Three-body resonances by complex scaling

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It is demonstrated that the complex scaling method can be used in practical calculations to localize three-body resonances. Our model example emphasizes the fact that in three-body systems several essentially different asymptotic behaviors can appear. We show that the possibility of these different asymptotic configurations can lead to an apparent, resonance-like structure in the threebody continuum.

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Three-body resonances (systems that decay into threebody final states) play an important role in few-body physics. The description of these states is somewhat easier than that of scattering processes that lead to three (or more) particles in the outgoing channel. The study of three-body resonances therefore will help to clarify some aspects of the many-body scattering problem.

One of the main difficulties in the general formulation of the quantum mechanical X-body resonance (and scattering) problem is the specification of the asymptotic behavior. There is a fundamental difference between problems where only short-range interactions occur and those where a long-range force (e.g., Coulomb force) is present [1]. There are methods that avoid explicit reference to the unknown or partially known asymptotics (e.g., the Jmatrix method [2] or the potential separable expansion method [3]) but until now these methods have been developed only for two-body systems. In the case of bound states the question of the asymptotic behavior is not a serious problem, and the majority of the methods work because, in most cases, the bound state asymptotics hardly affect the physically observable quantities. However, the asymptotic behavior is crucial for resonances and scattering states.

The complex scaling method (CSM) [4] reduces the description of resonant states to that of bound states, thus avoiding the problem of asymptotics. This method handles the non-Coulomb and Coulomb cases on equal footing and can be extended to two-body scattering states [5]. The possibility of generalizing this method to general many-body scattering states is therefore intriguing. Until now, three-body resonances have been investigated using the Faddeev method [6], real stabilization [7], and the time delay matrix formalism $[8]$. In this paper we study them using the complex scaling method. Although the CSM has been used to describe three-body systems above three-body breakup [9], those authors did not specify how they identified three-body resonances. The present

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work was prompted by the contradictory theoretical results concerning the existence of a soft dipole resonance in the neutron halo nucleus 6 He [10,11]. This problem is complicated by a mixture of the underlying nuclear physics and three-body dynamics. Here we clarify some points about the three-body dynamics.

We begin by recalling the main points of the CSM in the two-body context. In coordinate space, resonance eigenfunctions, corresponding to the complex energy solutions of the Schrödinger equation

$$
\widehat{H}|\Psi\rangle = (\widehat{T} + \widehat{V})|\Psi\rangle = E|\Psi\rangle, \qquad (1)
$$

show oscillatory behavior in the asymptotic region with exponentially growing amplitude, $\sim \exp[i(\kappa - i\gamma)r]$ $(\kappa, \gamma > 0)$. Thus, the resonance eigenfunctions are not square integrable. In the complex scaling method the eigenvalue problem of the transformed Hamiltonian $\widehat{H}_{\theta} = \widehat{U}(\theta) \widehat{H} \widehat{U}^{-1}(\theta)$:

$$
\widehat{H}_{\theta}|\Psi_{\theta}\rangle = E_{\theta}|\Psi_{\theta}\rangle \tag{2}
$$

is solved instead of Eq. (1). $\hat{U}(\theta)$ is an unbounded similarity transformation [12], which, in coordinate space, acts on a function $f(r)$ such that

$$
\widehat{U}(\theta)f(r) = e^{3i\theta/2}f(re^{i\theta}).
$$
\n(3)

[If θ is real, $\widehat{U}(\theta)$ means a rotation into the complex coordinate plane, if it is complex, it means a rotation and scaling. The two problems are connected by the Aguilar-Balslev-Combes theorem [13]: If \widehat{V} is a (dilation) analytic operator, then (i) the bound eigenstates of \widehat{H} are the eigenstates of \widehat{H}_{θ} , for any value of θ within $0 \leq \theta < \pi/2$; (ii) the continuous spectrum of \widehat{H} will be rotated by an angle 2θ ; (iii) a complex generalized eigenvalue of Eq. (2) , $E_{res} = \varepsilon - i\frac{1}{2}\Gamma$, $\varepsilon, \Gamma > 0$ (with the wave number $k_{\rm res} = \kappa-i\gamma,\, \kappa,\gamma>0),$ belongs to the proper spectrum of \widehat{H}_{θ} provided $2\theta > |\arg E_{\text{res}}|$. Roughly speaking, the complex scaling transformation changes the asymptotic wave function from $\exp[i(\kappa - i\gamma)r]$ to $\exp[i(\kappa - i\gamma)r \exp(i\theta)],$ which, in the case of $2\theta > |\arg E_{\text{res}}| = 2|\arg k_{\text{res}}|$, localizes the diverging wave function.

