Scattering amplitude without an explicit enforcement of boundary conditions

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It has been known for some time that for short range potentials scattering observables can be calculated using complex coordinates. We will show that the standard uniform complex scaling can be applied to calculate the scattering amplitude even in the presence of a long range interaction. The main advantage of the application of the complex scaling to the scattering problem is that the direct imposition of the complicated scattering boundary condition can be avoided. As a result, the scattering problem can be solved using only square integrable functions. The method will be applied not only for potential scattering but for the coupled-channel reaction model. As an application we calculate the phase shifts of the charge exchange reaction ^{3}H(p, n)^{3}He.

I. INTRODUCTION

The method of complex scaling (CS) is well known among few-body physicists as a tool to calculate the half-life time of a resonance state. The CS is widely used in many areas of quantum physics. The applications began in atomic and molecular physics in the early 60s of the last century. A general review of the principles and applications is given in [1,2]. It is very important that the theory of the CS has been founded mathematically [3] and it can easily be applied. The CS method later has become popular also in nuclear physics. Most of the states of a nucleus are decaying ones and this fact gives a great opportunity for the applications of the CS method in nuclear physics. Indeed many calculations have been devoted to find resonance states of cluster nuclei [4–7] or to calculate resonances of nuclear three-body problems [8–11].

Carrying out the diagonalization of the complex scaled Hamiltonian, we can gain information about the bound and resonance states. Besides the observation of the quantized bound and resonance states, the majority of information about nuclei comes from scattering experiments. It would be very expedient that in the framework of the CS procedure, the scattering amplitude could be calculated. Recently, in an indirect way, some scattering observables are calculated using the CS [12] but it is not obvious how to generalize it to coupled channels or to three-body problems. Direct calculations of scattering amplitudes in the framework of the CS have been achieved very early on [13,14] but a drawback of the standard CS (or the uniform CS) emerged. It can be safely applied only for short range potentials [13,15]. This is indeed serious since the Coulomb interaction cannot be neglected in problems of atomic and nuclear physics. There were several ideas of how to modify the basic procedure to overcome this problem [16,17] but none of them gained a widespread acceptance. After these

initial applications, the scattering aspect of the CS has received negligible interest. The turning point is the work [18] where it has been shown that, scattering calculations with the exterior CS can be successfully performed for long range interactions too. Since this pioneering work, the method has been applied for three-body Coulomb scattering even above the three-body breakup threshold [19–21].

The potential benefits to use the CS are the following: We can avoid the explicit construction of the boundary condition [22] and scattering observables can be calculated with the help of square integrable functions. If the Coulomb interaction presents, scattering calculations using CS can be carried out only with the the exterior form of the CS [18–22]. Although a modification of the standard CS was suggested in [23], it was applied only for a potential which is slowly decreasing and it was not checked to see how it performs for the truly long range Coulomb interaction.

The aim of this paper is to show that the standard CS can also be applied in the presence of the long range Coulomb interaction. We will consider nuclear systems where a potential term having Coulomb asymptotic is added to the short range nuclear interaction. We will show that, by separating the Coulomb and nuclear amplitudes, the standard CS can be applied for the calculation of the nuclear scattering amplitude. In Sec. II A for completeness, we review how to apply the CS in the case of short range forces for the calculation of scattering phase shift. Later in Sec. II B, we present our method to handle the long range interactions. We will give two methods to calculate the scattering amplitude. The first one is based on the separation of the wave function into two parts. The second one uses an expansion of the Green operator (Sec. II C). At first glance, they may seem to be different methods but we will show that they give exactly the same scattering amplitude. We will show that both methods can be derived from the same variational principle taking trial functions of special forms. In Sec. II D, we will describe how to generalize the method presented in the previous sections to the coupled-channel reaction model. This model is very successfully and extensively applied in nuclear physics. Finally, in Sec. III,

we present our numerical calculations. Here we discuss the scattering of a neutron on ^{3}He and a proton on ^{3}H in order to show the performance of our method for short and long range forces. In this part, we also solve a coupled-channel problem using the CS. As a realistic application, we will calculate the phase shifts of the charge exchange reaction ^{3}H$(p, n)^3$He described in the two-channel Lane model.

II. COMPLEX SCALING AND SCATTERING STATES

First we consider the potential scattering case when one particle moves in a central symmetric potential. In order to calculate scattering states, the radial Schrödinger equation

$$H_l \psi_{l,k}^{(+)}(r) = E \psi_{l,k}^{(+)}(r) \tag{1}$$

has to be solved with the appropriate boundary conditions. The Hamiltonian in the partial wave l is given by

$$H_l = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r). \tag{2}$$

A. Short range interaction

In the case of a short range potential, the boundary conditions for the physical solution can be given as follows: the wave function is regular at $r = 0$, i.e., $\psi_{l,k}^{(+)}(0) = 0$ and asymptotically behaves as [24]

$$\psi_{l,k}^{(+)}(r) \underset{r\to\infty}{\to} \hat{j}_l(kr) + k f_l(k)\hat{h}_l^{(+)}(kr). \tag{3}$$

Due to the centrifugal barrier, we have $\psi_{l,k}^{(+)}(r) \to c_l \times r^{l+1}$ if $r \to 0$, where c_l is related to the Jost function.

For a given energy $E > 0$, the wave number is denoted by $k = (\frac{2m}{\hbar^2}E)^{1/2} > 0$ and the scattering amplitude is signed by $f_l(k)$. In Eq. (3), we have introduced the Ricatti-Bessel and Ricatti-Hankel functions, $\hat{j}_l(kr)$ and $\hat{h}_l^{(+)}(kr)$, respectively, taking the standard definitions.

