Structure of positive energy states in a deformed mean-field potential

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Abstract

We investigate the properties of single-particle resonances in a non-spherical potential by solving the coupled-channels equations for the radial wave functions. We first generalize the box discretization method for positive energy states to a deformed system. As in the spherical case, we find that the discretized energy is stabilized against the box size when a resonance condition is met. Using the wave functions thus obtained, we then discuss the energy and the radial dependences of scattering wave functions in the vicinity of an isolated resonance. In the eigenchannel basis, where the $S$-matrix is diagonal, we propose a generalized expression for the factorization formula for the multi-channel wave function. We find that the factorized wave function agrees well with the exact solution inside the centrifugal barrier when the energy distance from the resonance is less than the resonance width.
I. INTRODUCTION

Recent experimental activities on drip-line nuclei have opened up a renewed interest in the continuum spectra of finite many-body systems. These nuclei are often weakly bound, or may even be unbound, and a proper treatment of the positive-energy states is crucial for their theoretical description. The continuum influences the properties of loosely bound nuclei mainly through the resonant states, which have a dominant contribution both in the ground state, e.g., through the correlations induced by the virtual pair scattering, and in the excited states [1–9]. It is thus becoming more and more important to approach the structure of unstable nuclei from the nuclear reaction point of view [10,11]. Recent developments of shell model calculations for weakly-bound systems by Id Betan et al. [1] and by Michel et al. [2] clearly indicate this direction.

A single-particle resonance state can be obtained relatively easily when the mean field potential has a spherical shape. In this case, the single-particle angular momentum is conserved, and the Schrödinger equation is reduced to a one dimensional differential equation for the radial motion. Approximated resonance states are easily found by putting a system in a box and imposing a condition that the wave function vanishes at the edge of the box. With this boundary condition, the continuum spectra are discretized. It has been recognized that, for a resonance state, the single-particle energy is stabilized against the box size, while it changes significantly as a function of the box radius for non-resonant continuum states [12–14].

A more consistent treatment for the resonance state is also possible for a spherical system. The resonance states are associated with poles of the S-matrix in the complex energy plane. One way to obtain the resonance states is to impose the outgoing wave boundary condition in the asymptotic region with a complex energy. The state which satisfies this boundary condition is referred to as the Gamow state in the literature. A similar approach is used in the complex scaling method, which has been developed originally in atomic and molecular physics [15] and subsequently been applied to nuclear systems [16,17]. Alternatively, the resonance states can also be found by monitoring the energy derivative of the phase shift along the real energy axis [18], where a maximum appears at the resonance energy. For a scattering wave function in a spherical potential, a simple factorization formula has been derived for its energy and radial dependences in the vicinity of an isolated resonance state [18–20]. This factorization property has been used recently in order to estimate the effect of resonant states on pairing correlations in loosely bound nuclei [5].

A resonance structure is much more complicated for a deformed system, where several angular momentum components of the single-particle wave function are coupled to each other. A standard method to solve this problem is to expand the wave function on a discrete basis, which may be deformed harmonic oscillator wave functions [21,22] or eigenfunctions of a spherical potential [23,24]. The positive energy states obtained by diagonalizing the Hamiltonian in such basis can describe properly the main properties of the resonant states [13,14], but this may require a large number of the basis set. A more direct method to obtain resonance states in a deformed system is to setup the coupled-channels equations for the radial motion and solve them for a complex energy by imposing the outgoing wave boundary condition at infinity for all the open channels [25]. Recently, this method has been successfully applied to the proton emission decay of proton-rich nuclei [26,27].
method has an advantage over the matrix diagonalization method that the wave functions are subject only to the radial mesh discretization error for the Schrödinger equation and that the desired asymptotic boundary condition can be imposed independently of the size of the mesh interval. However, the description of resonant states with such complex wave functions is generally difficult to use in nuclear models, since all the evaluated observables become complex quantities if the rest of the complex non-resonant states is not taken into account. We thus prefer to keep the energy as a real variable here.

The aim of this paper is to develop a practical method to obtain scattering wave functions in the vicinity of a multi-channel resonance state. A difficulty is that there are \( N \) linearly independent solutions of the coupled-channels equations at a given energy \( E \) (\( N \) is the number of included channels), whose asymptotic behavior are all different. For example, a physical scattering boundary condition is defined by requiring that asymptotically there is an incoming wave only in the incident channel. In this case, the equations have \( N \) degenerate solutions depending on which channel is the incident one. Since any linear combination of these \( N \) solutions is also a solution of the coupled-channels equations, a problem arises as to which combination one should take in order to study efficiently a multi-channel resonance state. If the resonance width is extremely small, as in the case of proton decay, one can easily construct a resonance wave function by matching to a standing wave solution [28–30]. However, this procedure is not applicable to a broad resonance.

