Complex scaling in the cluster model: Resonances in ^{8}Be

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To find the positions and widths of resonances, a complex scaling of the intercluster relative coordinate is introduced into the resonating-group model. In the generator-coordinate technique used to solve the resonating-group equation, the complex scaling requires minor changes in the formulas and code. The finding of the resonances does not need any preliminary guess or explicit reference to any asymptotic prescription. The procedure is applied to the resonances in the relative motion of two ground-state α clusters in ^{8}Be, but is appropriate for any systems consisting of two clusters.

I. INTRODUCTION

The energy spectrum of a Hamiltonian operator H consists of a negative-energy discrete and a positive-energy continuous part. The continuum is, however, structured. The phase shift function $\delta(E)$ may show steep rises of $\sim\pi$; these phenomena are called resonances. The position E_r and width Γ of a resonance may be defined as the inflexion point of $\delta(E)$ and $\Gamma=2/(d\delta/dE)_{E=E_r}$, respectively. Mathematical considerations reveal that this behavior of the phase shift may be associated with a pole of the scattering amplitude at $E_{\rm res}\approx E_r-i\Gamma/2$, which may serve as an alternative definition of the resonance parameters. At these discrete complex energy values the solution Ψ of the Schrödinger equation $H\Psi=E\Psi$ is an eigenfunction that satisfies the asymptotic boundary condition prescribing a purely outgoing wave (with a complex wave number). Since the tail of a bound-state wave function obeys a special case of this boundary condition (with a positive imaginary wave number), these Gamow or Siegert solutions[1] can be viewed as generalizations of bound states. Although they do not belong to the Hilbert space, they can be treated in close analogy with bound-state wave functions.[2]

This picture makes it possible to apply bound-state techniques to resonant states. We may, e.g., discretize the continuum on a square-integrable basis. Then the discrete eigenvalues that correspond to resonances will be distinguishable from the rest by being stable against certain changes in the basis. The methods exploiting this observation are called stabilization methods.

The real version[3,4] of the stabilization method is based on the approximate equivalence of using a square-integrable basis to closing the system in a box. The complex stabilization method[5,6] to be adopted in this work is a variational method applied to a transformed problem. The complex transformation or "scaling" invoked here rotates the continuum into the complex energy plane but keeps the discrete eigenvalues stable at their original positions. It transforms the Gamow, but not the scattering, wave functions into square-integrable functions. We used the complex scaling recently in a nontrivial nuclear one-body problem with fair success.[7]

The aim of the present paper is to apply this method to simple resonances of a microscopically described nuclear multiparticle system. We shall consider the resonances of ^{8}Be that can be observed in the relative motion of two (unexcited) α particles.[8] The framework we shall work with is therefore the microscopic cluster model.[9]

The concept of a resonance as a complex pole had already been introduced in the cluster model.[10–12] The novelty of using the complex scaling technique is that in this way the explicit construction of the asymptotic outgoing wave can be entirely avoided. The problem can be formulated in the conceptually transparent framework of the resonating-group method (RGM), but for the actual calculations it can be rewritten into a bound-state problem in the technically simpler generator-coordinate method (GCM). For the variable in which the complex scaling is to be applied, we choose the relative coordinate of the RGM. Since the scaling makes the resonance wave function square-integrable, the RGM relative wave function can be expanded in terms of shifted Gaussians. It is this expansion that reduces the RGM problem to a GCM one.

We formulate the physical problem, introduce the complex scaling, and apply it to the problem in Sec. II. We present the numerical results in Sec. III and discuss them in Sec. IV. Some technical points concerning the application of the complex scaling to the GCM are given in the Appendix.

II. FORMULATION

A. The cluster model

Now we collect the main formulas of the model as applied to ^{8}Be. The generalization to other systems is straightforward. We think of ^{8}Be as a fully antisymmetrized system of eight pairwise interacting nucleons grouped into two α clusters.

The wave function of ^{8}Be is taken in the form

$$\Psi=\mathcal{A}_{12}[\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}F(\mathbf{r}_{12})]\ , \tag{2.1}$$

where $\Phi_\alpha^{\rm int}$ is the intrinsic harmonic oscillator shell model ground state of an α particle, $F(\mathbf{r}_{12})$ is the unknown relative-motion function, $\mathcal{A}_{12}$ is the intercluster antisymmetrizer.

