Application of the complex-scaling method to few-body scattering

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A formalism based on the complex-scaling method is developed for solving the few-particle scattering problem, in terms of bound state boundary conditions. Several applications are presented to demonstrate the efficiency of the method for computing the elastic and three-body breakup reactions in systems described by Hamiltonians which may include both short- and long-range interactions.

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I. INTRODUCTION

The exact solutions of the quantum-mechanical problem of interacting particles are of fundamental importance in theoretical physics, and open a broad field of applications related to the description of the microscopic world. The fast development of the computational techniques, followed by the rapid evolution of the computational power, provoked a sizable advance in the multiparticle bound state problem: the rigorous and accurate description of systems composed of several or even dozens of particles have been obtained [1–4]. The progress in the multiparticle scattering problem is however still moderated. The major obstacle turns out to be the rich variety of the reactions one has to consider simultaneously and the resulting complexity of the wave function asymptotic structure. Till now only the three-body system has been treated in its full extent, including elastic and breakup channels [5–9], whereas a rigorous description by the same methods in the four-particle scattering remains limited to the elastic and rearrangement channels [10–12]. Recently, a very courageous effort has been undertaken to apply Green function Monte Carlo [13] and no-core shell model [14] techniques to the nucleon scattering on $A \geqslant 4$ nuclei. Nevertheless these promising approaches remains limited to the description of the binary scattering process. 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 would be of great importance.

The complex scaling method has been proposed [15,16] and successfully applied to the resonance scattering [17]; as has been demonstrated recently this method can be extended also for the scattering problem [18,19]. In this study we propose a novel method to solve the quantum few-particle scattering problem based on complex scaling method, which allows us to use trivial boundary conditions. We will demonstrate its applicability in calculating both elastic and three-particle breakup observables.

II. FORMALISM: TWO-BODY CASE

A. Short-range interaction

The complex scaling method has been proposed a while ago to treat the scattering problem for the exponentially bound potentials [15]. The underlying idea is quite simple and can be summarized as follows. First, one recasts the Schrödinger equation into an inhomogeneous (driven) form by splitting the system wave function into the sum $\Psi = \Psi^{\rm sc} + \Psi^{\rm in}$ containing the incident (free) $\Psi^{\rm in}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})$ and the scattered $\Psi^{\rm sc}(\mathbf{r})$ waves as

$$[E - \widehat{H}_0 - V(\mathbf{r})]\Psi^{\rm sc}(\mathbf{r}) = V(\mathbf{r})\Psi^{\rm in}(\mathbf{r}). \tag{1}$$

The scattered wave in the asymptote is represented by an outgoing wave $\Psi^{\rm sc} \sim \exp(ikr)/r$. If one scales all the particle coordinates by a constant complex factor, i.e., $\overline{r}_i = e^{i\theta} r_i$ with $\mathrm{Im}(e^{i\theta}) > 0$, the corresponding scattered wave $\overline{\Psi}^{\rm sc}$ vanishes exponentially as $\overline{\Psi}^{\rm sc} \sim \exp(-kr\sin\theta)$ with increasing particle separation r. Moreover if the interaction is of short range (exponentially bound), the right-hand side of Eq. (1) also tends to zero at large r, enabling us to solve the former equation in a similar way as for a bound state problem, that is, by using a compact basis or by solving a differential equation on a finite domain by imposing $\overline{\Psi}^{\rm sc}$ to vanish on its borders.

In practice, one uses to solve the two-body problem by expanding the Schrödinger wave function into partial waves:

$$\left[\frac{\hbar^2}{2\mu}k^2 - \widehat{H}_{0l}(r) - V_l(r)\right]\psi_l^{\rm sc}(r) = V_l(r)\psi_l^{\rm in}(r). \tag{2}$$

The radial part of the incoming wave is represented by the regular Bessel functions $\psi_l^{\rm in}(r) = j_l(kr)kr$, and the kinetic energy term is given by

$$\widehat{H}_{0l}(r) = \frac{\hbar^2}{2\mu}\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}\right]. \tag{3}$$

After the complex scaling, this equation becomes

$$\left[\frac{\hbar^2}{2\mu}k^2 - \widehat{H}_{0l}(re^{i\theta}) - V_l(re^{i\theta})\right]\overline{\psi}_l^{\rm sc}(r) = V_l(re^{i\theta})\overline{\psi}_l^{\rm in}(r). \tag{4}$$

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The complex scaled inhomogeneous term is easily obtained by using analytical expressions for the regular Bessel function $\overline{\psi}_l^{\rm in}(r) = j_l(kre^{i\theta})kre^{i\theta}$. The extraction of the scattering phase shift may be done directly by determining the asymptotic normalization coefficient of the outgoing wave:

$$\overline{\psi}_l^{\rm sc}(r) = A_l(r)\exp(ikre^{i\theta} - l\pi/2), \tag{5}$$

with scattering amplitude given by

$$kf_l = e^{i\delta_l}\sin\delta_l = A_l(r\to\infty). \tag{6}$$

Another well known alternative is to use an integral representation, which one gets after applying the Green theorem:

$$f_l = -\frac{2\mu}{\hbar^2}\int j_l(kre^{i\theta})V_l(re^{i\theta})\left[\overline{\psi}_l^{\rm sc}(r) + \overline{\psi}_l^{\rm in}(r)\right]re^{2i\theta}dr. \tag{7}$$