Our method presented in this paper is to start with discretized states whose wave functions vanish at a given radius. This is an extension of the box boundary condition for a spherical system into the deformed regime. As in the spherical case, resonances can be identified with those states whose energy is stabilized against the box size. This method provides the most convenient basis states, where the unperturbed states are already a good approximation to the true resonance states. In fact, as we will show below, the resonance energy thus estimated is close to the energy at which the first derivative of the eigenphase sum with respect to energy has a maximum. Here, the eigenphase sum is defined as the sum of the phase shifts for the eigenchannels, for which the \( S \)-matrix is diagonal [31]. In the field of electron-molecule scattering, it has been known that the eigenphase sum has the same energy dependence as the elastic phase shift in a one-channel case [32,33]. Using these unperturbed wave functions, we then employ the first order perturbation theory to construct wave functions around a resonance state.

The paper is organized as follows. In Sec. II, we discuss how to generalize the box boundary condition to a multi-channel case. This uses a generalized concept of node for a multi-channel wave function [34]. We also discuss the method based on the eigenphase sum and compare it with the multi-channel box discretization method. In Sec. III, we introduce the eigenchannels and discuss their usefulness. We consider several cases: the uncoupled (spherical) case, a very narrow resonance, and a case where the coupled-channels equations are decoupled. In Sec. IV, we discuss the factorization of the wave functions in the vicinity of an isolated resonance. We first consider a perturbation to the box discretized wave functions for a spherical system in order to re-formulate the factorization formula of Unger [19], which was originally derived using the \( R \)-matrix theory [10,35–37]. We then apply it to the eigenbasis wave functions, and derive a generalization of the factorization formula for a multi-channel wave function. We examine the validity of the factorization formula by comparing it with the exact solutions of the coupled-channels equations. The
II. SINGLE-PARTICLE RESONANCES AND BOX-DISCRETIZED STATES

Let us start with the following single-particle (s.p.) Hamiltonian:

\[ H = \frac{-\hbar^2}{2m} \nabla^2 + \hat{V}(r), \]  

(1)

where the potential \( \hat{V} \) may also contain a derivative operator such as a spin-orbit interaction. When the potential \( \hat{V} \) is non-spherical, the s.p. angular momentum is not conserved and the total s.p. wave function has the form

\[ \Psi(r) = \sum_{ljm} \frac{u_{ljm}(r)}{r} Y_{ljm}(\hat{r}), \]  

(2)

with

\[ Y_{ljm}(\hat{r}) = \sum_{s} \langle lm \frac{1}{2} m_s | jm \rangle Y_{lm}(\hat{r}) \chi_{ms}. \]  

(3)

Here, \( Y_{lm} \) are spherical harmonics and \( \chi_{ms} \) denotes the spin wave function. Projecting the Schrödinger equation, \( H\Psi = E\Psi \), on the spin-angular states \( Y_{ljm} \), the coupled-channels equations for the radial wave functions then read,

\[ \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} - E \right] u_{ljm}(r) + r \sum_{l'j'm'} \langle Y_{ljm} | \hat{V} | Y_{l'j'm'} \rangle \frac{u_{l'j'm'}}{r} = 0. \]  

(4)

These equations are solved with certain boundary conditions which depend on the problem of interest. A standard way to solve them is to generate \( N \) linearly independent solutions, \( N \) being the number of channel states to be included, and then to take a linear combination of these \( N \) solutions so that the relevant boundary condition is satisfied [28,38]. The linearly independent solutions can be obtained by taking \( N \) different sets of initial conditions at \( r = 0 \). We denote these solutions by \( \phi_{LL'}(r) \), where \( L \) refers to the channels while \( L' \) refers to a particular choice of initial conditions. Here, we use a shorthand notation, \( L = (ljm) \).

A simple choice for the \( N \) initial conditions is to impose

\[ \phi_{LL'}(r) \rightarrow r^{l+1} \delta_{L,L'} \quad \text{for} \quad r \rightarrow 0. \]  

(5)

The coupled-channels equations are solved outwards for each initial condition \( L' \). The wave functions \( u_L(r) \) in Eq.(4) are written in terms of the \( \phi_{LL'} \) as

\[ u_L(r) = \sum_{L'} C_{L'} \phi_{LL'}(r), \]  

(6)

where the coefficients \( C_{L'} \) are determined from the asymptotic behavior of \( u_L(r) \).
When the s.p. energy $E$ is positive, the physical wave function is a scattering wave with an incoming wave behaviour in some particular incident channel $L_0$ and outgoing waves in all channels $L$. Thus, the asymptotic boundary condition of the wave function $u_L(r)$ is given by

$$u_L(r) \rightarrow \sqrt{\frac{k}{\pi E}} \frac{i}{2} \left\{ e^{-i(kr-l\pi/2)} \delta_{L,L_0} - S_{LL_0} e^{i(kr-l\pi/2)} \right\} \text{ for } r \rightarrow \infty,$$