The equation for the relative wave function $F(\mathbf{r}_{12})$ arises from the projection equation

$$\langle\delta\Psi\,|\,H-E\,|\,\Psi\rangle=0\ , \tag{2.2}$$

where H is a many-body Hamiltonian,

$$H=-\frac{\hbar^2}{2m}\sum_{i=1}^{8}\Delta_{\mathbf{r}_i}+\sum_{i<j}^{8}V_{ij}(\mathbf{r}_i-\mathbf{r}_j)-T_{\rm c.m.}\ , \tag{2.3}$$

with $T_{\rm c.m.}$ being the kinetic energy operator of the center of mass. Using the ansatz (2.1) in Eq. (2.2), we get a one-channel resonating-group equation

$$\left[-\frac{\hbar^2}{2\mu}\Delta_{\mathbf{r}_{12}}+V_D(\mathbf{r}_{12})\right]F(\mathbf{r}_{12})+\int d\mathbf{r}'_{12}[H_E(\mathbf{r}_{12},\mathbf{r}'_{12})-EN_E(\mathbf{r}_{12},\mathbf{r}'_{12})]F(\mathbf{r}'_{12})=(E-2E_\alpha)F(\mathbf{r}_{12})\ , \tag{2.4}$$

where μ is the reduced mass of the two α clusters, and the other quantities are as follows. The definitions of the exchange kernels are

$$N_E(\mathbf{r},\mathbf{r}')=\langle\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\delta(\mathbf{r}_{12}-\mathbf{r})\,|\times\mathcal{A}'_{12}[\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\delta(\mathbf{r}_{12}-\mathbf{r}')]\rangle\ , \tag{2.5}$$

$$H_E(\mathbf{r},\mathbf{r}')=\langle\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\delta(\mathbf{r}_{12}-\mathbf{r})\,|\,H\,|\times\mathcal{A}'_{12}[\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\delta(\mathbf{r}_{12}-\mathbf{r}')]\rangle\ , \tag{2.6}$$

where $\mathcal{A}'_{12}=\mathcal{A}_{12}-1$, the direct potential term is

$$V_D(\mathbf{r})=\langle\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\delta(\mathbf{r}_{12}-\mathbf{r})\,|\times\sum_{i=1}^{4}\sum_{j=5}^{8}V_{ij}(\mathbf{r}_i-\mathbf{r}_j)\,|\,\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\rangle\ , \tag{2.7}$$

and the energy of the free α particle is

$$E_\alpha=\langle\Phi_\alpha^{\rm int}\,|\,H_\alpha\,|\,\Phi_\alpha^{\rm int}\rangle/\langle\Phi_\alpha^{\rm int}\,|\,\Phi_\alpha^{\rm int}\rangle\ , \tag{2.8}$$

with H_α being the intrinsic α Hamiltonian.

B. The complex scaling

The method of complex scaling, as applied to a single-particle problem, transforms the Hamiltonian $H(\mathbf{r})$ into

$$H(\mathbf{r},\Theta)=U(\Theta)H(\mathbf{r})U(\Theta)^{-1}\ , \tag{2.9}$$

where $U(\Theta)$ is defined by[13]

$$U(\Theta)f(\mathbf{r})=\exp(i\tfrac{3}{2}\Theta)f[\mathbf{r}\exp(i\Theta)]\ ,\quad 0<\Theta<\pi/2\ . \tag{2.10}$$

With the transformed Hamiltonian a transformed Schrödinger equation may be written as

$$H(\mathbf{r},\Theta)\Psi(\mathbf{r},\Theta)=E(\Theta)\Psi(\mathbf{r},\Theta)\ . \tag{2.11}$$

For a broad class of potentials Aguilar, Balslev, Combes, and Simon[5] have rigorously proven some remarkable properties of this transformation ("ABC theorem"). Namely, the continuum of $H(\mathbf{r})$ is rotated down by an angle of 2Θ onto the lower half of the second Riemann sheet of the complex energy surface, while the discrete (bound or resonant) eigenvalues of $H(\mathbf{r})$ remain in their original positions, so that if $2\Theta>|\arg E_{\rm res}|$, the complex eigenvalue $E_{\rm res}$ becomes "uncovered." The transformed eigenfunctions $\Psi(\mathbf{r},\Theta)$ belonging to such $E_{\rm res}$ become square integrable. The spectra of $H(\mathbf{r})$ and $H(\mathbf{r},\Theta)$ are shown schematically in Fig. 1.