B. Coulomb plus short-range interaction

If the interaction contains a long-range term, the problem turns out to be quite different. The right-hand side of Eq. (1)—after applying the complex scaling—diverges and the $\Psi^{\rm sc}(re^{i\theta})$ term is not anymore exponentially bound. In Refs. [18,19] the so-called "exterior complex scaling" was proposed as a solution to circumvent the problem created by the diverging term on the right-hand side of Eq. (1).

In this paper, when considering the problem of the interaction containing the short-range V^s plus the Coulomb term $V^C = \frac{\hbar^2\eta}{\mu r}$, we propose to keep the standard smooth scaling procedure, however, employing analytically continued Coulomb waves to circumvent the problem of the divergence. In this case the driven partial wave Schrödinger equation is written as

$$\left[\frac{\hbar^2}{2\mu}k^2 - H_{0l}(r) - V^s(r) - V^C(r)\right]\psi_l^{{\rm sc},C}(r) = V^s(r)\psi_l^{{\rm in},C}(r), \tag{8}$$

where $\psi_l^{{\rm in},C} = F_l(\eta, kr)$ is the regular solution of the former Hamiltonian containing Coulomb interaction only. Asymptotically, the scattered wave behaves as $\psi^{{\rm sc},C}\sim\exp(ikr - \eta\ln 2kr)$, and therefore vanishes exponentially after the complex scaling:

$$\overline{\psi}_{\rm sc}^C(r) = A_l(r)\exp(ikre^{i\theta} - \eta\ln 2kre^{i\theta} - l\pi/2). \tag{9}$$

Equation (8) may be readily solved with the vanishing boundary condition for $\overline{\psi}_{\rm sc}^C(r)$, provided one is able to continue analytically the regular Coulomb functions standing on the right-hand side.

The scattering amplitude and the Coulomb-corrected phase shifts due to the short-range interaction δ_l can be determined as previously from the asymptotic normalization coefficient:

$$e^{-i\sigma_l}f_l = e^{i(\delta_l+\sigma_l)}\sin\delta_l = A_l(r\to\infty), \tag{10}$$

where σ_l is the so-called Coulomb phase shift.

Alternatively, the Green theorem may be used to obtain an integral relation similar to Eq. (7):

$$f_l = -\frac{2\mu}{\hbar^2}e^{2i\sigma_l}\int F_l(\eta, kre^{i\theta})V^s(re^{i\theta})\overline{\Psi}^C(r)re^{2i\theta}dr. \tag{11}$$

III. FORMALISM: THREE-BODY CASE

A. Short-range interaction

For the sake of simplicity, let us consider a system of three identical spinless particles submitted to short-range pairwise interactions. Only two vector variables are needed in the barycentric system, which may be one of the Jacobi pairs $\mathbf{x}_i = \mathbf{r}_j - \mathbf{r}_k$ and $\mathbf{y}_i = \frac{2}{\sqrt{3}}[\mathbf{r}_i - (\mathbf{r}_k + \mathbf{r}_j)]$. The pair potential is assumed to support an arbitrary number of two-particle bound states $\phi_m(\mathbf{x}_i)$ with eigenvalues ϵ_m and angular momentum l_m. The corresponding continuum state has relative momenta q_m, satisfying the energy conservation relation $E = \frac{\hbar^2}{m}q_m^2 + \epsilon_m = \frac{\hbar^2}{m}K^2$; the second equality defines three-particle breakup momenta K.

The three-body problem is formulated by using Faddeev equations [20] in configuration space. By readily separating the incoming wave of the particle scattered on a bound pair in the state $\phi_m(\mathbf{x}_i)$, they result in a single equation:

$$[E - H_0 - V_i(\mathbf{x}_i)]\psi_{i,m}^{\rm sc}(\mathbf{x}_i,\mathbf{y}_i) - V_i(\mathbf{x}_i)\sum_{j\neq i}\psi_{j,m}^{\rm sc}(\mathbf{x}_j,\mathbf{y}_j) = V_i(\mathbf{x}_i)\sum_{j\neq i}\phi_m(\mathbf{x}_j)\exp(i\mathbf{q}_m\cdot\mathbf{y}_j), \tag{12}$$

where $\psi_{i,m}^{\rm sc}$ is the scattered part of the Faddeev amplitude, corresponding to the incoming particle i, and where we denote by V_i the pair interaction of the particles j and k.