(7)

where $k = \sqrt{2mE/\hbar^2}$ and $S_{LL_0}$ is the scattering $S$-matrix. The normalization is chosen so that the total wave function satisfies $\langle \Psi_{E,L_0} | \Psi_{E,L_0'} \rangle = \delta(E - E') \delta_{L_0,L_0'}$. Here, $|\Psi_{E,L_0}\rangle$ is given by Eq. (2), whose channel components $u_L(r)$ satisfy the boundary condition (7). In practice, the $S$-matrix can be obtained by decomposing $\phi_{LL'}(r)$ in the asymptotic region with spherical Hankel functions $h_l^{(\pm)}(kr)$ and comparing Eq. (6) with Eq. (7) [28,38].

The generalization of the concept of s.p. resonances from the spherical to the multi-channel cases is most conveniently done by monitoring the energy dependence of the eigenphase sum [32,33]. The eigenphases are related to the eigenvalues of the $S$-matrix through

$$(U^\dagger SU)_{aa'} = e^{2i\delta_a} \delta_{a,a'}.$$  

(8)

Hazi [33] has shown that, the sum of the eigenphases $\Delta(E) \equiv \sum_a \delta_a(E)$, has the same energy dependence around a resonance as the phase shift in a spherical system, i.e.,

$$\Delta(E) = \Delta_0(E) + \tan^{-1} \frac{\Gamma}{2(E_R - E)},$$  

(9)

where the slowly-varying quantity $\Delta_0(E)$ is the sum of the background eigenphases, and $E_R$ and $\Gamma$ are the multi-channel resonance energy and total width, respectively. Therefore, the properties of multi-channel resonances can be extracted directly by plotting $\Delta(E)$, or its energy derivative, as a function of $E$. The quantity $\Delta(E)$ is called the eigenphase sum, and it has been widely used in the context of electron-molecule scattering (see, e.g., Ref. [39] for a recent publication).

We illustrate the above discussion by the following example. We use a Woods-Saxon parametrization for the potential $\hat{V}$ which is given by

$$\hat{V}(r) = V_{\text{cent}}(r) + \nabla(V_{\text{ls}}(r)) \cdot (-i \nabla \times \sigma),$$  

(10)

with

$$V_{\text{cent}}(r) = V_0(r) - R \beta \frac{dV_0(r)}{dr} Y_{20}(\hat{r}),$$  

$$V_{\text{ls}}(r) = V_{\text{so}}(r) - R_{\text{so}} \beta \frac{dV_{\text{so}}(r)}{dr} Y_{20}(\hat{r}),$$  

(11)

where $V_0(r)$ and $V_{\text{so}}(r)$ have a Woods-Saxon shape:

$$V_0(r) = -V_0/[1 + \exp((r - R)/a)],$$  

$$V_{\text{so}}(r) = V_{\text{so}}/[1 + \exp((r - R_{\text{so}})/a_{\text{so}})].$$  

(13)

(14)
For simplicity, we have expanded the deformed Woods-Saxon potential and kept only the linear order of the deformation parameter $\beta$ [40]. Also, we assume an axial symmetry, where both the parity $\pi$ and the spin projection $K$ onto the $z$ axis are conserved. An explicit form of the coupled-channels equations is given in the Appendix. The parameters of the Woods-Saxon potential are taken to be $V_0=42.0$ MeV, $R = R_{so} = 1.27 \times 44^{1/3}$ fm, $a = a_{so} = 0.67$ fm, and $V_{so} = 14.9$ MeV/fm$^2$, to somehow simulate the neutron potential in the $^{44}$S region. As an example we calculate the neutron s.p. levels with $K^\pi = 5/2^+$ at $\beta=0.2$. We include the $d_{5/2}, g_{7/2}, g_{9/2}, i_{13/2}$, and $i_{11/2}$ states in the coupled-channels equations. Notice that the $s_{1/2}$ and $d_{3/2}$ states do not contribute to the $K^\pi = 5/2^+$ levels. We have checked that the results are not significantly altered even if we include higher angular momentum components.

The thick solid line in Fig. 1 shows the eigenphase sum and its energy derivative as a function of energy. The contributions from three main eigen-channels are also shown by thin lines. One clearly sees a maximum at $E_R= 3.44$ MeV in the first derivative of the eigenphase sum. The total width can be estimated to be $\Gamma= 0.46$ MeV.