Since any resonant eigensolution of $H(\mathbf{r})$ may be transformed into square-integrable $\Psi(\mathbf{r},\Theta)$ with a suitable choice for Θ, the whole variety of approximation methods developed for bound states is at one's disposal. One may proceed by approximating $\Psi(\mathbf{r},\Theta)$ by an expansion over a set of N linearly independent real square-integrable functions $\chi_i(\mathbf{r})$ $(i=1,\ldots,N)$:

$$\Psi_N(\mathbf{r},\Theta)=\sum_{i=1}^{N}c_i(\Theta)\chi_i(\mathbf{r})\ . \tag{2.12}$$

The unknown coefficients $c_i(\Theta)$ are then to be determined by a generalized variational principle[6,14,15]

$$\delta\left[\int d\mathbf{r}\,\bar{\Psi}_N(\mathbf{r},\Theta)^*H(\mathbf{r},\Theta)\Psi_N(\mathbf{r},\Theta)/\int d\mathbf{r}\,\bar{\Psi}_N(\mathbf{r},\Theta)^*\Psi_N(\mathbf{r},\Theta)\right]=0\ . \tag{2.13}$$

The bar on the functions means that only their angular factors are to be complex conjugated.[6,14,15] For $c_i(\Theta)$ we obtain

$$\sum_{j=1}^{N}(H_{ij}(\Theta)-EN_{ij})c_j(\Theta)=0\ , \tag{2.14}$$

where

$$H_{ij}(\Theta)=\int d\mathbf{r}\,\bar{\chi}_i(\mathbf{r})^*H(\mathbf{r},\Theta)\chi_j(\mathbf{r})\ ,\qquad N_{ij}=\int d\mathbf{r}\,\bar{\chi}_i(\mathbf{r})^*\chi_j(\mathbf{r})\ . \tag{2.15}$$

It is straightforward to verify that these matrix elements may as well be expressed as matrix elements of the unrotated operator $H(\mathbf{r})$ or 1 between the back-rotated basis functions

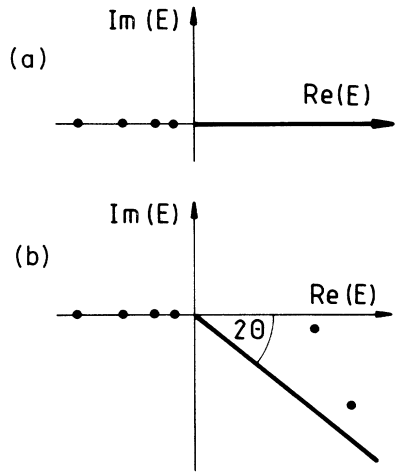

FIG. 1. The spectra of a typical Hamiltonian (a) $H(\mathbf{r})$ and of its transformed (b) $H(\mathbf{r},\Theta)$.

$$\chi_i(\mathbf{r},\Theta)=U(\Theta)^{-1}\chi_i(\mathbf{r})=\exp(-i\tfrac{3}{2}\Theta)\chi_i[\mathbf{r}\exp(-i\Theta)] \ . \tag{2.16}$$

Since we solve Eq. (2.11) approximately, it is expected that the ABC theorem is also fulfilled only approximately. For instance, there will be no eigenenergy that is completely independent of Θ. The resonance energies $E_{\rm res}(\Theta)$ will also move along trajectories in the complex energy plane as a function of Θ. It had been suggested,[16] and subsequently confirmed in many works,[6] that the best estimate for a resonance energy is given by the particular Θ value for which the rate of change with respect to Θ is minimal. This heuristic procedure has been justified by an extension of the virial theorem.[14,15,17]