The solution of Eq. (1) is searched in the form

$$\psi_{l,k}^{(+)}(r) = \hat{j}_l(kr) + \psi_{l,k}^{sc}(r). \tag{4}$$

For the unknown scattered part of the wave function, $\psi_{l,k}^{sc}(r)$, we can get an inhomogeneous equation

$$(E - H_l)\psi_{l,k}^{sc}(r) = V(r)\hat{j}_l(kr). \tag{5}$$

The scattered part of the wave function $\psi_{l,k}^{sc}(r)$ is not square integrable since asymptotically it has to behave as

$$\psi_{l,k}^{sc}(r) \underset{r\to\infty}{\to} k f_l(k)\hat{h}_l^{(+)}(kr), \tag{6}$$

and for the Hankel function, we have $\hat{h}_l^{(\pm)}(kr) \underset{r\to\infty}{\to} \exp\{\pm i(kr - \frac{l\pi}{2})\}$.

In the standard applications of the CS theory, the role of the CS is to turn a non square integrable function into a square integrable one. For example the wave function of a resonance state is not square integrable but after applying the CS, it

becomes square integrable and then it can be expanded on any square integrable basis. One can apply a similar trick in the case of a scattering problem. The main idea of the method is to carry out the CS not on the full scattering wave function $\psi_{l,k}^{(+)}$ but only on the scattered part of it.

The complex scaling operator is defined by $U(\theta)\phi(r) = \phi^\theta(r) = \exp(i\theta/2)\phi(r\exp(i\theta))$, where $\phi(r)$ is an arbitrary function and θ is a fixed real number. Using this notation, we get

$$\psi_{l,k}^{sc,\theta}(r) \underset{r\to\infty}{\to} e^{i\theta/2}k f_l(k)i^{-l}e^{ikr\cos\theta - kr\sin\theta}. \tag{7}$$

We can notice an important change as the function $\psi_{l,k}^{sc,\theta}(r)$ becomes square integrable provided $0 < \theta < \pi$. If we had applied the CS to the full wave function, it should not have become square integrable since its asymptotic part contains both incoming and outgoing Hankel functions.

It is easy to show that the complex scaled scattered part of the wave function satisfies the following equation:

$$(E - H_l(\theta))\psi_{l,k}^{sc,\theta}(r) = e^{i\theta/2}V(re^{i\theta})\hat{j}_l(kre^{i\theta}), \tag{8}$$

where the complex scaled Hamiltonian is

$$H_l(\theta) = -e^{-2i\theta}\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + e^{-2i\theta}\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(re^{i\theta}). \tag{9}$$

Since $\psi_{l,k}^{sc,\theta}(r)$ is square integrable we can approximate it with the following ansatz:

$$\psi_{l,k}^{sc,\theta}(r) \approx \sum_{i=1}^{N} c_i(\theta)\phi_i(r), \tag{10}$$

where $\phi_i(r), i = 1, \ldots, N$ are arbitrary known square integrable functions. Using Eq. (8) for the unknown linear expansion coefficients, we get the following inhomogeneous linear system of equations:

$$\sum_{j=1}^{N}\left\{E O_{ij} - H_{ij}^l(\theta)\right\}c_j(\theta) = b_i(\theta), \quad i = 1, \ldots N, \tag{11}$$

where

$$b_i(\theta) = e^{i\theta/2}\int_0^\infty dr\,\phi_i(r)V(re^{i\theta})\hat{j}_l(kre^{i\theta}). \tag{12}$$

In Eq. (11), we used the notations $O_{ij} = \langle\phi_i|\phi_j\rangle$ and $H_{ij}^l(\theta) = \langle\phi_i|H_l(\theta)|\phi_j\rangle$.

It remains to calculate the scattering amplitude. We use the well known expression [24]

$$f_l(k) = -\frac{2m}{\hbar^2 k^2}\int_0^\infty dr\,\hat{j}_l(kr)V(r)\psi_{l,k}^{(+)}(r). \tag{13}$$

Substituting Eq. (4) into Eq. (13), we can separate the Born term and we get

$$f_l(k) = f_l^{Born}(k) + f_l^{sc}(k), \tag{14}$$

where

$$f_l^{Born}(k) = -\frac{2m}{\hbar^2 k^2}\int_0^\infty dr\,\hat{j}_l(kr)V(r)\hat{j}_l(kr) \tag{15}$$

and

$$f_l^{sc}(k) = -\frac{2m}{\hbar^2 k^2} \int_0^\infty dr\, \hat{j}_l(kr) V(r) \psi_{l,k}^{sc}(r). \quad (16)$$

The Born term can be easily numerically integrated. In order to use the complex scaled solution $\psi_{l,k}^{sc,\theta}(r)$, we deform the integration contour of Eq. (16) into the complex r plane in the following way $r \to r \exp(i\theta)$. Using the Cauchy-theorem, we can express the scattering amplitude in terms of the complex scaled solution

$$f_l^{sc}(k) = -\frac{2m}{\hbar^2 k^2} e^{i\theta/2} \int_0^\infty dr\, \hat{j}_l(kr e^{i\theta}) V(r e^{i\theta}) \psi_{l,k}^{sc,\theta}(r). \quad (17)$$

Substituting the approximate scattered wave function Eq. (10) into the integral of Eq. (17), we get our final formula

$$f_l^{sc}(k) \approx -\frac{2m}{\hbar^2 k^2} \sum_{i=1}^N c_i(\theta) b_i(\theta). \quad (18)$$

B. Long range interaction

In this section, we assume that in addition to a short range interaction ($V_N(r)$) the Hamiltonian contains the pure Coulomb interaction $V_C(r) = Z_1 Z_2 e^2/r$ with charges Z_1 and Z_2. Using the previous notation, now, we have $V(r) = V_N(r) + V_C(r)$. We will denote the corresponding Hamiltonian by H_l^C and the corresponding scattering solution by $\psi_l^{C(+)}(r)$. We will apply similar arguments and steps as we have done in the case of the short range interaction.