Let us now compare this continuum result with the s.p. spectrum of a box-discretized calculation. From the structure (6) of the general solution, it is clear that one can impose the boundary condition that the total wave function $\Psi(r)$ vanishes at a radius $R_{\text{box}}$. This is equivalent to putting the nucleus in an impenetrable spherical box of radius $R_{\text{box}}$. If the condition

$$\det(\phi_{LL'}(R_{\text{box}})) = 0 \quad (15)$$

is satisfied, then Eq.(6) has a non-trivial solution for $C_L$ such that $u_L(R_{\text{box}}) = 0$ for all the channels $L$. This is a natural extension of the well-known box discretization method for a spherical system. We notice that Johnson [34] has advocated to use $\det(\phi(r))$ as a generalized concept of node for a multi-channel wave function. We have recently used this method to find all the bound state solutions of a deformed Skyrme-Hartree-Fock mean field.

Figure 2 shows s.p. energies obtained with the box discretization method as a function of the box size $R_{\text{box}}$. One can clearly see that there are two classes of s.p. levels. One consists of those whose energy changes significantly as the box radius $R_{\text{box}}$ increases, and the other contains those whose energy is almost constant as a function of $R_{\text{box}}$. This behavior is similar to that of box-discretized s.p. energies for a spherical system where the stabilized levels correspond to resonances [12]. This example shows that, in the deformed case it is also possible to generate a complete set of box-discretized states and that some of these states can be a good approximation to multi-channel s.p. resonances.

III. EIGENCHANNEL REPRESENTATION

The states obtained with the box discretization method in the previous section are the eigenstates of a potential which is the same as the original potential for $r < R_{\text{box}}$, and infinite for $r \geq R_{\text{box}}$. They thus form a complete set, and any regular function defined in the domain $r < R_{\text{box}}$ can be expanded on this basis. In the next section, we discuss the factorization property of the scattering wave function around a resonance in terms of this basis set. To this end, it appears convenient to introduce the eigenchannel wave functions [31] defined in terms of the unitary matrix $U$ of Eq. (8),
\[ \tilde{\Psi}_{E,a}(r) \equiv \sum_{L_0} \Psi_{E,L_0}(r) U_{L_0 a}. \]  

We refer to the channels \( L \) as the physical channels, in order to distinguish them from the eigenchannels \( a \). Substituting Eqs. (7) and (8), one can find that the eigenchannel wave functions behave asymptotically as

\[ \tilde{\Psi}_{E,a}(r) \to \frac{1}{r} \sum_{L} \sqrt{\frac{k}{\pi E}} \frac{i}{2} \left\{ e^{-i(kr-l\pi/2)} - e^{2i\delta_a} e^{i(kr-l\pi/2)} \right\} U_{La} Y_{ljm}(\hat{r}) \quad \text{for} \quad r \to \infty. \]  

For each eigenchannel, the asymptotic radial wave functions thus behave in the same way for all angular momentum components, and the coupling is greatly simplified. Loomba et al. argued that the eigenchannel wave functions provide the most direct way to visualize a resonance state [31]. The eigenchannels were also used in the context of the \( R \) matrix theory [37,41,42]. We also mention that the eigenchannel approach has been widely used in the field of heavy-ion fusion reactions in the context of fusion barrier distributions [43–47]. In this section, we discuss the usefulness of this approach for multi-channel resonances by considering several cases.

### A. Spherical systems

In spherical systems, the s.p. angular momentum is conserved and the \( S \)-matrix is diagonal in the physical channel representation \( L \), i.e., the physical channels are equivalent to the eigenchannels. Likewise, the wave function \( \phi_{LL'}(r) \) with the initial condition (5) is diagonal at all the values of \( r \), and \( C_L \) in Eq. (6) is proportional to \( \delta_{LL_0} \) for the incident channel \( L_0 \). From this consideration, it is apparent that the eigenchannel wave functions \( \tilde{\Psi}_a \) exhibits a resonance behavior for a spherical system if the resonance condition is met for an incident channel \( a = L_0 \).

### B. Two-channel decoupled system

We next consider a special case where the coupled-channels equations are completely decoupled by a transformation of the basis. For this purpose, we consider the following two-channel model [43],

\[ \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) - E \right) \begin{pmatrix} u_1(r) \\ u_2(r) \end{pmatrix} + \begin{pmatrix} 0 & F(r) \\ F(r) & 0 \end{pmatrix} \begin{pmatrix} u_1(r) \\ u_2(r) \end{pmatrix} = 0. \]  

This corresponds to a system where the incident channel couples to a spinless vibrational state whose excitation energy is zero [43,44,47]. This model has been used by Dasso et al. in order to understand the coupling-assisted tunneling phenomena in heavy-ion fusion reactions [43].