C. Complex scaling in the cluster model

The RGM equation (2.4) has the form of a Schrödinger equation with a very complicated effective potential. Let us approximate $F(\mathbf{r}_{12})$ with a combination of shifted Gaussians centered around suitable points $\mathbf{s}_k$:

$$F(\mathbf{r}_{12})=\sum_{k=1}^{N} f_k \exp[-\gamma(\mathbf{r}_{12}-\mathbf{s}_k)^2] \ . \tag{2.17}$$

This expansion is widely used in resonating group calculations for bound-state wave functions and for the interior of scattering wave functions.[8,18] It may also be used for scattering states in the exterior region and, in combination with the real stabilization technique, for resonances as well.[4]

When γ is chosen equal to the common oscillator parameter $\beta_\alpha=m\omega/\hbar$ of the α particles, the expansion (2.17) reduces the RGM to the conventional GCM. Because of the complex scaling, however, for our purpose it is important to keep γ independent of β_α. In this case the RGM reduces to Tohsaki-Suzuki's "new" GCM.[19]

In the spirit of Sec. II B, we subject the coordinate $\mathbf{r}_{12}$ in the basis function to a complex rotation. According to Eq. (2.16), we arrive at

$$F(\mathbf{r}_{12},\Theta)=\sum_{k=1}^{N} f_k(\Theta)\exp(-i\tfrac{3}{2}\Theta) \times\exp\{-\gamma[\mathbf{r}_{12}\exp(-i\Theta)-\mathbf{s}_k]^2\} \tag{2.18}$$

or, equivalently, at

$$F(\mathbf{r}_{12},\Theta)=\sum_{k=1}^{N} f_k(\Theta)\exp\{-i\tfrac{3}{2}\Theta\}\exp[-\gamma_\Theta(\mathbf{r}_{12}-\tau_k^\Theta)^2] \ , \tag{2.19}$$

where

$$\gamma_\Theta=\gamma\exp(-i2\Theta) \ , \quad \tau_k^\Theta=\mathbf{s}_k\exp(i\Theta) \ . \tag{2.20}$$

Putting the form (2.19) into (2.13), we get for the coefficients $f_k(\Theta)$ the discretized form of the generalized Griffin-Hill-Wheeler integral equation

$$\sum_{j=1}^{N}[h_{ij}(\Theta)-En_{ij}(\Theta)]f_j(\Theta)=0 \ , \tag{2.21}$$

where

$$\begin{aligned} h_{ij}(\Theta)&=\langle\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\overline{\exp[-\gamma_\Theta(\mathbf{r}_{12}-\tau_i^\Theta)^2]}\,|\,H\,|\,\mathcal{A}_{12}(\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\exp\{-\gamma_\Theta(\mathbf{r}_{12}-\tau_j^\Theta)^2\})\rangle \ , \\ n_{ij}(\Theta)&=\langle\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\overline{\exp[-\gamma_\Theta(\mathbf{r}_{12}-\tau_i^\Theta)^2]}\,|\,\mathcal{A}_{12}(\Phi_\alpha^{\rm int}\Phi_\alpha^{\rm int}\exp\{-\gamma_\Theta(\mathbf{r}_{12}-\tau_j^\Theta)^2\})\rangle \ . \end{aligned} \tag{2.22}$$

The matrix elements given above are generalizations of Tohsaki-Suzuki's "new GCM kernels" to complex γ and generator coordinate. In the appendix we give a derivation of these kernels.

We should like to point out that once the kernels in the "new GCM space" are known for real parameters γ and $\mathbf{s}$, the change to the complex case, $\gamma\exp(-2i\Theta)$ and $\mathbf{s}\exp(i\Theta)$, implies only minor modifications of the kernels. With these minor alterations, any existing new generator coordinate code can be used to compute resonances.

III. NUMERICAL RESULTS

In the numerical example, for the sake of comparison, we have chosen the same parameters as in Refs. 10 and

TABLE I. The complex energies $E_r - i\Gamma/2$ (MeV) of some resonances in ^{8}Be.