The asymptotic form of the wave function is known

$$\psi_{l,k}^{C(+)}(r) \underset{r\to\infty}{\to} F_l(kr) e^{i\sigma_l} + k f_l(k) e^{2i\sigma_l} u_l^{C(+)}(kr), \quad (19)$$

where we have introduced the outgoing Coulomb wave $u_l^{C(\pm)}(kr) = (\pm i F_l(kr) + G_l(kr)) e^{\mp i\sigma_l}$. The regular and irregular Coulomb functions are denoted by $F_l(kr)$ and $G_l(kr)$, the Coulomb phase shift is signed by σ_l and the nuclear scattering amplitude is marked by $f_l(k)$. Decomposing the total wave functions into two pieces

$$\psi_{l,k}^{C(+)}(r) = F_l(kr) e^{i\sigma_l} + \psi_{l,k}^{C,sc}(r), \quad (20)$$

we can easily derive the following equation:

$$\left(E - H_l^C\right) \psi_{l,k}^{C,sc}(r) = e^{i\sigma_l} V_N(r) F_l(kr). \quad (21)$$

Now we can repeat the steps of the previous section. The asymptotic behavior of the outgoing Coulomb function is given by $u_l^{C(\pm)}(kr) \underset{r\to\infty}{\to} \exp\{\pm i(kr - \eta \ln 2kr - \frac{l\pi}{2})\}$. Using this form, we can realize that the $U(\theta) \psi_{l,k}^{C,sc}(r)$ function goes to zero exponentially fast as r tends to infinity since

$$\psi_{l,k}^{C,sc,\theta}(r) \underset{r\to\infty}{\to} e^{i\theta/2} k f_l(k) e^{2i\sigma_l} i^{-l}$$
$$\times e^{i(kr\cos\theta - \eta \ln 2kr)} \cdot e^{-kr\sin\theta + \eta\theta}. \quad (22)$$

This conclusion is valid if $0 < \theta < \pi$.

The complex scaled analog of Eq. (21) reads

$$\left(E - H_l^C(\theta)\right) \psi_{l,k}^{C,sc,\theta}(r) = e^{i\theta/2} e^{i\sigma_l} V_N(r e^{i\theta}) F_l(kr e^{i\theta}), \quad (23)$$

where $H_l^C(\theta) = U(\theta) H_l^C U(\theta)^{-1}$. Due to the square integrability of $\psi_{l,k}^{C,sc,\theta}(r)$, we can also approximate it in the form

$$\psi_{l,k}^{C,sc,\theta}(r) \approx \sum_{i=1}^N c_i^C(\theta) \phi_i(r). \quad (24)$$

Using Eq. (23), we can derive the following set of equations:

$$\sum_{j=1}^N \{E O_{ij} - H_{ij}^{C,l}(\theta)\} c_j^C(\theta) = b_i^C(\theta). \quad (25)$$

The inhomogeneous term is given by

$$b_i^C(\theta) = e^{i\theta/2} e^{i\sigma_l} \int_0^\infty dr\, \phi_i(r) V_N(r e^{i\theta}) F_l(kr e^{i\theta}). \quad (26)$$

This integral exists since only the short range potential appears in it.

The nuclear amplitude can be calculated from the expression

$$f_l(k) = -\frac{2m}{\hbar^2 k^2} e^{-i\sigma_l} \int_0^\infty dr\, F_l(kr) V_N(r) \psi_{l,k}^{C(+)}(r). \quad (27)$$

Substituting the decomposition of Eq. (20) into the integral above, we can separate the Born term. The total amplitude can be written also in the form of Eq. (14). The Born term is

$$f_l^{\text{Born}}(k) = -\frac{2m}{\hbar^2 k^2} \int_0^\infty dr\, F_l(kr) V_N(r) F_l(kr) \quad (28)$$

and the second term of Eq. (14) now looks like

$$f_l^{sc}(k) = -\frac{2m}{\hbar^2 k^2} e^{i\theta/2} e^{-i\sigma_l}$$
$$\times \int_0^\infty dr\, F_l(kr e^{i\theta}) V_N(r e^{i\theta}) \psi_{l,k}^{C,sc,\theta}(r), \quad (29)$$

where we have used the Cauchy-theorem. If we make the approximation of Eq. (24), we can write

$$f_l^{sc}(k) \approx -\frac{2m}{\hbar^2 k^2} e^{-2i\sigma_l} \sum_{i=1}^N c_i^C(\theta) b_i^C(\theta). \quad (30)$$

C. The Green operator method

In the previous section, the application of the CS to a scattering problem is based on calculating the scattering wave function. Using the Green-operator formalism, we can give the scattering amplitude without an explicit reference to the scattering function. The scattering amplitude correction to the Born term can be cast into the form

$$f_l^{sc}(k) = -\frac{2m}{\hbar^2 k^2} \int dr dr'\, F_l(kr)$$
$$\times V_N(r) G_l(E; r, r') V_N(r') F_l(kr'). \quad (31)$$

The coordinate space representation of the full Green operator is denoted by $G_l(E; r, r') = \lim_{\epsilon \to +0} \langle r | (E + i\epsilon - H_l^C)^{-1} | r' \rangle$. If we transform the integration contours into the complex r and r' planes in the same way as we have done in Sec. II A and use the Cauchy theorem, we can turn Eq. (31) into the form

$$-e^{2i\theta} \frac{2m}{\hbar^2 k^2} \int dr dr' F_l(kre^{i\theta}) V_N(re^{i\theta})$$
$$\times G_l(E; re^{i\theta}, r'e^{i\theta}) V_N(r'e^{i\theta}) F_l(kr'e^{i\theta}). \quad (32)$$

We can realize that we can rewrite this integral in a form which contains the Green operator of the complex scaled Hamiltonian

$$-e^{i\theta} \frac{2m}{\hbar^2 k^2} \int dr dr' F_l(kre^{i\theta}) V_N(re^{i\theta})$$
$$\times G_l^\theta(E; r, r') V_N(r'e^{i\theta}) F_l(kr'e^{i\theta}), \quad (33)$$

where $G_l^\theta(E) = (E - H_l^C(\theta))^{-1}$. In order to be able to calculate the integral above, we need a good approximation for the Green-operator of $H_l^C(\theta)$.