The decomposition of the total wave function into three Faddeev amplitudes permits us to separate the two-cluster particle channels, whereas the three-body breakup component remains shared by the three Faddeev amplitudes. In the $y_i\to\infty$ asymptote, the scattered part of the Faddeev amplitude i takes form

$$\psi_{i,m}^{\rm sc}(\mathbf{x}_i,\mathbf{y}_i) \underset{y_i\to\infty}{=} A_m(\widehat{x}_i,\widehat{y}_i,x_i/y_i)\frac{\exp(iK\rho)}{\rho^{5/2}} + \sum_n f_{nm}(\widehat{y}_i)\phi_n(\mathbf{x}_i)\frac{\exp(iq_n y_i)}{|y_i|}, \tag{13}$$

where $\rho = \sqrt{x_i^2 + y_i^2}$ is the hyperradius, $A_m(\widehat{x}_i,\widehat{y}_i,x_i/y_i)$ is the three-particle breakup amplitude, and $f_{mn}(\widehat{y}_i)$ is denotes the two-body transition amplitude from channel m to channel n. In this expression, the sum runs over all open binary channels n.

One may easily see that the scattered part of the Faddeev amplitude vanishes for a large hyperradius if the particle coordinates are properly complex scaled: $\overline{\mathbf{x}}_i = \mathbf{x}_i e^{i\theta}$, $\overline{\mathbf{y}}_i = \mathbf{y}_i e^{i\theta}$, and $\rho = \rho e^{i\theta}$. However in order to obtain a solution of the problem on a finite grid, one should ensure that the inhomogeneous term, standing in the right-hand side of Eq. (12), also vanishes outside the resolution domain. The inhomogeneous term is indeed null, damped by the potential term, if x_i is large and falls outside of the interaction region. Alternatively for $x_i \ll y_i$, the modulus of the transformed

Jacobi coordinates approach $x_j \approx \frac{\sqrt{3}}{2} y_i$, $y_j \approx \frac{y_i}{2}$, and

$$\phi_n(\mathbf{x}_j e^{i\theta}) \exp(i\mathbf{q}_n \cdot \mathbf{y}_j e^{i\theta}) \propto \phi_n(\mathbf{x}_j e^{i\theta}) \frac{\exp(-iq_n y_j e^{i\theta})}{|y_j| e^{i\theta}} \propto \exp\left(- k_n \frac{\sqrt{3}}{2} y_i \cos\theta \right) \times \frac{\exp\left(q_n \frac{y_i}{2} \sin\theta\right)}{y_i}. \quad (14)$$

Here we exploited the fact that the bound state wave function decreases exponentially in the asymptote with momenta $k_n = \sqrt{m|\epsilon_n|}/\hbar$. The last expression vanishes for large y_i only if the condition

$$\tan\theta < \frac{k_n\sqrt{3}}{q_n} = \sqrt{\frac{3|\epsilon_n|}{E + |\epsilon_n|}} \quad (15)$$

is satisfied.[1] Notice that if the scattering energy is large, one is obliged to restrict the complex scaling angle to very small values.

The extraction of the scattering observables may be realized as in the two-body case following two different ways. The straightforward way is to extract the transition amplitudes from the $y_i \to \infty$ asymptote of the solution $\overline{\psi}_i^{\rm sc}(\mathbf{x}_i, \mathbf{y}_i)$, using the fact that different scattering channels are orthogonal to each other:

$$f_{nm}(\widehat{y_i}) = C_n^{-1} |y_i| \exp(-iq_n y_i e^{i\theta}) \times \int \phi_n^*(\mathbf{x}_i e^{-i\theta}) \overline{\psi}_{i,m}^{\rm sc}(\mathbf{x}_i, \mathbf{y}_i) e^{3i\theta} d^3\mathbf{x}_i, \quad (16)$$

where C_n is the normalization coefficient of the two-body wave function

$$\int \phi_n^*(\mathbf{x}_i e^{-i\theta}) \phi_n(\mathbf{x}_i e^{i\theta}) e^{3i\theta} d^3\mathbf{x}_i = C_n.$$

The breakup amplitude can be extracted from the $\overline{\psi}_{i,m}^{\rm sc}(\mathbf{x}_i, \mathbf{y}_i)$ once all the two-body transition amplitudes are calculated by using Eq. (16).

Alternatively, one can employ the Green theorem. In this case, the integral relations might be obtained both for the breakup and for the two-body transition amplitudes. For the transition amplitude one has

$$f_{nm}(\widehat{y_i}) = -C_n^{-1} \frac{m}{\hbar^2} \int\int \phi_n^*(\mathbf{x}_i e^{-i\theta}) \frac{\exp(-iq_n y_i e^{i\theta})}{|y_i|} [V_j(\mathbf{x}_j e^{i\theta}) + V_k(\mathbf{x}_k e^{i\theta})] \overline{\Psi}_m(\mathbf{x}_i, \mathbf{y}_i) e^{6i\theta} d^3\mathbf{x}_i d^3\mathbf{y}_i. \quad (17)$$

These integrals are convergent on the finite domain, if the following condition is satisfied:[2]

$$\tan\theta < \frac{\sqrt{3}k_m}{q_m + 2q_n} = \frac{\sqrt{3|\epsilon_m|}}{\sqrt{|\epsilon_m| + E} + 2\sqrt{|\epsilon_n| + E}}, \quad (18)$$

which is stronger than the condition given by Eq. (15).