Model			$J^\pi=0^+$	$J^\pi=2^+$	$J^\pi=4^+$
Present work	$\beta_\alpha=0.53$,	$\gamma=0.4$[a]	$0.558-i0.097$	$3.168-i1.226$	$12.10-i3.86$
	$\beta_\alpha=0.47$,	$\gamma=0.4$	$0.585-i0.120$	$3.069-i1.196$	$11.56-i3.53$
	$\beta_\alpha=0.47$,	$\gamma=0.32$	$0.588-i0.121$	$3.068-i1.195$	$11.60-i3.52$
Ref. 11	$\beta_\alpha=0.47$	Gamow	$0.59-i0.120$	$3.34-i1.240$	$11.36-i2.47$
		Scattering	$0.59-i0.135$	$3.08-i1.495$	$11.70-i3.79$
Ref. 10	$\beta_\alpha=0.47$	Gamow		$3.16-i1.205$	$12.20-i3.88$
		Scattering		$3.16-i1.565$	$12.20-i4.27$

[a]The zero of the energy scale is -54.17 MeV (otherwise -53.41 MeV).

11. For the nuclear part of the two-body interaction we used the Volkov 1 force[20] with Majorana exchange parameter $m=0.6$. The Coulomb interaction is included in the form of a fairly accurate expansion in terms of Gaussians.[21] The oscillator size parameter in the intrinsic wave function was chosen to be $\beta_\alpha=0.470\,31$ fm^{-2} in accordance with Refs. 10 and 11 in most of the calculations, or to be $\beta_\alpha=0.529\,06$ fm^{-2}, which gives the best α binding energy. The arbitrary γ parameter was taken to be 0.32 fm^{-2}, or, for test purposes, 0.40 fm^{-2}. The number of basis functions was 24, and the values s_i of the generator coordinate were distributed equidistantly in the interval (1 fm, 24 fm). A test calculation showed that this density of s_i is adequate for the resonance energy. The zero of the energy scale in all cases was set equal to twice the actual α binding energy.

Our results for the three resonances ($J^\pi=0^+,2^+,4^+$) of ^{8}Be are displayed in Table I, together with the corresponding numbers of Refs. 10 and 11. We see that the three different methods give the same results for all states considered with accuracies well within the predicted widths of the resonances. As for the γ dependence, it can be interpreted in terms of a generalized scaling.[6] In fact, with the distance and number of s_i points assumed to be appropriate, one can prove that a change of γ is equivalent to a dilation transformation of the problem.

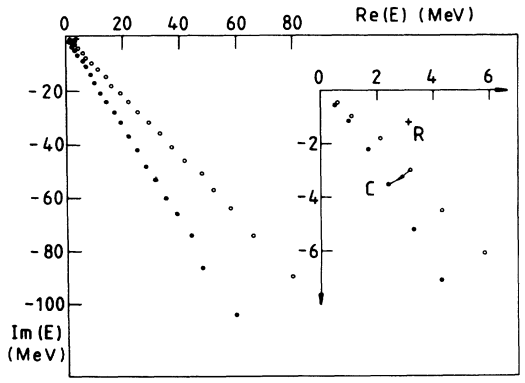

FIG. 2. The $J^\pi=2^+$ energy values as given by Eq. (2.21) solved on a 24-term complex basis ($\gamma=0.32$ fm^{-2}) with $\Theta=0.4$ (○) and $\Theta=0.5$ (●); the point + belongs to both Θ values. The inset shows the area near the origin on an enlarged scale.

The ABC theorem was actually proved for a combination of the complex rotation with such a dilation. The stability of $E_{\rm res}$ with respect to γ can thus be viewed as an analog of its stability to Θ.

In Figs. 2–5, the working mechanism of our method can be followed in full detail. Figure 2 shows the energy values yielded by Eq. (2.21) with $N=24$, with two different Θ values. For each Θ, N discrete complex E values are obtained. The one denoted by a cross (in the insert by R) is stuck to the same place irrespective of the value of Θ. This point is to be regarded as a resonance. The remaining values, for a fixed Θ, are lined up on a straight line declining by 2Θ from the real energy axis, so they should be looked upon as a discretization of the rotated continuum.