To get such an approximation for $G_l^\theta(E)$, we consider the eigenvalue problem of the complex scaled Schrödinger equation $H_l^C(\theta) \psi_\alpha^\theta = E_\alpha^\theta \psi_\alpha^\theta$. An approximate solution is searched in the form

$$\tilde{\psi}_\alpha^\theta = \sum_i^N a_{\alpha,i}^C(\theta) \phi_i(r). \quad (34)$$

The approximate eigenvalues—bound, resonance, and discretized continuum ones—are denoted by $\epsilon_\alpha(\theta)$ and they can be calculated by solving a generalized matrix eigenvalue problem

$$\sum_{j=1}^N \{\epsilon_\alpha(\theta) O_{ij} - H_{ij}^{C,l}(\theta)\} a_{\alpha,j}^C = 0, \quad i = 1, \dots N, \quad (35)$$

where $H_{ij}^{C,l} = \langle \phi_i | H_l^C(\theta) | \phi_j \rangle$. Using these approximate eigensolutions, the Green-operator appearing in Eq. (33) can be expanded in the form [25,26]

$$G_l^\theta(E; r, r') \approx \sum_{\alpha=1}^N \frac{\tilde{\psi}_\alpha^\theta(r) \tilde{\psi}_\alpha^\theta(r')}{E - \epsilon_\alpha(\theta)}. \quad (36)$$

Substituting this expansion into Eq. (33), we get for the amplitude

$$f_l^{sc}(k) \approx -e^{i\theta} \frac{2m}{\hbar^2 k^2} \sum_\alpha \frac{d_\alpha^C(\theta) d_\alpha^C(\theta)}{E - \epsilon_\alpha(\theta)}, \quad (37)$$

where

$$d_\alpha^C(\theta) = e^{-i\theta/2} e^{-i\sigma_l} \sum_j^N a_{\alpha,j}^C(\theta) b_j^C(\theta). \quad (38)$$

We will refer to the calculation based on Eq. (37) as the CS-GO method and a procedure outlined in the previous section as the CS-WF method [Eq. (30)].

The Green-operator $G_l^\theta(E; r, r')$, considering it as a function of the energy, has pole and cut singularities. It is a bounded operator if E is different from the singularities, unbounded if E is from the cut and undefined if E is a pole. It is expected and numerical studies confirmed, that the finite basis set expansion (36) is a good approximation if the energy E is different from the cut [17]. Thanks to the complex scaling, the cut of $G_l^\theta(E; r, r')$ is moved from the real axis to the complex plane. Therefore for real E we can use Eq. (36). Since the threshold remains on the real axis, the applicability of Eq. (36) is questionable at threshold. In the numerical calculations, we have not experienced any problem due to the fact that $\epsilon_\alpha(\theta)$ in Eq. (36) is never equal to the threshold energy as far as we use a finite basis set.

It is worthwhile to mention here that in the standard application of the CS, Eq. (35) has to be solved in order to determine the bound and resonance states of the system. We have shown that we can also determine the scattering amplitude using this solution. The extra computational effort to calculate the amplitude is negligible [see Eqs. (37) and (38)]. In other words, we can say that it is possible to get the scattering information in the continuum energy region simultaneously, in addition to information on the bound and resonant states by solving the eigenvalue problem Eq. (35).

The remaining part of this section is devoted to show the equivalence of the CS-GO and CS-WF methods. We take two arbitrary but fixed square integrable functions $|\chi\rangle$ and $|\chi'\rangle$ and consider the calculation of the matrix element

$$D = \langle \chi' | G_l^\theta(E) | \chi \rangle. \quad (39)$$

For this purpose we will use a functional F with two trial functions $|\phi'\rangle$ and $|\phi\rangle$

$$F = \langle \chi' | \phi \rangle + \langle \phi' | \chi \rangle - \langle \phi' | (E - H_l^C(\theta) | \phi \rangle. \quad (40)$$

It is easy to show that D is the stationary value of the functional F. The Euler-Lagrange equations for F are $|\chi\rangle = (E - H_l^C(\theta)) | \phi \rangle$ and $|\chi'\rangle = (E - H_l^C(\theta)^\dagger) | \phi' \rangle$. The formal solutions can be immediately written down $|\phi\rangle = G_l^\theta(E) | \chi \rangle$ and $|\phi'\rangle = G_l^\theta(E)^\dagger | \chi' \rangle$, where the adjoint of an operator is denoted by the upper sign †. Substituting these solutions into Eq. (40), we get $F = D$. The functional introduced in Refs. [27,28] has the same form as Eq. (40) but in our case a non-Hermitian operator the complex scaled Hamiltonian appears in it. An another difference is that the energy E is real. We do not have to worry about condition $Im E \neq 0$ of Refs. [27,28] since we have changed the Hamiltonian. The condition of the applicability of the functional Eq. (40) is as follows: the energy E has to differ from the poles and cut of the Green-operator $G_l^\theta(E)$.