For the breakup amplitude several different relations can be obtained [21]. It seems that the one employing two-body outgoing states $\overline{\phi}^{(+)}(p, \mathbf{x}_i)$, generated by the correspondingly scaled strong potential at relative momenta p, is the most reliable numerically:

$$A_{i,m}(\widehat{x_i}, \widehat{y_i}, x_i/y_i) = \frac{m}{\hbar^2} \int\int \overline{\phi}^{(+)}(K x_i/y_i, \mathbf{x}_i) \frac{\exp(-iq_n y_i e^{i\theta})}{|y_i|} \times V_i(\mathbf{x}_i e^{i\theta}) (\overline{\psi}_{j,m} + \overline{\psi}_{k,m}) e^{6i\theta} d^3\mathbf{x}_i d^3\mathbf{y}_i. \quad (19)$$

In practice, calculations are performed by expanding the former equations into partial waves. This pure technical issue is not the subject of this paper, and we refer the interested reader to [21] for the details on the partial wave Faddeev equations. One should however notice that the partial wave expansion has no effect on the validity of the presented method.

B. Coulomb plus short-range interaction

The former discussion can be readily extended to the case of particles interacting via short-range plus Coulomb forces. In this case we prefer to use Faddeev-Merkuriev equations [22], which generalizes the Faddeev formalism in order to accommodate Coulomb forces.

Indeed, the Faddeev original equations suppose free asymptotic behavior of the particles and in the presence of long-range interaction become ill behaved due to the noncompactness of their kernel. These equations can still provide satisfactory solution for the bound state problem, but are impractical for dealing with the scattering case.[3] Faddeev equations do not shed any light on the asymptotic behavior of the separate amplitudes when long-range interaction is present.

The seminal idea of Merkuriev work [22] was to split the Coulomb potential V^C into a short- plus a long-range part, $V^C = V^{s.C} + V^{l.C}$, by means of some arbitrary cutoff function χ:

$$V_i^{s.C}(x_i, y_i) = V_i^C(x_i)\chi_i(x_i, y_i), \quad (20)$$

$$V_i^{l.C}(x_i, y_i) = V_i^C(x_i)[1 - \chi_i(x_i, y_i)], \quad (21)$$

[1] One must note that this condition is derived for a system of three particles with identical masses. For the case of three particles with arbitrary masses, one gets $\tan\theta < \sqrt{\frac{|\epsilon_n| M m_k}{(E+|\epsilon_n|) m_j m_i}}$, where m_i is the mass of the incoming particle and $m_k \leqslant m_j$, the binding energy $|\epsilon_n|$ corresponds to the weakest bound state of the particle pair (jk) open for scattering, and $M = m_i + m_j + m_k$ is a total mass of the system.

[2] For the case of three particles with arbitrary masses, one gets $\tan\theta < \sqrt{m_k M |\epsilon_m|}/[\sqrt{m_j m_i (|\epsilon_m| + E)} + \sqrt{(M - m_i)(M - m_k)(|\epsilon_n| + E)}]$, where $|\epsilon_n|$ is the ground state binding energy of the particle pair (ij).

[3] In principle, Faddeev equations may be also solved for the long-range scattering problem after the complex scaling. However only the vanishing of the total wave function and not of the separate Faddeev amplitudes (ones work with) is assured in this case.

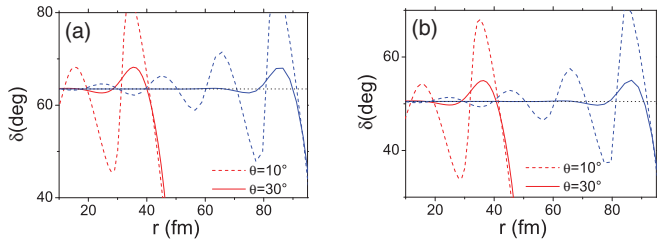

FIG. 1. (Color online) $NN\ ^1S_0$ phase shifts at $E_{\rm cm} = 1$ MeV extracted using relations Eqs. (5) and (6) and Eqs. (9) and (10) for panels (a) and (b), respectively. Calculations were performed with a cutoff imposed at $r_{\rm max} = 50$ (in red, curves diverging close to 50 fm) and 100 fm (in blue, curves diverging close to 100 fm) using a complex rotation angle $\theta = 10^\circ$ (dashed lines) and 30° (solid line). The pure strong interaction result is presented in panel (a) and calculations including repulsive Coulomb interaction for a pp pair are presented in panel (b). They are compared to the exact results indicated by a dotted horizontal line.

and properly reshuffle the long-range terms. One is then left with a system of equivalent equations having the form:

$$\begin{aligned}&\left(E - H_0 - W_i - V_i^s\right)\psi_i^{\rm sc} - V_i^s \sum_{i\neq j}\left(\psi_j^{\rm sc} + \psi_{j,m}^{\rm in}\right)\\ &\quad = \left(W_i - V_i^l - V_i^{C,\rm res}\right)\psi_{i,m}^{\rm in}\,, \quad W_i = V_i^l + V_j^l + V_k^l \end{aligned} \tag{22}$$

where $V_i^s = V_i^{s,C} + V_i$ denote the sum of the short-range interaction $V_i(x_i)$ of the pair (jk) plus the short-range part of the Coulomb force (20).