In Fig. 3 the stability of the point R is displayed on an enlarged scale together with the trajectory of a nearby continuum point, denoted by C in the inset of Fig. 2. According to the ABC theorem, the continuum point is to be moved along an arc given by the equation

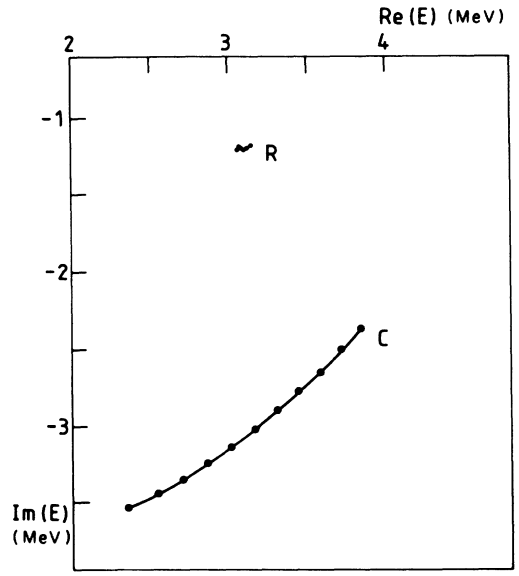

FIG. 3. The Θ trajectories of the resonance (R) and of a continuum point (C) of Fig. 2. Both for R and C, Θ varies from the right to the left between 0.3 and 0.5.

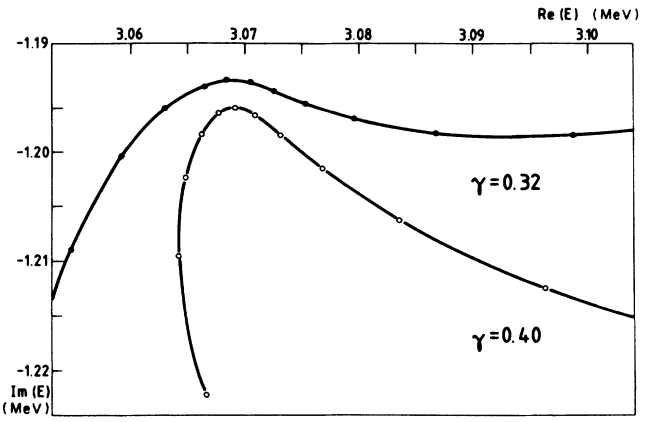

FIG. 4. Magnified plot of the Θ trajectory of R from Fig. 3 (●) and the same with $\gamma=0.4$ fm^{-2} (○). Θ varies from 0.34 to 0.54 by steps of 0.02.

$E\exp(-2i\Theta)$. The small deviation from the straight lines in Fig. 2 and from the circular arc in Fig. 3 are due to the finiteness of the basis set.

Figures 2 and 3 illustrate that the ABC theorem is fulfilled approximately and thereby justify the approximation method we used to solve the rotated RGM equation. In this respect it is worth noting that in a sense the method checks itself. Not only the stability of the resonance measures the overall accuracy but also the deviation of the slope of the rotated continuum from 2Θ. This helps to choose a reasonable basis.

Now let us turn to the precise determination of the position and width of the resonance. Figure 4 presents the relevant part of the Θ trajectory thoroughly magnified. Here insight can be gained into the "slowing down" of the trajectory. The subsequent points belong to equal steps in Θ. The resonance position is taken as the $dE/d\Theta\approx 0$ point. That is how the values of Table I were obtained. Figure 5 shows the convergence of the stable energy point with increasing basis size.

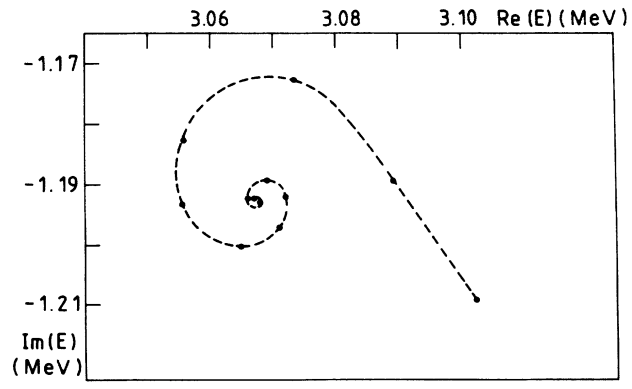

FIG. 5. The N trajectory of the resonance energy (R) belonging to $\gamma=0.32$ fm^{-2} and $\Theta=0.46$. From the right to the left $N=12$, 13, 14, 15, 16, 17, 18, 19, 20, 22, 24, and 28.