We refer to the basis in the coupled-channels equations (18) as \(|1\rangle\) and \(|2\rangle\). For symmetry reasons the \( S\)-matrix in this system satisfies \( S_{11} = S_{22} \) and \( S_{12} = S_{21} \), and the total wave functions are given by
\[ \Psi_1 = \frac{1}{r} [u_1(r)|1\rangle + u_2(r)|2\rangle], \tag{19} \]
\[ \Psi_2 = \frac{1}{r} [u_2(r)|1\rangle + u_1(r)|2\rangle]. \tag{20} \]

Here, the asymptotic behaviors of the wave functions \( u_1(r) \) and \( u_2(r) \) are
\[ u_1(r) \to e^{-ikr} - S_{11} e^{ikr}, \tag{21} \]
and
\[ u_2(r) \to -S_{12} e^{ikr}, \tag{22} \]
respectively. By diagonalizing the \( S \) matrix, the eigenchannel wave functions read
\[ \tilde{\Psi}_1 = \frac{1}{\sqrt{2}} (\Psi_1 + \Psi_2) = \frac{1}{r} (u_1(r) + u_2(r)) \cdot \frac{|1\rangle + |2\rangle}{\sqrt{2}}, \tag{23} \]
\[ \tilde{\Psi}_2 = \frac{1}{\sqrt{2}} (\Psi_1 - \Psi_2) = \frac{1}{r} (u_1(r) - u_2(r)) \cdot \frac{|1\rangle - |2\rangle}{\sqrt{2}}. \tag{24} \]

Notice that the coupling matrix in the coupled-channels equations (18) can be diagonalized independently of \( r \) with the same unitary operator \( U \). Transforming Eqs. (18) with this unitary operator leads to
\[ \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) - E \right) \begin{pmatrix} u_1(r) + u_2(r) \\ u_1(r) - u_2(r) \end{pmatrix} + \begin{pmatrix} F(r) & 0 \\ 0 & -F(r) \end{pmatrix} \begin{pmatrix} u_1(r) + u_2(r) \\ u_1(r) - u_2(r) \end{pmatrix} = 0. \tag{25} \]

The coupled-channels equations are thus decoupled with this basis. The radial wave functions for the eigenchannel wave functions \( \tilde{\Psi}_{1,2} \) obey a one-dimensional Schrödinger equation with a potential given by \( V(r) \pm F(r) \), respectively. Therefore, if the one-dimensional potential \( V(r) + F(r) \) holds a resonance state at an energy \( E_R \), the eigenchannel wave function \( \tilde{\Psi}_1 \) exhibits a resonance behavior while the wave function \( \tilde{\Psi}_2 \) does not, and vice versa. The energy dependence of the wave functions with the physical basis \( \Psi_{1,2} \) is much more complicated. Although, in general cases, the coupled-channels equations are not decoupled if different angular momentum components are coupled to each other, it is evident from this example that the eigenchannel basis provides a much simpler image of a multi-channel resonance than the physical basis.

C. Very narrow resonance

As a final example, we consider a case where the resonance width is very small, as in proton or alpha decays. In Refs. [28–30], the energy of a multi-channel resonance for a proton emission decay was found by imposing the asymptotic boundary condition that the channel wave functions are proportional to \( G_l(kr) \) for all the channels, where \( G_l(kr) \) is the irregular Coulomb wave function. From Eq. (17), one can see that this state should correspond to one of the eigenbasis wave functions whose eigenphase is \( \pi/2 \). In this subsection, we would like to demonstrate that the total width is exhausted by only one eigenchannel when it is very small.
To this end, let us start with the Breit-Wigner expression for a multi-channel S-matrix \[10,35–37\]. If there is only one isolated resonance of energy \(E_R\) in the energy region of interest, the S-matrix can be approximated in the vicinity of this resonance as
\[
S_{LL'} = e^{2i\phi_L \delta_{LL'}} - e^{i(\phi_L + \phi_{L'})} \frac{i\sqrt{\Gamma_L \Gamma_{L'}}}{E - E_R + i\Gamma/2},
\]
where \(\phi_L\) is the background phase shift and \(\Gamma\) is the total width given as a sum of partial widths \(\Gamma_L\). For a very narrow resonance, the background phase shifts can often be neglected. The left hand side of Eq. (8) then reads
\[
(U^\dagger SU)_{aa'} = \delta_{a,a'} - \frac{i\sqrt{\Gamma_a \Gamma_{a'}}}{E - E_R + i\Gamma/2},
\]
where \(\sqrt{\Gamma_a} = \sum_L \sqrt{\Gamma_L} U_{La}\) is related to the partial width for the eigenchannel \(a\). By definition of the unitary operator \(U\), the off-diagonal components of the right hand side of Eq. (27) should vanish. The only possibility for this to be satisfied is that \(\Gamma_a\) is zero except for one particular channel \(a_0\). Thus, around the resonance the eigenphase shifts are given by \(\delta_{a_0} = \tan^{-1}[\Gamma/(2(E_R - E))]\) for the eigenchannel \(a_0\), and \(\delta_a = 0\) for the other channels. Again, this example clearly shows that the eigenchannel representation provides the most direct manifestation of a multi-channel resonance state.