For the calculation of scattering amplitudes, a similar functional as Eq. (40) was introduced in [13]. This method was used only for short range potentials. The functional Eq. (40) was used also in [17] where it was outlined how a method, similar to the CS-GO method, can be derived from Eq. (40) using the locally complex distortions technique instead of uniform CS. Here we show how the CS-WF and CS-GO methods can be derived from Eq. (40) in the presence of long range potentials. Let us choose the function $|\chi\rangle$ to the

right hand side of Eq. (23)

$$\chi(r) = e^{i\theta/2}e^{i\sigma_l}V_N(re^{i\theta})F_l(kre^{i\theta}) \tag{41}$$

and furthermore we take $|\chi'(r)\rangle = |\chi^*(r)\rangle$. The function $|\chi\rangle$ is square integrable since the diverging asymptotic behavior of $F_l(kre^{i\theta})$ is compensated by the short range potential $V_N(re^{i\theta})$. For the solutions we have $|\phi'(r)\rangle = |\phi^*(r)\rangle$ since the complex scaled Hamilton operator is complex symmetric. With these choices, D happens to be proportional to $f_l^{sc}(k)$ [see Eqs. (31) and (33)]. We have the relationship

$$f_l^{sc}(k) = -e^{-2i\sigma_l}\frac{2m}{\hbar^2 k^2}D. \tag{42}$$

If we approximate $|\phi(r)\rangle$ in the form $\sum_{i=1}^{N}f_i(\theta)\phi_i(r)$ then the calculation of the stationary value of the functional Eq. (40) leads to the equation

$$\sum_{j=1}^{N}\left(EO_{ij} - H_{ij}^{C,l}(\theta)\right)f_j(\theta) = b_i^C(\theta). \tag{43}$$

For the correction to the Born term from Eqs. (40) and (42), we get

$$f_l^{sc}(k) \approx -e^{-2i\sigma_l}\frac{2m}{\hbar^2 k^2}\sum_{i=1}^{N}f_i(\theta)b_i^C(\theta), \tag{44}$$

where we have used Eq. (43). We notice that the coefficients $f_i(\theta)$ and $c_i^C(\theta)$ satisfy the same set of equations [see Eqs. (25) and (43)] so $f_i(\theta) = c_i^C(\theta)$. Taking into account this fact we can conclude that the variational principle with this choice of trial functions leads to the method CS-WF [see Eq. (30)].

An important property of a variational principle is that the result depends only on the subspace where the "best" solution is searched. The functions $\phi_i(r), i = 1, \ldots N$ span a linear subspace. However this subspace is also spanned by the functions of Eq. (34) therefore if we search the stationary solution $|\phi(r)\rangle$ of Eq. (40) in the form $\sum_{\alpha=1}^{N}g_\alpha(\theta)\tilde{\psi}_\alpha^\theta(r)$ we have to get the same result for D as before. Varying $g_\alpha(\theta)$ in the functional Eq. (40), we get the condition of stationarity

$$\sum_{\beta=1}^{N}\left(E\delta_{\alpha,\beta} - H_{\alpha\beta}^{C,l}(\theta)\right)g_\beta(\theta) = e^{i\theta/2}e^{i\sigma_l}d_\alpha^C(\theta), \tag{45}$$

where $H_{\alpha\beta}^{C,l}(\theta) = \langle\tilde{\psi}_\alpha|H_l^C(\theta)|\tilde{\psi}_\beta\rangle$. Using Eq. (35), we can solve the previous equation and the result is

$$g_\alpha^\theta = e^{i\theta/2}e^{i\sigma_l}\frac{d_\alpha^C(\theta)}{E - \epsilon_\alpha(\theta)}. \tag{46}$$

Calculating the value of D with this solutions ($D \approx F = e^{i\theta/2}e^{i\sigma_l}\sum_{\alpha=1}^{N}g_\alpha(\theta)d_\alpha^C(\theta)$) and using Eq. (42), we realize that the result agrees with the expression that we get with the CS-GO method, i.e., with Eq. (37).

It goes without saying that the CS-WF and the CS-GO methods should produce the same result if $N \rightarrow \infty$, however we have proved that the CS-WF and CS-GO methods give the same scattering amplitude even if N is a finite number.

D. Coupled-channel problem

The applications of the coupled-channel reaction model lead to a system of coupled-differential or integrodifferential equations. For simplicity we restrict ourselves to the first case and show how to apply our CS-WF method in the coupled-channel problem. We assume that the total number of channels is M. The set of equations we have to solve is

$$(E - H_c)\psi_c - \sum_{c'=1}^{M}V_{cc'}\psi_{c'} = 0, \quad c = 1, \ldots, M, \tag{47}$$

where the radial channel functions are denoted by ψ_c. The diagonal V_{cc} and coupling potentials $V_{cc'}, c \neq c'$ have short ranges and the channel Hamiltonian H_c is given by

$$H_c = -\frac{\hbar^2}{2\mu_c}\frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu_c}\frac{l_c(l_c + 1)}{r^2} + V_c^L(r) + E_c, \tag{48}$$

where μ_c and l_c are the reduced mass and the orbital angular momentum, respectively, in the channel c, and the pure Coulomb potentials are V_c^L. The symbol E_c denotes the sum of the energies of fragments which belong to the channel c. For the channel wave numbers, we use the notation $k_c = (2\mu_c(E - E_c)/\hbar^2)^{1/2}$. The number of closed channels, where the wave number is pure imaginary, is denoted by M^B. We assume that for a given sequence the open channels follow the closed ones. The boundary conditions are the standard ones employed in the coupled-channel reaction model. The incoming wave is contained in the channel c_0.