The incoming state is defined by

$$\psi_{i,m}^{\rm in}(\mathbf{x}_i, \mathbf{y}_i) = \phi_m(\mathbf{x}_i)\varphi^C(q_m, \mathbf{y}_i), \tag{23}$$

where $\varphi^C(q_m, \mathbf{y}_i)$ is an incoming Coulomb plane wave of the incident particle i interacting with a cluster of particles (jk) via the Coulomb potential: $V_i^{C,\rm res}(y_i) = \frac{4\hbar^2\eta_{i,jk}}{\sqrt{3}my_i}$. The $\phi_m(\mathbf{x}_i)$ is the eigenfunction of the mth bound state of the particle pair (jk).

The former equations are solved and the scattering observables extracted in a similar way as for the Coulomb free case. For example the transition amplitudes are given, via the Green theorem, by

$$\begin{aligned} f_{nm}^C(\widehat{y_i}) = -C_n^{-1}\frac{m}{\hbar^2}\int\!\!\int \phi_n^*(\mathbf{x}_i e^{-i\theta})\varphi^{C*}(q_m, \mathbf{y}_i e^{-i\theta})\big[V_j^s(\mathbf{x}_j e^{i\theta})\\ + V_k^s(\mathbf{x}_k e^{i\theta}) + W_i(\mathbf{x}_i e^{i\theta}, \mathbf{y}_i e^{i\theta}) - V^{C,\rm res}(y_i e^{i\theta})\\ - V_i(x_i e^{i\theta})\big]\overline{\Psi}_m(\mathbf{x}_i, \mathbf{y}_i)e^{6i\theta}d^3\mathbf{x}_i d^3\mathbf{y}_i\,, \end{aligned} \tag{24}$$

with $V_i(x_i)$ representing the full interaction between particle pair (jk).

There is however a formal difficulty associated with the extraction of the breakup amplitude for the case when all three particles are charged, since the asymptotic form of the breakup wave function is not known. In this case one may still rely on the approximate relation employing the Peterkop integral [23] as it was claimed in [24].

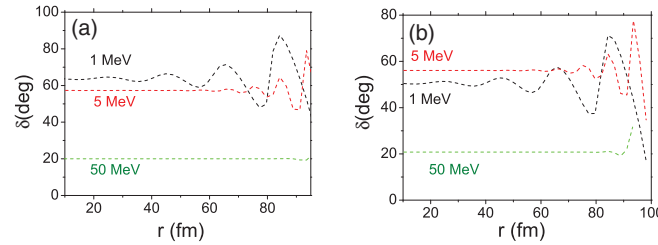

FIG. 2. (Color online) $NN\ ^1S_0$ phase shifts calculation at $E_{\rm cm} =$ 1, 5, and 50 MeV extracted using relations Eqs. (5) and (6) and Eqs. (9) and (10), respectively for panels (a) and (b). Calculations were performed with a cutoff imposed at $r_{\rm max} = 100$ fm using the complex rotation angle $\theta = 10^\circ$. The pure strong interaction results are presented in panel (a), and those including repulsive Coulomb interaction for a pp pair are presented in panel (b).

C. Numerical solution

To solve the three-body problem, the Faddeev amplitudes are expanded in the basis of partial angular momentum, spin and isospin variables, according to

$$\psi_i^{\rm sc}(\vec{x}_i, \vec{y}_i) = \sum_\alpha \frac{\mathcal{F}_i^\alpha(x_i, y_i)}{x_i y_i} Y_i^\alpha(\hat{x}_i, \hat{y}_i). \tag{25}$$

Here $Y_i^\alpha(\hat{x}_i, \hat{y}_i)$ denote the generalized bipolar harmonics containing spin, isospin, and angular momentum variables of the three particles. The so-called Faddeev partial amplitudes $\mathcal{F}_i^\alpha(x_i, y_i)$ are continuous functions in radial variables x, y. The label α represents the set of intermediate quantum numbers. By projecting Eq. (12) or Eq. (22) on the partial wave basis $Y_i^\alpha(\hat{x}_i, \hat{y}_i)$, a set of two-dimensional integro-differential equations is obtained.