IV. FACTORIZATION OF SCATTERING WAVE FUNCTIONS

We now consider the most general case for a multi-channel resonance, i.e., when the resonance width is not very small. For a spherical system having an isolated single-particle resonance at energy \(E_R\), Unger [19] has shown that the scattering radial wave function at energy \(E\) whose asymptotic form is
\[
\psi_E(r) \to \sqrt{\frac{k_e}{\pi E}} e^{i\delta(E)} \sin(kr - l\pi/2 + \delta(E)) \quad \text{for} \quad r \to \infty,
\]
can be approximately factorized into a product of an \(r\)-independent function \(F(E)\) times the wave function at resonance energy. This factorization property holds if
\[
|E - E_R| \ll |V(r)|,
\]
a condition which is realized generally in the internal region of the potential when \(|E - E_R|\) is less than the resonance width \(\Gamma\). In Ref. [19] the function \(F(E)\) is written in terms of a Breit-Wigner function, but for an isolated resonance it is easy to relate this to the derivative of the phase shift with respect to energy, so that the factorization property can be expressed as
\[
\psi_E(r) \sim e^{i\delta(E)} \sqrt{\frac{1}{\pi \frac{d\delta}{dE}}} \frac{\psi_{E_R}(r)}{\left[\int_0^R dr |\psi_{E_R}(r)|^2\right]^{1/2}},
\]
under the condition (29). Thus, the factorization function \(F(E)\) is just \(e^{i\delta(E)} \sqrt{\frac{d\delta}{dE}}\) except for a normalization factor. In this section, we generalize this formula to a deformed system. We
do not attempt to give an analytic derivation, which could be done by using multi-channel Jost functions \[48\], but we would like to have a hint on how should be the generalized form of Eq.(30). To this end we find it useful to use the box discretized states of Sec. II to express the function \( F(E) \), first in the familiar spherical case, then in the general case.

### A. Spherical system

The infinite set of all discretized states \( X_{\lambda}(r) \) with corresponding eigen-energies \( E_{\lambda} \) calculated in a box of radius \( R_{\text{box}} \) form a complete orthonormal set, and one can expand on this basis any regular function defined in the domain \([0, R_{\text{box}}[ \) (the domain excludes \( r = R_{\text{box}} \)). In particular, the inner part of the scattering wave function \( \psi_E(r) \) can be expanded as

\[
\psi_E(r) = \sum_{\lambda} C_{\lambda}(E) X_{\lambda}(r) \quad r \in [0, R_{\text{box}}[, \tag{31}
\]

with

\[
C_{\lambda}(E) = \int_0^{R_{\text{box}}} dr \, X_{\lambda}(r) \psi_E(r). \tag{32}
\]

Notice that this expansion does not hold at \( r = R_{\text{box}} \) in general. Here and in the following, all integrals \( \int_0^{R_{\text{box}}} dr \) are meant to be \( \lim_{\varepsilon \to 0} \int_0^{R_{\text{box}}-\varepsilon} dr \). With this definition, the expansion (31) is still meaningful even when the radius \( r \) is infinitesimally smaller than \( R_{\text{box}} \). Since the wave functions \( X_{\lambda}(r) \) and \( \psi_E(r) \) obey the same Schrödinger equation (but with different energies from each other),

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi_E}{dr^2} + \left( V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E \right) \psi_E = 0 ,
\]

\[
-\frac{\hbar^2}{2m} \frac{d^2 X_{\lambda}}{dr^2} + \left( V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E_{\lambda} \right) X_{\lambda} = 0 . \tag{33}
\]

the expansion coefficients \( C_{\lambda}(E) \) are given by

\[
C_{\lambda}(E) \equiv \frac{1}{E - E_{\lambda}} \frac{\hbar^2}{2m} \int_0^{R_{\text{box}}} dr \left( \psi_E \frac{d^2 X_{\lambda}}{dr^2} - X_{\lambda} \frac{d^2 \psi_E}{dr^2} \right),
\]

\[
= \frac{1}{E - E_{\lambda}} \frac{\hbar^2}{2m} \psi_E(R_{\text{box}}) X'_{\lambda}(R_{\text{box}}) \psi_E(R_{\text{box}}) X_{\lambda}(r). \tag{34}
\]

In the last step we have used the boundary condition \( X_{\lambda}(R_{\text{box}}) = 0 \).