We decompose the radial functions in the same form as we have done in the previous section [see Eq. (20)]

$$\psi_c(r) = e^{i\sigma_c}F_{l_c}(k_cr)\delta_{c,c_0} + \psi_c^{sc}(r), c = M^B + 1, \ldots, M. \tag{49}$$

However we make this decomposition only for the open channels. We do not touch the square integrable channel functions of closed channels. One can easily get a system of equations for the unknown functions $\psi_c(r), c = 1, \ldots M^B$ and $\psi_c^{sc}(r), c = M^B + 1, \ldots, M$. If we carry out the complex scaling of this equation, we get

$$\left(E - H_c^\theta\right)\psi_c^\theta - \sum_{c'=1}^{M^B}V_{cc'}^\theta\psi_{c'}^\theta - \sum_{c'=M^B+1}^{M}V_{cc'}^\theta\psi_{c'}^{sc,\theta}$$
$$= e^{i\theta/2}e^{i\sigma_{c_0}}V_{cc_0}(re^{i\theta})F_{l_{c_0}}(k_{c_0}re^{i\theta}), c = 1, \ldots, M^B \tag{50}$$

and

$$\left(E - H_c^\theta\right)\psi_c^{sc,\theta} - \sum_{c'=1}^{M^B}V_{cc'}^\theta\psi_{c'}^\theta - \sum_{c'=M^B+1}^{M}V_{cc'}^\theta\psi_{c'}^{sc,\theta}$$
$$= e^{i\theta/2}e^{i\sigma_{c_0}}V_{cc_0}(re^{i\theta})F_{l_{c_0}}\left(k_{c_0}re^{i\theta}\right),$$
$$c = M^B + 1, \ldots, M. \tag{51}$$

The complex scaled channel Hamiltonian is $H_c^\theta = U(\theta)H_cU(\theta)^{-1}$. The result of the action of the CS operator on a given function is denoted in the same way as earlier, i.e., $\psi_c^\theta = U(\theta)\psi_c$ and similarly for ψ_c^{sc}.

Since the functions $\psi_c^\theta, c = 1, \ldots, M^B$ and $\psi_c^{sc,\theta}, c = M^B + 1, \ldots, M$ are square integrable, we can approximate them in the following form:

$$\psi_c^\theta(r) = \sum_{i=1}^{N} t_{c;i}(\theta)\phi_i(r), \quad c = 1, \ldots, M^B \qquad (52)$$

and

$$\psi_c^{sc,\theta}(r) = \sum_{i=1}^{N} t_{c;i}(\theta)\phi_i(r), \quad c = M^B + 1, \ldots, M. \quad (53)$$

If we substitute Eqs. (52) and (53) into Eqs. (50) and (51), we can get an inhomogeneous system of linear equations for $t_{c;i}(\theta)$

$$\sum_{j=1}^{N} \left\{ (EO_{ij} - H_{c;ij}^\theta) t_{c;j}(\theta) - \sum_{c'=1}^{M} V_{cc';ij}^\theta t_{c';j}(\theta) \right\}$$
$$= b_{cc_0;i}^\theta, c = 1, \ldots, M, \qquad (54)$$

where we used the abbreviations

$$b_{cc';i}^\theta = e^{i\theta/2} e^{i\sigma_{c'}} \langle \phi_i | V_{cc'}(re^{i\theta}) | F_{l_{c'}}(k_{c'}re^{i\theta}) \rangle. \qquad (55)$$

The rest of the notations are obvious.

The scattering amplitude for the $c_0 \to c$ transition can be turned into the form

$$f_{cc_0} = -\frac{2(\mu_c\mu_{c_0})^{1/2}}{\hbar^2 k_c k_{c_0}} e^{-i\sigma_c} e^{i\theta/2}$$
$$\times \sum_{c'=1}^{M} \int dr F_{l_c}(k_c r e^{i\theta}) V_{cc'}(re^{i\theta}) \psi_{c'}^\theta(r). \quad (56)$$

Using the decomposition of the open channels given in Eq. (49) and the expansions of Eqs. (52) and (53), we can write the correction to the Born term in the form

$$f_{cc_0}^{sc} \approx -\frac{2(\mu_c\mu_{c_0})^{1/2}}{\hbar^2 k_c k_{c_0}} e^{-2i\sigma_c} \sum_{c'=1}^{M} \sum_{i=1}^{N} t_{c';i}(\theta) b_{c'c;i}^\theta. \quad (57)$$

III. NUMERICAL RESULTS

Because nuclear forces are charge independent, it is often useful to use isospin representation. To be specific we will consider the proton scattering on the ground state of a nuclei A with isopin $T_A = 1/2$ and projection $T_{z,A} = 1/2$ (e.g., ^{3}H). The isobaric analog nucleus $\bar{A}$ also has isospin T_A but with projection $T_{z,\bar{A}} = -1/2$ (in the specific case $\bar{A} = {}^3$He). From the states $|pA\rangle$ and $|n\bar{A}\rangle$ with superposition, one can construct wave functions with the total isospins 0 and 1. These states are coupled due to the isovector part of the interaction. In the uncoupled representation, the total wave function is $|pA\rangle \chi_p(\mathbf{r}) + |n\bar{A}\rangle \chi_n(\mathbf{r})$, where the relative motion of proton and neutron are described by $\chi_p(\mathbf{r})$ and $\chi_n(\mathbf{r})$, respectively. The coupled equations of Lane [29] refer to these relative motion functions. If $p + A$ is the entrance channel with the Lane equation, we are describing the $A(p, p)A$ elastic scattering and the $A(p, n)\bar{A}$ charge exchange scattering.