If we have N particles, we can transform the problem from one-particle coordinates to certain interparticle rel-

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ative coordinates (Jacobi coordinates):

$$
{\mathbf r}_1, {\mathbf r}_2, \ldots, {\mathbf r}_N \} \to {\mathbf t}_1, {\mathbf t}_2, \ldots, {\mathbf t}_{N-1}, \qquad (4)
$$

where the origin is fixed at the center of mass, so that $\sum_{i=1}^{N} m_i \mathbf{r}_i = 0$, where m_i are the particle masses. The application of the CSM in this case means that we transform all relative coordinates under the action of $\dot{U}(\theta)$. Note that the transformation (4) is linear. Therefore the complex scaling transformation in a certain set of Jacobi coordinates results in the same transformation in all other possible sets of relative coordinates. As a consequence, we cannot choose the rotation angles independently in the different configurations, like in the multichannel CSM [14].

Our present model problem consists of three particles with masses m_1, m_2 , and m_3 . In order to have only two different systems of Jacobi coordinates, we choose $m_1 =$ $m₂$. The interactions between the particles are separable forces

$$
\widehat{V}_{ij} = |\varphi_0(b)\rangle \lambda_{ij} \langle \varphi_0(b)|, \quad j > i = 1, 2, 3,
$$
 (5)

where $|\varphi_0(b)\rangle$ is the eigenfunction of the three dimensional harmonic oscillator with $n = l = 0, b$ is the oscillator size parameter, and λ_{ij} are the potentia strengths. In coordinate space the interactions depend on the various relative coordinates. Each interaction has a natural Jacobi coordinate system in which it has the simplest form: e.g., in the (12)3 coordinate system [there is a relative coordinate between particles 1 and 2, t_{12} and another between (1,2) and 3, $t_{(12)3}$ the V_{12} interaction depends only on t_{12} .

The kinetic energy operator is easy to express in any coordinate system: e.g., in (12)3 it is given by

$$
T = -\frac{\hbar^2}{2} \left[\frac{1}{\mu_{12}} \Delta_{\mathbf{t}_{12}} + \frac{1}{\mu_{(12)3}} \Delta_{\mathbf{t}_{(12)3}} \right],
$$
 (6)

where the Laplace operators are differential operators in the appropriate Jacobians. It is easy to show that the application of the complex scaling transformation (3) to our potential and kinetic energy operators is equivalent with the change of b to $b \exp(i\theta)$ in (5) and the multiplication of the right-hand side of (6) by $\exp(-2i\theta)$.

As the CSM localizes the resonant wave functions, we can use any bound state method to describe them. Here we use the wave function expansion method. We consider three different trial functions. In coordinate space

$$
\Psi_1 = \sum_{ij} c_{ij} \varphi_i(\mathbf{t}_{12}) \varphi_j(\mathbf{t}_{(12)3}), \tag{7}
$$

$$
\Psi_2 = \sum_{ij} d_{ij} \varphi_i(\mathbf{t}_{23}) \varphi_j(\mathbf{t}_{(23)1}), \qquad (8)
$$

and the sum of these two, $\Psi_3 = \Psi_1 + \Psi_2$. The expansion coefficients c and d are to be determined from a variational principle. As our potentials act only between 8 waves, each oscillator function carries zero angular momentum in (7) and (8). We choose the oscillator size parameter of the wave functions, b , different from b in order to make the trial functions more Bexible. The summation limits in the wave functions are chosen to reach stable convergence.

For the necessary matrix elements we need to calculate the overlap of the product oscillator states between different Jacobi coordinate systems, and the Laplace operator between such states. Using the Talmi-Moshinsky-Tobocman transformation [15] we can express a product of oscillator states, given in a certain Jacobi coordinate system (α) , in terms of product oscillator states in another system (α') , e.g.,

$$
\varphi_i^{\alpha}(\mathbf{t}_{23})\varphi_j^{\alpha}(\mathbf{t}_{(23)1})=\sum_{\mathbf{k},l}a_{ijkl}^{\alpha\alpha'}\varphi_k^{\alpha'}(\mathbf{t}_{12})\varphi_l^{\alpha'}(\mathbf{t}_{(12)3}),\quad(9)
$$

where the sum is finite, and the transformation coefficients can be calculated, for example, by the program developed in [16]. Using these transformations, and in addition the overlap between two oscillator functions with different size parameters, and the matrix element of the Laplace operators between such oscillator functions (for the formulas see, e.g., $[17]$), all necessary matrix elements can be calculated analytically.

We choose $m_1 = m_2 = 2$, and $m_3 = 4$, $b = 1.0$, and $\bar{b} = 2.0$ ($\hbar = 1$ and atomic mass units are used). The use of separable interactions allows us to set up their strengths in such a way that resonances occur at prescribed energies in the two-body subsystems [18]. The choice $\lambda_{12} = 0.6377 + i0.0697$ results in a resonance in the (1,2) subsystem at $E = 1.5 - i0.5$. The $\lambda_{13} = \lambda_{23} = 1.0$ strengths give a resonance in the $(1,3)$ and $(2,3)$ subsystems at $1.7553 - i0.2438$ energy. As an illustrative example we show in Fig. 1(a) the result of a CSM calculation for the (1,2) subsystem. The operation of the CSM is evident: the discretized continuum points are rotated, and the resonance is revealed.