IV. DISCUSSION AND SUMMARY

The study we have presented here has several aspects. As an approach to resonant states, our method is a direct method, which solves the dynamical equation with purely outgoing asymptotics and associates the real and imaginary parts of the complex energy eigenvalues with the positions and widths of the resonances. Owing to the complex scaling, which is becoming commonplace in atomic and molecular physics,[6] but is still counted a novelty in nuclear physics, this method excels among the direct methods[10–12] in two respects: First, there is no explicit reference to the asymptotics required, and second, we need no advance guess for the approximate position and width of the resonance either. Ostensibly, Okhrimenko's method[11] shares this latter advantage with ours. However, Okhrimenko's method yields a great number of resonances in each J^π, out of which our method reproduces only one. We think that the other resonances are spurious and could be best eliminated by invoking a first guess. A scrutiny into the reasons of the appearance of the spurious resonances in Ref. 11 is underway and will be published elsewhere.

As for the approximation used to solve the dynamical equation, this work belongs to the stabilization methods. It expands the trial function on a square-integrable basis, and singles out the resonances by a stability condition. Just as in the method proposed earlier,[4] the basis consists of shifted Gaussians, which reduces the underlying RGM model to a GCM model. The advantage over real stabilization methods arises from the fact that the scaled resonance wave function is square integrable: the expansion of such a function over a square-integrable basis may be duly expected to be more accurate.

It is also for this reason that, in contrast to the real stabilization methods, which cannot identify resonances without solving the problem with several bases of different sizes, the complex stabilization method reveals the existence of a resonance by a single calculation with a (sufficiently large) basis provided the rotation angle Θ is appropriate. A precise determination of the position and the width requires repetitions of the calculation at various Θ.

With the scaling shifted from the Hamiltonian to the basis functions, the procedure requires minor technical changes in the computation of the generator-coordinate kernels, which can easily be introduced in existing GCM codes.

Finally, we should like to point out that no use was made of the equal size of the clusters in our numerical example. With the complex rotation performed on the size parameter (and centers) of the Gaussians of the relative motion, this size parameter becomes at any rate detached from those of the internal motions. Therefore, no advantage can be derived from the equality of the internal size parameters. Thus, since our case is not special in this respect, the method is valid to any system containing two clusters, which are not even necessarily in their ground states. An application to a multichannel description of some resonances of ^{8}Be that involve excited α clusters is underway.

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APPENDIX

Here we show how the complex rotated GCM formalism derives from the conventional GCM formalism. The usual GC trial function has the form

$$\Psi(\mathbf{t}_A,\mathbf{t}_B)=\mathcal{A}_{12}\left\{\Phi_A^{\rm int}\Phi_B^{\rm int}\exp\left[-\frac{A\beta_A}{2}(\mathbf{r}_A-\mathbf{t}_A)^2-\frac{B\beta_B}{2}(\mathbf{r}_B-\mathbf{t}_B)^2\right]\right\}, \tag{A1}$$

where $\Phi_A^{\rm int}$ and $\Phi_B^{\rm int}$ are the translational-invariant harmonic-oscillator shell-model ground-state wave functions of clusters A and B having different oscillator width parameters, β_A and β_B, respectively, and $\mathbf{r}_A$ and $\mathbf{r}_B$ are the center-of-mass coordinates of A and B, respectively. By integrating over $\mathbf{T}=(A\mathbf{t}_A+B\mathbf{t}_B)/(A+B)$, we get rid of the spurious center-of-mass motion[22] and obtain (apart from a constant factor)

$$\Psi(\gamma_0,\mathbf{t})=\mathcal{A}_{12}\{\Phi_A^{\rm int}\Phi_B^{\rm int}\exp[-\gamma_0(\mathbf{r}_{12}-\mathbf{t})^2]\}\ , \tag{A2}$$

where

$$\gamma_0=A\beta_A B\beta_B/2(A\beta_A+B\beta_B)\ , \tag{A3}$$

and $\mathbf{t}=\mathbf{t}_A-\mathbf{t}_B$.