In the ^{3}H$(p, n)^3$He case, carrying out the partial wave expansion, we get the following coupled equations:

$$\left[-\frac{\hbar^2}{2\mu_{^3\text{H}+p}} \left(\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} \right) + V_d(r) \right.$$
$$\left. + V_{Coul}(r) - E_{^3\text{H}+p} \right] \chi_p(r) = V_c(r)\chi_n(r), \quad (58)$$

$$\left[-\frac{\hbar^2}{2\mu_{^3\text{He}+n}} \left(\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} \right) \right.$$
$$\left. + V_d(r) - E_{^3\text{He}+n} \right] \chi_n(r) = V_c(r)\chi_p(r), \quad (59)$$

where $E_{^3\text{H}+p} = E - \epsilon_{^3\text{H}+p}$ and $E_{^3\text{He}+n} = E - \epsilon_{^3\text{He}+n}$ are the center-of-mass energy of the relative motion of ^{3}H $+ p$, ^{3}He $+ n$ systems, $\mu_{^3\text{H}+p}$ and $\mu_{^3\text{He}+n}$ are the reduced masses of ^{3}H$+p$, ^{3}He$+n$ systems, respectively. We use the experimental threshold energy difference, $\epsilon_{^3\text{He}+n} - \epsilon_{^3\text{H}+p} = 0.763$ MeV, between ^{3}He $+ n$ and ^{3}H $+ p$ systems.

The diagonal and coupling potentials (V_d and V_c) are expressed by $T = 0$ and $T = 1$ components as

$$V_d = \frac{1}{2} \left\{ V^{k,T=1} \exp\left[-\left(\frac{r}{b_{k,T=1}} \right)^2 \right] \right.$$
$$\left. + V^{k,T=0} \exp\left[-\left(\frac{r}{b_{k,T=0}} \right)^2 \right] \right\}, \quad (60)$$

$$V_c = \frac{1}{2} \left\{ V^{k,T=1} \exp\left[-\left(\frac{r}{b_{k,T=1}} \right)^2 \right] \right.$$
$$\left. - V^{k,T=0} \exp\left[-\left(\frac{r}{b_{k,T=0}} \right)^2 \right] \right\}, \quad (61)$$

where k denotes the partial wave component $^{2S+1}L_J$. The parameters b_k and V^k were obtained to reproduce the experimental phase shift [30] and shown in Table I for ^3P_J. The long range part of the Coulomb potential between ^{3}H and p is

$$V_{Coul}(r) = \frac{e^2}{r} \text{erf}(\sqrt{\alpha}r), \quad (62)$$

where α is taken to be 0.66 fm^2. In order to apply the CS, we have to separate off a pure Coulomb part in the diagonal potentials. Using the notation of Sec. II D, we have $V_{11}(r) = V_d(r) + V_{Coul}(r) - e^2/r$ and $V_1^L(r) = e^2/r$. For the second

TABLE I. The $3N$-N potential parameters for $T = 1$ and $T = 0$ channels.

	$k = {}^{2S+1}L_J$	b_k[fm]	V_0^k [MeV]
$T = 1$	$^3P_0$	1.54	-91.54
	$^3P_1$	3.06	-18.83
	$^3P_2$	3.03	-22.93
$T = 0$	$^3P_0$	2.5	-49.5
	$^3P_1$	3.0	-8.0
	$^3P_2$	3.5	-20.0

TABLE II. The value of the $^3P_1$ state phase shift at different basis sizes using two distinct values for the CS parameter θ expressed in degree. The center-of-mass energy is 1.00 MeV.

N	^{3}He+n		^{3}H+p	
	$\theta = 15$	$\theta = 25$	$\theta = 15$	$\theta = 25$
15	4.618	4.685	3.229	3.273
20	4.912	4.939	3.433	3.425
25	4.932	4.933	3.419	3.418
30	4.933	4.933	3.418	3.418
exact	4.933		3.418	

channel, we can write $V_{22}(r) = V_d(r)$ and $V_2^L(r) = 0$ and for the coupling $V_{12}(r) = V_c(r)$.

It remains to specify our basis functions. For the partial wave L, we use Gaussian functions with different size parameters

$$\psi_i(r) = N_L(b_i) \cdot r^{L+1} \exp\left[-\frac{1}{2b_i^2} r^2 \right],$$

$$N_L(b_i) = b_i^{-3/2-L} \left\{ \frac{2^{L+2}}{(2L+1)!!\sqrt{\pi}} \right\}^{1/2},$$

(63)

where the parameters $\{b_i : i = 1, 2, \ldots, N\}$ are given by a geometric progression of the form $b_i = b_0 \gamma^{i-1}$. Here, b_0 and γ are the first term and the common ratio, respectively. These type of basis functions are frequently used [31]. We here employ $b_0 = 0.2$ fm and $\gamma = 1.2$ values in the following calculations.

First we check our method in the potential scattering case. For the one channel calculations we will use for the protons Eq. (58) and for neutrons Eq. (59). Understandingly now we will put the coupling potential $V_c(r)$ identically to zero and similarly $\epsilon_{^3\text{He}+n} = \epsilon_{^3\text{H}+p} = 0$. We will show that the rate of the convergence does not depend on the nature (short or long range) of the potential. Table II shows the calculated phase
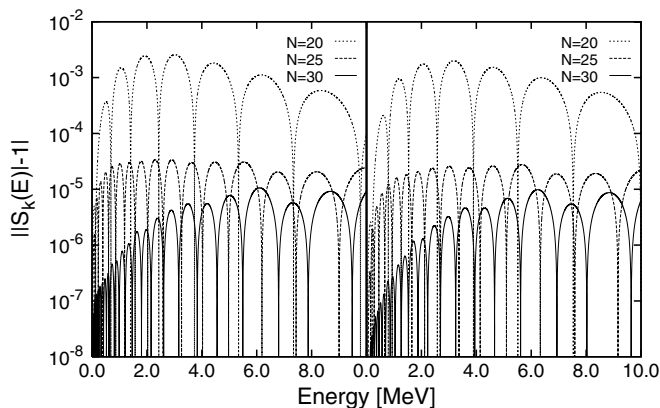