In Figs. $1(b)$ –(d) we show the results of three-body CSM calculations using the Ψ_1 , Ψ_2 , and Ψ_3 trial functions, respectively. We can see that as the rotation angles are large enough to localize the resonances in the subsystems, there are discretized continuum points lying on straight half-lines that start from the position of the resonances of the subsystems. These starting points act as nonreal thresholds. For example, in Fig. 1(b) the halfline starts at $1.5 - i0.5$, which is the resonance energy in the (12) subsystem. This is in full agreement with the mathematical theorems [19,20].

In addition to the continuum points, there is an isolated point at $4.128 - i0.337$ in each figure. The position of this solution is stable against the variation of the rotation angle θ . We can identify this point as a three-body resonance. The fact that this point occurs in each figure shows that this state of the three-body system can exhibit both (12)3 and (23)1 asymptotic behaviors, exactly as expected for a three-body resonance. This behavior gives us a method to identify three-body resonances in practical calculations. But what can we say about the continuum states that lie on the half-lines starting from the resonance energies of the subsystems' For example, in the (23)1 configuration there is a resonant state in the $(2, 3)$ system and a scattering state between 1 and $(2, 3)$. These continuum states are essentially different from a pure three-body scattering state, which is represented by

FIG. 1. Energy eigenvalues (in atomic units) of a complex scaled (a) two-body problem with $m_1 = m_2 = 2$, and $\lambda_{12} = 0.6377 + i0.0697$; (b)-(d) three-body problem with m_1 $=$ m_2 $=$ $2,$ m_3 $=$ $4,$ λ_{12} = 0.6377 + i0.0697, and $\lambda_{13} = \lambda_{23} = 1.0$. The trial wave function is (b) Ψ_1 , (c) Ψ_2 , and (d) Ψ_3 . The θ rotation angle is 0.4 rad in each figure.

the continuum points lying on the half-lines that start at the origin. These resonance+scattering continuum states represent a kind of sequential decay, where the lifetime of a quasistationary subsystem $(2, 3)$ is longer than the time needed for the 1 and (2, 3) scattering.

The fact that different types of continuum states can be present in a three-body system means that the threebody continuum has structure beyond that of the threebody resonances. Let us speculate a bit about this additional structure. In Fig. 2 we show the distribution (in energy bins 0.2 wide) of the continuum points of the model whose wave function is Ψ_3 . We note here that there is no qualitative difference between unscaled $(\theta = 0)$ and complex scaled results because the CSM causes only a contraction of the continuum points, while the resonances remain stable. We can see in Fig. 2 the resonant structure around 4.2. But, in addition, there are concentrations of the continuum points around 1.6 and 2.0, which coincide with the real parts of the resonance energies of the subsystems. These resonance-like structures are apparent and they are the consequence of the fact that if the energy is larger than the threshold energy of a subsystem's resonance, a new, resonance+scattering, asymptotic behavior can appear.

We should note that the shape of the background distribution in Fig. 2 is surprising. In the case of two particles, the wave function expansion method can be thought of as enclosing our system in a box whose size is the 6 nite spatial region of the trial function. This leads to a spectrum $E_n \sim n^2$ $(n = 1, 2, \ldots)$, and the number of continuum points that are in an interval ΔE around E (if ΔE is small) is $\Delta N \sim \Delta E/\sqrt{E}$. We have checked in a two-body model that this is a good approximation. However, our three-body spectrum in Fig. 2 differs strongly from such a shape. In the case of three particles, the radial Schrödinger equation in the hyperspherical coordinate can be cast into a form which is similar to a twobody equation (see, e.g., Ref. [21]). If all angular momenta are zero, a centrifugal barrier occurs in this reformulated Schrödinger equation with $L = 3/2$. This nonzero L leads to a reduction of the low energy solutions, but this is a marginal decrease. There must be another effect which supresses the low energy spectrum.

In conclusion, we have shown that the complex scaling method can be used in practical three-body calculations. In this method, three-body resonances can be identified as those resonant energy solutions that appear in all Jacobi coordinate systems. We have pointed out that the possibility of resonant+scattering-type asymptotic behavior can lead to an apparent structure in the three-body continuum. The case of the 6He soft dipole mode is very similar to our present example. That nucleus is a genuine three-body, $\alpha + n + n$, system [22,23].

> 14 12 10

8 $N(E)$ $\overline{6}$ $\overline{4}$ $\overline{2}$ $\mathbf 0$

There are two resonances in the $\alpha + n$ subsystem at $0.89 - i0.60$ MeV and $4 - i4$ MeV energies [24]. (And there is an antibound state in the $n+n$ subsystem, which is beyond the scope of this Brief Report.) From what we can learn from our present model, it is quite possible that the structure in the 6 He continuum, which has been interpreted as a signature of a three-body resonance (the so-called soft dipole resonance), is nothing but a consequence of the three-body dynamics.

Of course we have considered here only one side of the problem. The question of the 6 He soft dipole resonance can only be answered in a model that contains both the

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correct nuclear physics and the proper three-body dynamics. The application of the complex scaling method to such a realistic model of 6 He is in progress.

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