In the vicinity of \( E_R \simeq E_{\lambda_R} \), the contribution from \( \lambda = \lambda_R \) dominates the expansion (31). Retaining only this term in the expansion (this corresponds to the one term approximation in the \( R \)-matrix theory \([10,35–37]\)), the scattering wave function around the resonance and inside the potential barrier reads

\[
\psi_E(r) \simeq \frac{1}{E - E_{\lambda_R}} \cdot \frac{\hbar^2}{2m} \psi_E(R_{\text{box}}) X'_{\lambda_R}(R_{\text{box}}) X_{\lambda_R}(r). \tag{35}
\]
We now set the $R$-matrix radius $R$ to be $R_{\text{box}}$, approximate $X_{\lambda R}(r)$ by the resonance wave function $\psi_{E R}(r)$ (except for the normalization) and finally assume that $kR_{\text{box}}$ is sufficiently large so that the $\psi_E(r)$ at $R_{\text{box}}$ can be replaced by its asymptotic form (28). Then, a comparison between Eqs. (30) and (35) leads to
\[
e^{i\delta(E)} \sqrt{\frac{1}{\pi}} \frac{d\delta}{dE} = \frac{\hbar^2}{2m} \sqrt{\frac{k}{\pi E}} e^{i\delta(E)} \sin(kR_{\text{box}} - l\pi/2 + \delta(E)) \frac{X'_{\lambda R}(R_{\text{box}})}{\left[ \int_0^{R_{\text{box}}} dr |X_{\lambda R}(r)|^2 \right]^{1/2}}.
\] (36)

We have thus established the relation between the function $F(E)$ (except for a normalization factor) and the derivative of the discretized state $X_{\lambda R}(r)$ at $r = R_{\text{box}}$. This relation is our guideline for obtaining the generalized function $F(E)$ in the deformed case. Notice that we have explicitly written down the normalization of $X_{\lambda R}(r)$ so that Eq. (36) can be used also when the function $X_{\lambda R}(r)$ is not normalized.

B. Deformed system

The procedure is very similar to that of the spherical case. Using the complete set of discretized wave functions introduced in Sec.II:
\[X_{\lambda}(r) = \sum_L \frac{X_{L\lambda}(r)}{r} \mathcal{Y}_L(\hat{r}),\] (37)
we expand the eigenchannel wave functions $\Psi_{E,a}(r)$:
\[\tilde{\Psi}_{E,a}(r) = \sum_L \frac{u_{L}^{(a)}(r)}{r} \mathcal{Y}_L(\hat{r}),\]
\[= \sum_{\lambda} C_{\lambda}(E) X_{\lambda}(r),\] (38)
with
\[C_{\lambda} = \sum_L \int_0^{R_{\text{box}}} dr X_{L\lambda}(r) u_{L}^{(a)}(r).\] (39)

The coupled-channels equations (4) lead to
\[C_{\lambda}(E) = \frac{1}{E - E_{\lambda}} \cdot \frac{\hbar^2}{2m} \sum_{L} u_{L}^{(a)}(R_{\text{box}}) X'_{L\lambda}(R_{\text{box}}).\] (40)

As in the spherical system, we retain only the contribution from $\lambda = \lambda_R$ in the expansion (38) for $E \simeq E_{\lambda_R}$. In the asymptotic region (for a large $R_{\text{box}}$) the wave function $u_{L}^{(a)}(r)$ has exactly the same asymptotic form (except for a factor $U_{La}$) as the scattering wave function $\psi_{E}(r)$ in the spherical system (see Eqs. (17) and (28)), the only difference being that the spherical phase shift $\delta(E)$ is replaced by the eigenphase $\delta_a$. Thus, we can replace in Eq.(40) $u_{L}^{(a)}(R_{\text{box}})$ by $\psi_{E}(R_{\text{box}}) U_{La}$ with $\psi_E$ represented by its asymptotic form (28). Comparing
the resulting expression with Eq. (36), we obtain the desired factorization formula for a multi-channel resonance,

\[
C_{\lambda R} \sim e^{i\delta_a(E)} \sqrt{\frac{1}{\pi} \frac{d\delta_a}{dE}} \left( \sum_L \left[ \int_0^{R_{\text{box}}} dr |X_{\lambda R}^L(r)|^2 \right]^{1/2} U_{La} \right).
\]  

(41)

Here, \( \sum_L \left[ \int_0^{R_{\text{box}}} dr X_{\lambda R}^L(r)^2 \right]^{1/2} U_{La} \) is the probability of finding the particle inside the box for the eigenchannel \( a \).

