + y^2 + z^2 \) and \( \theta \) is the complex scaling angle, of free choice. The action of the complex scaling operator on outgoing wave gives

\[ \hat{S} \exp(ikr) = \exp(-kr \sin \theta) \exp(ikr \cos \theta). \]
FIG. 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.

Therefore if one acts on $K^{out}$ (or $H^{out}$) with the complex scaling operator (5), by keeping the complex scaling angle in the range $0 < \theta < \pi/2$, one gets exponentially decreasing functions 

$$\tilde{K}^{out} \equiv \hat{S}K^{out} \quad \text{and} \quad \tilde{H}^{out} \equiv \hat{S}H^{out}.$$ 

By acting with the same operator on equations (3-4), one gets equivalent equations for the scaled FY components $\tilde{K}^{out}$ and $\tilde{H}^{out}$:

$$\hat{S} \left( E - H_0 - V_{12} \right) \hat{S}^{-1} \tilde{K}^{out} - \hat{S}V_{12} \hat{S}^{-1} (P^+ + P^-) \left[ (1 + Q) \tilde{K}^{out} + \tilde{H}^{out} \right] = \hat{S}V_{12} \hat{S}^{-1} (P^+ + P^-) \left[ (1 + Q) \tilde{K}^{in} + Q \tilde{K}^{out} \right], \quad (7)$$

$$\hat{S} \left( E - H_0 - V_{12} \right) \hat{S}^{-1} \tilde{H}^{out} - \hat{S}V_{12} \hat{S}^{-1} \hat{P} \left[ (1 + Q) \tilde{K}^{out} + \tilde{H}^{out} \right] = \hat{S}V_{12} \hat{S}^{-1} \hat{P} \left[ (1 + Q) \tilde{K}^{in} \right], \quad (8)$$

The functions to determine in the last equation, notably $\tilde{K}^{out}$ and $\tilde{H}^{out}$, are exponentially bound. Thus, in principle, bound-state techniques based on square integrable basis functions, may be employed to solve these equations. Nevertheless, one should still ensure that the inhomogeneous terms on the right hand side of eqs. (7-8) is also square integrable. Indeed, after the complex scaling, the incoming waves $\tilde{K}^{in}$ and $\tilde{H}^{in}$, diverge when the inter-cluster separation increases. This divergence should be screened by the short range potential term $\hat{S}V_{12} \hat{S}^{-1}$. Nevertheless, the direction in which propagates the incoming wave does not coincide completely with the direction of the potential term.

\[\footnote{Note, that the four-body incoming wave components $K^{in}$ (or $\tilde{K}^{in}$) and $H^{in}$ (or $\tilde{H}^{in}$) are constructed from the corresponding bound-state wave functions of 3- and 2-particle systems respectively.}\]
particles, the inhomogeneous terms are exponentially bound if the following conditions are satisfied:

\[ \tan \theta < \sqrt{\frac{2B_3}{E_{cm}}} \],

(9)
in case of incoming wave of 1 + 3-type – \( B_3 \) being the binding energy of 3-particle cluster – and

\[ \tan \theta < \sqrt{\frac{2B_2}{E_{cm}}} \],

(10)
when considering incoming wave of 2 + 2-type with a binding energy of 2-particle cluster equal \( B_2 \). \( E_{cm} \) denotes the energy of the two scattering clusters in the center of mass frame. Similar conditions for a 3-body problem have been derived in [5].

The scattering amplitudes are extracted from the solutions of eqs. (7-8) by using integral relations, obtained through the Green’s theorem [5, 10]. Equations (7-8) are solved using the method described in our previous works [5, 11, 12]. Namely, first spin, isospin and angular dependence of the FY components is expanded using partial-waves. The radial dependence of the FY components, in variables (x,y,z), is expanded by means of cubic spline basis and vanishing boundary conditions are implemented at the borders of the chosen 3-dimensional grid.

III. RESULTS

We will present in this section some chosen results obtained by applying the complex scaling method to 3- and 4-body systems. In table I we summarize the phase shifts and inelasticity parameters calculated for S-wave nucleon-deuteron scattering, using MT I-III potential [13]. Very nice agreement is obtained compared to the benchmark calculation of reference [16, 17], both by neglecting (n-d) as well as including (p-d) repulsive Coulomb interaction. Differential break-up amplitudes may be equally extracted with very nice accuracy [5], although they are not reported in this work.