This set of equations is solved by expanding the partial Faddeev amplitudes in the basis of piecewise Hermite

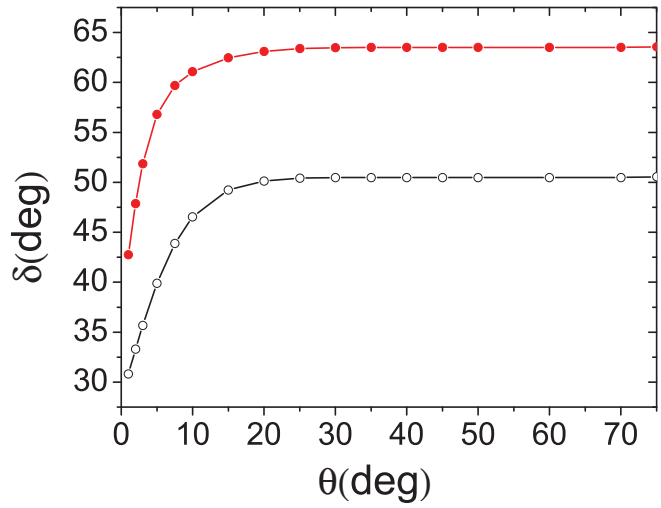

FIG. 3. (Color online) Dependence of the calculated $NN\ ^1S_0$ phase shift using an integral expression as a function of the complex rotation angle. The grid was limited to $r_{\rm max} = 100$ fm. The upper curve corresponds to the Coulomb-free case and the bottom one includes Coulomb.

TABLE I. Calculation of the scattering phase shift using integral expressions at $E_{\rm cm} = 1$ MeV.

	MT I-III				MT I-III+Coulomb			
$r_{\rm max}$ (fm)	5°	10°	30°	50°	5°	10°	30°	50°
10	44.420	49.486	55.790	56.676	33.999	36.390	41.528	43.805
25	34.704	44.211	62.654	63.743	24.772	34.910	50.693	50.698
50	56.812	61.083	63.482	63.512	39.895	46.546	50.487	50.491
100	66.502	63.822	63.512	63.512	55.463	50.811	50.491	50.491
150	62.497	63.485	63.512	63.512	49.317	50.474	50.491	50.491
exact			63.512				50.491	

polynomials (splines):

$$\mathcal{F}_i^{\alpha}(x, y) = \sum c_{i,jk}^{\alpha} S_j(x) S_k(y). \tag{26}$$

The spline functions are defined in a rectangular grid inside the domain $[0, x_{\rm max}] \times [0, y_{\rm max}]$ and are such that $S_j(x = 0) \equiv 0$ and $S_k(y = 0) \equiv 0$ as well as $S_j(x \geqslant x_{\rm max}) \equiv 0$ and $S_k(y \geqslant y_{\rm max}) \equiv 0$. We have alternatively used a cubic and quintic spline basis. This implies that $\mathcal{F}_i^{\alpha}(x, y)$ are regular at the origin and vanish on the borders $x = x_{\rm max}$ and $y = y_{\rm max}$.

Using this technique, the set of integro-differential equations are converted into a linear algebra problem with the unknown complex spline expansion coefficients $c_{i,jk}^{\alpha}$ to be determined. Nowadays, the computational resources permit us to perform rather elaborate three- and two-body calculations. Therefore the spline basis has been chosen to be sufficiently large in order to assure four digits accuracy in three-body calculation and five digits accuracy in the two-body case. For the three-body problem we were using from one to two hundred spline functions in each direction (x and y). The convergence of the results has been checked by increasing the number of splines until the desired number of digits is unchanged. We have also checked the stability of the final result by changing the cubic spline basis into the quintic one. One should mention however that three digits accuracy may readily be obtained by using a spline basis containing as few as 30–40 elements. For more details of the numerical method, the interested reader may refer to [25].

IV. RESULTS

To test the applicability of our approach, we consider a system of three identical nucleons with mass $\frac{\hbar^2}{m} = 41.47$ MeV fm^2, where the strong part of the nucleon-nucleon (NN) interaction is described by the spin-dependent S-wave Malfliet and Tjon potential, MT I-III, defined as

$$V_S(r) = -A_S \frac{\exp(-1.55r)}{r} + 1438.72 \frac{\exp(-3.11r)}{r}, \tag{27}$$

where $V_S(r)$ is in MeV and r is in femtometers. The attractive Yukawa strength is given by $A_{s=0} = -513.968$ MeV fm and $A_{s=1} = -626.885$ MeV fm for the two-nucleon interaction in spin singlet and triplet states respectively.

The MT I-III potential has been chosen for two reasons. On one hand it is a widely employed potential for which accurate benchmark calculations exist. On the other hand this potential, being a combination of the attractive and repulsive Yukawa terms, reflects well the structure of the realistic nucleon-nucleon interaction: it is strongly repulsive at the origin; however it has a narrow attractive well situated at $r \approx 1$ fm. Note that many numerical techniques fail for the potentials that, like MT I-III, contain a repulsive core.