FIG. 1. The quantity $||S_k(E)| - 1|$ for the partial wave $k = {}^3P_1$ as the function of the energy using different number of basis functions. $S_k(E)$ is the partial wave S-matrix. The complex scaling parameter is 20°.
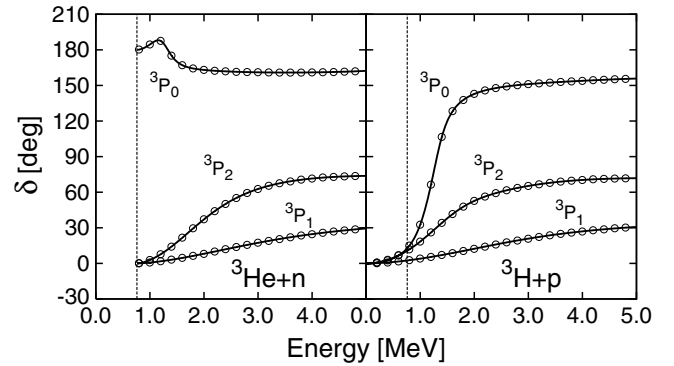

FIG. 2. The P-wave phase shifts of the charge exchange reaction ^{3}H$(p, n)^3$He. The solid lines are determined by CS calculation and the circles are calculated by integrating the differential equations with the Runge-Kutta method. The vertical dashed lines show the threshold energy of the channel ^{3}He+n.

shift at different basis sizes at two different values of the CS parameter θ.

The results of Table II clearly show that the rate of convergence is independent from the short or long range nature of the potential. This table also demonstrates that the converged result is independent, as it should be, from the value of the complex scaling parameter θ. We also notice that the rate of convergence is the same for both θ values.

In order to judge the quality of our method, we present Fig. 1. This figure shows the quantity $||S_k(E)| - 1|$ as the function of the energy. Results of calculations carried out by different basis sizes are displayed. Since the S-matrix is unitary the quantity $||S_k(E)| - 1|$ should be very close to zero. Figure 1 shows that 10^{-5} accuracy is achieved on a large energy region.

For the charge exchange reaction ^{3}H$(p, n)^3$He first we show the calculated phase shift for a P wave compared to the exact solution. This later one is determined by numerically integrating the coupled-differential equation with the Runge-Kutta method. The scattering phase shifts are shown in Fig. 2. We mention that the rate of convergence is the same as in the one channel case. Also the quality of the complex scaled calculation remained unchanged. This was checked by calculating the quantity $||\det(S_k(E))| - 1|$, where $S_k(E)$ is the
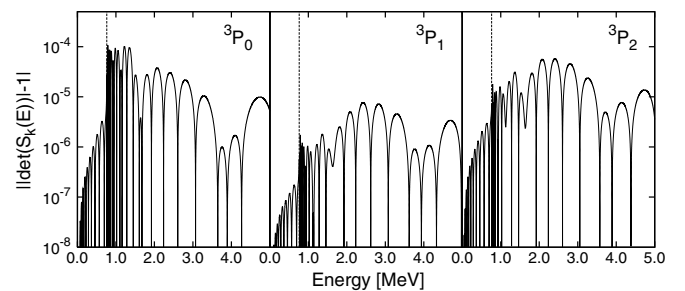

FIG. 3. The quantity $||\det(S_k(E))| - 1|$ for different partial waves as the function of the energy. The CS calculation is carried out using 30 basis functions. $S_k(E)$ is the 2×2 S-matrix in the partial wave $k = {}^{2S+1}L_J$. The complex scaling parameter is 20°. The vertical dashed lines show the threshold energy of the channel ^{3}He+n.

2×2 S-matrix in the partial wave k. We display the quantity $||\det(S_k(E))| - 1|$ in Fig. 3 as the function of the energy using 30 basis functions for three different partial waves. We see that in the coupled-channel problem we have achieved the same accuracy as in the potential scattering case.

IV. SUMMARY

In the coordinate space, boundary conditions have to be given in order to get a unique solution of the Schrödinger equation. In any approximation method, these boundary conditions have to be satisfied. However, the explicit implementation can be avoided. We have presented a method which overcomes the difficulty of the construction of the correct asymptotic form of a scattering wave function. We have achieved this using the method of the CS. It has been known for some time that such a procedure is possible for short range potentials. We have generalized this method to long range potentials, i.e., potentials with Coulombic asymptotic. The method is based on the fact that the total scattering amplitude is the sum of the Coulombic and nuclear amplitudes. As a by-product of our method, it turned out that in order to treat long range potentials it is enough to use the standard CS and that the application of the exterior scaling is not necessary. We have also shown how

to apply the method in the framework of the coupled-channel reaction theory.

Nowadays the CS method is a standard tool to find resonances. The standard application of the CS method requires the solution of a complex symmetric matrix eigenvalue problem. Having solved this equation, the physically important bound and resonance states of the considered system can be determined. We have showed that using the output of the standard CS calculation we can also determine the scattering amplitude. In addition to the Hamiltonian matrix we need only one new matrix: the matrix elements of the transition potential between the basis functions and the regular solution ($\hat{j}_l$ or F_l). The computational cost of this task is negligible. Now we can claim that the CS method has become a unique technical tool since the bound, resonance and scattering state calculations can be done in one run using only square integrable functions.

The scattering boundary condition is especially complicated in the case of three charged particles. We are presently working on how to generalize the presented ideas in the case of the Coulombic three-body problem.

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