More recently, calculations in 3-body sector have been extended to the study of reactions including compound nucleus. Here we present the results concerning \( d + ^{12}C \rightarrow p + ^{13}C \) scattering, which were obtained within a three-body model containing \( n, p \) and \( ^{12}C \) clusters. The interaction between the free nucleons is described by the realistic AV18 potential [14], whereas the \( N - ^{12}C \) interaction is described by the optical CH89 potential [15]. The \( n-^{12}C \)
TABLE I: Phase shifts and inelasticity parameters calculated for S-wave nucleon-deuteron scattering, using MT I-III potential [13]

| P.W. $E_{lab}$ (MeV) | n-d | p-d |
|----------------------|-----|-----|
|                      | This work | Ref. [16, 17] | This work | Ref. [16] |
| $^2S_{1/2}$ 14.1    | $Re(\delta)$ 105.5 | 105.49 | 108.4 | 108.41[3] |
|                     | $\eta$ 0.465 | 0.4649 | 0.498 | 0.4983[1] |
| $^4S_{1/2}$ 14.1    | $Re(\delta)$ 69.0 | 68.95 | 72.6 | 72.60 |
|                     | $\eta$ 0.978 | 0.9782 | 0.983 | 0.9795[1] |
| $^2S_{1/2}$ 42.0    | $Re(\delta)$ 41.5 | 41.35 | 43.8 | 43.68[2] |
|                     | $\eta$ 0.502 | 0.5022 | 0.505 | 0.5056 |
| $^4S_{1/2}$ 42.0    | $Re(\delta)$ 37.7 | 37.71 | 40.1 | 39.96[1] |
|                     | $\eta$ 0.903 | 0.9033 | 0.904 | 0.9046 |

potential in the $^2P_{1/2}$ partial wave is made real and is adjusted to support the ground state of $^{13}C$ with 4.946 MeV of binding energy; the parameters are taken from Ref. [18]. This adjustment is made in order to reproduce $p-^{13}C$ threshold in the transfer reactions. These results are summarized in Fig. 2 and compared to the ones obtained by the Lisboa group [19], who used the formalism of Alt-Grassberger-Sandhas (AGS) equations in momentum space. One may see an excellent agreement between these two calculations for $d+^{12}C$ and $p+^{13}C$ elastic cross sections, as well as for the transfer $d+^{12}C \rightarrow p+^{13}C$ cross section.

Concerning the four-body case, we present in table III a calculation of the integrated elastic and break-up cross sections for $n-^3H$ collisions. These results are obtained for the total isospin $T = 1$ channel, using MT I-III potential [13]. A rather reasonable agreement is obtained with the experimental values, although the agreement worsens at higher energies. MT I-III potential, being restricted to the S-waves, is not appropriate to this high energy domain. In figure 3 the corresponding differential elastic cross sections are displayed, calculated for incident neutrons at laboratory energy 14.4 MeV (left panel) and 22.1 MeV (right panel). One may notice that a rather good agreement is obtained also in this case. Only at the minimum region, for 14.4 MeV neutrons, the theoretical results underestimate the experimental values. These small discrepancies are due to the simplicity of the MT I-III potential. It has been shown recently [7] that the realistic interactions further improve the
FIG. 2: Comparison of the momentum space AGS results (solid curves) and the current paper ones (dashed-dotted curves). They contain the deuteron-\(^{12}\)C scattering at 30 MeV deuteron laboratory energy (left panel) and the proton-\(^{13}\)C elastic scattering at 30.6 MeV proton laboratory energy (right panel). Differential cross sections for the elastic scattering and neutron stripping reaction are presented as a ratio to the Rutherford cross section \(d\sigma/d\Omega\). The proton analyzing power is displayed in the bottom of the right panel figure. The experimental data are taken from Refs. [20–22].

TABLE II: Neutron-triton elastic (\(\sigma_e\)), inelastic (\(\sigma_b\)) and total (\(\sigma_t\)) scattering cross sections (in mb) for the selected neutron laboratory energies (in MeV) compared with the experimental data.

| \(E_{lab}\) (MeV) | \(\sigma_e\) | \(\sigma_b\) | \(\sigma_t\) | [Ref.] |
|-------------------|------------|------------|------------|-------|
| 14.4              | 922        | 11         | 933        | 978±70 | [25]  |
| 18.0              | 690        | 25         | 715        | 750±40 | [25]  |
| 22.1              | 512        | 38         | 550        | 620±24 | [26]  |

results, providing almost perfect agreement with the data, both for the differential as well as for the integrated elastic cross sections.
FIG. 3: Calculated $n-^3H$ elastic differential cross sections for neutrons of laboratory energy 14.4 MeV (left panel) and 22.1 MeV (right panel) compared with experimental results of Frenje et al. [27], Debretin et al. [23] and Seagrave et al. [24].

IV. CONCLUSIONS

A method based on the complex scaling is presented to solve the scattering problem above the break-up thresholds. This method does not require the implementation of highly non-trivial boundary conditions and allows to solve the few-body scattering problem using square-integrable functions. Scattering problem might thus be solved using configuration space bound state techniques in complex arithmetics.

Reliable and accurate results have already been obtained for the 3- and 4-body elastic and break-up processes, including optical potentials as well as long-range Coulomb repulsion. This method opens a way to explore the many-body scattering and breakup reactions and allows an accurate treatment of a rich variety of problems in molecular as well as in nuclear physics.

Acknowledgments

This work was granted access to the HPC resources of IDRIS under the allocation 2009-i2009056006 made by GENCI (Grand Equipement National de Calcul Intensif). We thank
the staff members of the IDRIS for their constant help.

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