We have first considered the two-body case. In Fig. 1 we present our results for the NN $^1S_0$ phase shifts at $E_{\rm cm} =$ 1 MeV. Two calculation sequences have been performed by forcing $\overline{\psi}_l^{\rm sc}$ to vanish at the border of the numerical grid set at $r_{\rm max} = 50$ fm (in red) and $r_{\rm max} = 100$ fm (in blue), respectively, whereas the complex scaling angle θ has been chosen to be 10° (dashed lines) and 30° (solid lines). The phase shifts are extracted from the $\overline{\psi}_l^{\rm sc}(r)$ value at fixed distance r, according to Eqs. (5) and (6) for the Coulomb free case [Fig. 1(a)] and Eqs. (9) and (10) for the case of short range plus Coulomb interaction [Fig. 1(b)]. As one can see, the extracted phase shifts oscillate with r. This oscillatory behavior is due to the premature enforcement of $\overline{\psi}_l^{\rm sc}(r)$ to vanish at the border of the

TABLE II. Calculation of the scattering phase shift using integral expressions at $E_{\rm cm} = 50$ MeV.

	MT I-III				MT I-III+Coulomb			
$r_{\rm max}$ (fm)	3°	5°	10°	30°	3°	5°	10°	30°
10	19.400	19.719	19.923	19.605	19.795	20.245	20.610	20.313
25	20.788	20.135	20.027	20.032	21.530	20.864	20.755	20.760
50	20.014	20.026	20.027	20.027	20.734	20.754	20.755	20.755
100	20.027	20.027	20.027	20.027	20.755	20.755	20.755	20.755
exact			20.027				20.755	

TABLE III. Neutron-deuteron scattering phase shift and inelasticity parameter as a function of the complex rotation angle θ compared with benchmark results of [26,27]. Our calculations has been performed by setting $y_{\max} = 100$ fm.

	3°	4°	5°	6°	7.5°	10°	12.5°	Refs. [26,27]
				nd doublet at $E_{\rm lab} = 14.1$ MeV				
Re(δ)	105.00	105.43	105.50	105.50	105.50	105.49	105.48	105.49
η	0.4559	0.4638	0.4653	0.4654	0.4653	0.4650	0.4649	0.4649
				nd doublet at $E_{\rm lab} = 42$ MeV				
Re(δ)	41.71	41.63	41.55	41.51	41.45	41.04		41.35
η	0.5017	0.5015	0.5014	0.5014	0.5015	0.5048		0.5022
				nd quartet at $E_{\rm lab} = 14.1$ MeV				
Re(δ)	68.47	68.90	68.97	68.97	68.97	68.97	68.97	68.95
η	0.9661	0.9762	0.9782	0.9784	0.9783	0.9782	0.9780	0.9782
				nd quartet at $E_{\rm lab} = 42$ MeV				
Re(δ)	37.83	37.80	37.77	37.77	37.74	38.06		37.71
η	0.9038	0.9034	0.9032	0.9030	0.9029	0.8980		0.9033

grid $r_{\max}$. The phase shifts extracted close to $r_{\max}$ are strongly affected by the cutoff and are thus not reliable. The amplitude of the close-border oscillations is sizeably reduced by either increasing $r_{\max}$ or θ, i.e., by reducing the sharpness of the numerical cutoff. The extracted phase shifts corresponding to the calculation with $r_{\max} = 100$ fm and $\theta = 30^\circ$ are stable in a rather large window, which starts at $r \sim 5$ fm (right outside the interaction region) and extends up to $r \sim 70$ fm. Beyond this value the effect due to cutoff sets in. In the stability region the extracted phase shifts agree well with the "exact" results (dotted line), obtained by solving the scattering problem using the standard (i.e., not complex rotated) boundary condition technique.

In Fig. 2 we have compared the $NN\ ^1S_0$ phase shifts at different energies ($E_{\rm cm} = 1$, 5, and 50 MeV) by fixing $r_{\max} =$ 100 fm and $\theta = 10^\circ$. One can see that when increasing the energy, the effect of the cutoff reduces, sizeably improving the stability of the extracted phase shifts. The inclusion of the repulsive Coulomb term does not have any effect on the quality of the method.

One may improve considerably the accuracy of the phase shifts calculations by using the integral relation given in Eq. (7). The results are displayed in Tables I and II and in Fig. 3. The phase shifts converge to a constant value by either increasing the cutoff radius $r_{\max}$ or the complex rotation angle. An accuracy of five digits is easily reached. One should notice however that the use of very large values of θ should be avoided, due to the fact that the function $\overline{\psi}_l^{\rm sc}(r)$ as well as the complex scaled potential $V(re^{i\theta})$ might become very steep and rapidly oscillating. At a higher energy, the function $\overline{\psi}_l^{\rm sc}(r)$

TABLE IV. Proton-deuteron scattering phase shift and inelasticity parameter as a function of the complex rotation angle θ compared with benchmark values of [27]. Our calculations has been performed by setting $y_{\max} = 150$ fm.