Because of the scaling, however, we would like to use basis functions $\Psi(\gamma,\mathbf{t})$, which contain γ unrelated to β_A,β_B. Since it is $\Psi(\gamma_0,\mathbf{t})$ whose kernels are easy to calculate,[23] it would be useful to express $\Psi(\gamma,\mathbf{t})$ in terms of $\Psi(\gamma_0,\mathbf{t})$. This may be done, e.g., through the double Fourier transformation

$$\Psi(\gamma,\mathbf{s})=\left[\frac{\gamma_0}{4\pi^2\gamma}\right]^{3/2}\int d\mathbf{k}\exp(\mathbf{k}^2/4\gamma_0-\mathbf{k}^2/4\gamma-i\mathbf{k}\mathbf{s})\times\int d\mathbf{t}\exp(i\mathbf{k}\mathbf{t})\Psi(\gamma_0,\mathbf{t})\ . \tag{A4}$$

A straightforward application of this generating function may be shown to lead to Tohsaki-Suzuki's "new GCM."[19]

However, for $\gamma<\gamma_0$ (γ and $\mathbf{s}$ are still real), we may simplify (A4) by interchanging the two integrations and obtain

$$\Psi(\gamma,\mathbf{s})=\left[\frac{\gamma_0^2}{\pi(\gamma_0-\gamma)}\right]^{3/2}\int d\mathbf{t}\exp\left[-\frac{\gamma_0\gamma}{\gamma_0-\gamma}(\mathbf{s}-\mathbf{t})^2\right]\Psi(\gamma_0,\mathbf{t})\ . \tag{A5}$$

We can make a similar simplification for $\gamma>\gamma_0$ as well:

$$\Psi(\gamma,\mathbf{s})=i\left[\frac{\gamma_0^2}{\pi(\gamma-\gamma_0)}\right]^{3/2}\int_{-i\infty}^{i\infty}d\mathbf{t}\exp\left[-\frac{\gamma_0\gamma}{\gamma_0-\gamma}(\mathbf{s}-\mathbf{t})^2\right]\Psi(\gamma_0,\mathbf{t})\ , \tag{A6}$$

where the integration is to be performed along the imaginary axes t_x, t_y, and t_z.

The conventional GCM kernels are matrix elements between $\Psi(\gamma_0,\mathbf{t})$ and $\Psi(\gamma_0,\mathbf{t}')$. Equations (A5) and (A6) show, that once these have been calculated, the new kernels, i.e., the matrix elements of $\Psi(\gamma,\mathbf{s})$ and $\Psi(\gamma,\mathbf{s}')$, require just integrations over $\mathbf{t}$ and $\mathbf{t}'$. In this way Tohsaki-Suzuki's kernels can be calculated by a simplified procedure.

Equations (A5) and (A6) can be generalized to complex γ and $\mathbf{s}$, which give rise to complex scaled basis functions. The equation corresponding to (A5) reads [$\mathrm{Re}(\gamma_\Theta)<\gamma_0$]

$$\Psi(\gamma,\mathbf{s},\Theta)=\left|\frac{\gamma_0^2}{\pi(\gamma_0-\gamma_\Theta)}\right|^{3/2}\exp\left[i\tfrac{3}{2}\arg\frac{\gamma_0^2}{\gamma_0-\gamma_\Theta}\right]\times\int d\mathbf{t}\exp\left[-\frac{\gamma_0\gamma_\Theta}{\gamma_0-\gamma_\Theta}(\tau_\Theta-\mathbf{t})^2\right]\Psi(\gamma_0,\mathbf{t})\ , \tag{A7}$$

where $\gamma_\Theta=\gamma\exp(-2i\Theta)$ and $\tau_\Theta=\mathbf{s}\exp(i\Theta)$. Comparing (A7) and (A5), one can show that the calculation of the complex rotated kernels differs from the real case only in appropriate phase factors and modulus signs.

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