	3°	4°	5°	6°	7.5°	10°	12.5°	Ref. [27]
				pd doublet at $E_{\rm lab} = 14.1$ MeV				
Re(δ)	108.46	108.43	108.43	108.43	108.43	108.43	108.42	108.41[3]
η	0.5003	0.4993	0.4990	0.4988	0.4986	0.4984	0.4981	0.4983[1]
				pd doublet at $E_{\rm lab} = 42$ MeV				
Re(δ)	43.98	43.92	43.87	43.82	43.78	44.83		43.68[2]
η	0.5066	0.5060	0.5056	0.5054	0.5052	0.5488		0.5056
				pd quartet at $E_{\rm lab} = 14.1$ MeV				
Re(δ)	72.70	72.65	72.65	72.64	72.64	72.63	72.62	72.60
η	0.9842	0.9827	0.9826	0.9826	0.9826	0.9828	0.9829	0.9795[1]
				pd quartet at $E_{\rm lab} = 42$ MeV				
Re(δ)	40.13	40.11	40.08	40.07	40.05	40.35		39.96[1]
η	0.9052	0.9044	0.9039	0.9036	0.9034	0.9026		0.9046

TABLE V. Neutron-deuteron $^3S_1$ breakup amplitude calculated at $E_{\rm lab} = 42$ MeV as a function of the breakup angle ϑ.

	0°	10°	20°	30°	40°	50°	60°	70°	80°	90°
This work Re($^3S_1$)	1.49[−2]	8.84[−4]	−3.40[−2]	3.33[−2]	7.70[−2]	2.52[−1]	4.47[−1]	6.47[−1]	6.30[−1]	−1.62[−1]
This work Im($^3S_1$)	1.69[0]	1.74[0]	1.87[0]	1.92[0]	1.80[0]	1.68[0]	1.70[0]	1.96[0]	2.23[0]	3.17[0]
Ref. [26] Re($^3S_1$)	1.48[−2]	9.22[−4]	−3.21[−2]	3.09[−2]	7.70[−2]	2.52[−1]	4.51[−1]	6.53[−1]	6.93[−1]	−1.05[−1]
Ref. [26] Im($^3S_1$)	1.69[0]	1.74[0]	1.87[0]	1.92[0]	1.80[0]	1.67[0]	1.70[0]	1.95[0]	2.52[0]	3.06[0]

vanishes faster, and thus one achieves a convergent result by employing smaller values of $r_{\rm max}$ and/or θ.

Our analysis has been extended to the three-body case. We have considered the nucleon-deuteron (N-d) $L = 0$ scattering in spin-doublet ($S = 1/2$) and spin-quartet ($S = 3/2$) states. Calculations have been performed both below and above the three-particle breakup threshold. Below the breakup threshold the results are stable and independent of the scaling angle, in a similar way as for the two-body case. Phase shifts might be accurately extracted using either differential or integral expressions.

The application of the differential relations for extracting scattering phase shifts and inelasticities above the breakup threshold does not lead to very convincing results. It is always a difficult task to find the stability domain. We have therefore employed integral expressions Eqs. (24) and (19), obtained using the Green theorem, which once again proved their worth. We have summarized some obtained results in Tables III and IV, respectively, for n-d and p-d scattering above the breakup threshold. Very accurate results are obtained for both the phase shifts and inelasticity parameters, once the complex scaling angle is chosen in the interval [4°, 12.5°] for incident neutrons with energy $E_{\rm lab} = 14.1$ MeV and in the range [3°, 7.5°] at $E_{\rm lab} = 42$ MeV. A stability of the final result within at least three significant digits is assured, providing an excellent agreement with the benchmark calculations of [26,27]. The calculated integral gradually ceases to converge on the finite domain for the calculations when higher complex scaling angles are chosen. This happens due to the fact that the condition of Eq. (18)—which set as a limit $\theta_{\rm max} = 14.2°$ and 8.9° at $E_{\rm lab} = 14.1$ and 42 MeV, respectively—is violated.

We have displayed in Table V the $^3S_1$ n-d breakup amplitude as a function of the breakup angle ϑ, which defines the pair and spectator wave numbers via $k = K\cos(\vartheta)$ and $q = 2K\sin(\vartheta)/\sqrt{3}$, respectively. A nice agreement is obtained with the benchmark calculation of [26]. Some small discrepancy appears only for the ϑ values close to 90°, which corresponds to a geometric configuration where, after the breakup, one pair of particles remains at rest. This is due to the slow convergence of the integral (19) for $\vartheta \to 90°$ in the y direction. A special procedure must be undertaken in this particular case to evaluate the contribution of the slowly convergent integral outside the border of resolution domain limited by $y_{\rm max}$.

V. CONCLUSION

We have presented in this work a method based on the complex scaling, which enables us to solve the few-nucleon scattering problem using square-integrable functions, without an explicit implementation of the boundary conditions. The validity of the method has been demonstrated for two- and three-particle scattering, including the three-particle breakup case with repulsive Coulomb interaction. A three-digit accuracy may be easily obtained using this method.

As it is well known in the two-body case, the complex scaling angle is, in principle, only limited to 90°. We have shown that in order to solve the three-body breakup problem, the scaling angle must be, on the contrary, strongly restricted from above according to Eq. (18). For the scattering at high energy the scaling angle should be limited to very small values. Nevertheless this limitation does not spoil the method at high energies, since after the complex scaling a fast vanishing of the outgoing wave is ensured by the large wave number values.

This method opens a way to 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.

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