In practice, one may replace the box wave function \( X_{\lambda R} \) in Eq. (41) by the scattering wave functions at the resonance, for each eigenchannel \( a \), i.e.,

\[
\tilde{\Psi}_{E,a}(r) \sim C_a(E) \tilde{\Psi}_{E_R,a}(r)/C_a(E_R)
\]

(42)

with

\[
C_a(E) = \sqrt{\frac{1}{\pi} \frac{d\delta_a}{dE}} \frac{\sum_L \left[ \int_0^{R_{\text{box}}} dr |u_{L}^{(a)}(r)|^2 \right]^{1/2} U_{La}(E)}{\left[ \sum_L \int_0^{R_{\text{box}}} dr |u_{L}^{(a)}(r)|^2 \right]^{1/2}},
\]

(43)

where the wave functions \( u_{L}^{(a)}(r) \) are evaluated at the resonance energy \( E_R \). One may also choose the phase factor of the eigenchannel wave functions \( \tilde{\Psi}_{E,a} \) for each channel \( a \) and energy \( E \) so that the factor \( e^{i\delta_a} \) does not appear in Eq. (43). With this, the wave functions become real numbers.

Figure 3 shows the applicability of the factorization formula for the system considered in Figs. 1 and 2. At the resonance energy, \( E = E_R = 3.44 \) MeV, the eigenphase shifts \( \delta_a/\pi \) are calculated as 0.559, 2.53\times10^{-3}, 4.12\times10^{-2}, 1.06\times10^{-5}, \) and 2.79\times10^{-5} for the five eigenchannels (see the thin lines in Fig. 1). Therefore, there is one eigenchannel which dominates the eigenphase sum \( \Delta(E) \) around the resonance. In the figure, the \( d_{5/2}, g_{7/2}, \) and \( g_{9/2} \) wave function components are shown for this particular eigenchannel. The exact wave functions at the resonance energy are denoted by the thick solid line, while those at \( E = 3.54 \) MeV are given by the thin solid line. The dashed line is the result of the factorization formula (42) and (43). We take \( R_{\text{box}} = 20 \) fm to evaluate the integrations in the formula. For the \( l = 4 \) components, one clearly sees that the energy dependence, as well as the radial dependence for \( r \leq 10 \) fm, of the radial wave functions are well expressed by the factorization formula. We have confirmed that the agreement is even better for the \( l = 6 \) components (not shown). For the \( l = 2 \) component, the wave function is not localized inside the barrier, and the factorization formula does not work well. As expected, the factorization approximation is better for high \( l \) states, which are more localized by the centrifugal barrier.

Figure 4 shows the spin projected total wave function (multiplied by \( r \)),

\[
\langle \chi_{1/2} | r \tilde{\Psi}_{E,a}(r) \rangle = \sum_{lj} u_{lj}^{(a)}(r) \cdot \langle l, K - \frac{1}{2}, \frac{1}{2} | j K \rangle Y_{l+1/2}(\hat{r}),
\]

(44)

for this eigenchannel \( a \). The upper and the lower panes are the wave functions as a function of \( r \) for \( (\theta, \phi) = (\pi/4, 0) \) and \( (\theta, \phi) = (\pi/2, 0) \), respectively. (Note that the total wave function vanishes along \( \theta = 0 \) for \( K = 5/2 \).) As we have shown in fig. 3, the factorization formula works reasonably well, especially inside the potential barrier, i.e., \( r \leq 4.23 \) fm.
In Fig. 5, we show more in detail the energy dependence of the main component of the multi-channel wave function (i.e., the $g_{9/2}$ component) around the resonance energy, and its comparison with the factorization method. At $E = E_R + 0.1\Gamma$, the factorization formula works, and the exact radial dependence of the wave function is well reproduced, as we already showed in Fig. 3. As the energy increases, the performance of the factorization becomes worse. At $E = E_R + \Gamma$, the factorization still works inside the potential, but the deviation becomes significant in the outside (see the middle panel). By the energy $E_R + 2\Gamma$, the wave function does not resemble the resonance wave function, and the factorization formula looses its applicability, as was already known for the spherical system [20].

In Ref. [49], Lejeune and Mahaux used a solvable two-level model to argue that the energy dependence of the wave function components is quite different from each other and a simple scaling does not hold. However, this does not come out in the present study. The energy dependences are similar for all the angular momentum components, except for the $d$-wave which shows a non-resonant behavior. This different conclusion may come from the fact that here the calculations are done with the eigenchannel basis, in contrast to Lejeune and Mahaux, who worked with the physical basis. This fact again suggests that the eigenchannel basis provides a powerful means to study a multi-channel resonance.

V. SUMMARY

We have used the eigenchannel representation of the multichannel wave function to investigate the properties of a single-particle resonance in a deformed system. We first showed that the box boundary condition can be generalized to deformed systems if one uses the generalized concept of the wave function node, that is to impose the condition that the determinant of the wave function matrix vanishes at the boundary of a spherical box. We have solved the coupled-channels equations with this boundary condition and showed that the discretized energy is nearly a constant as a function of the box size for a multichannel resonance state. The energy $E_R$ and the width $\Gamma$ of the resonant state were also calculated by using the energy dependence of the eigenphase sum. We have next studied the properties of the eigenbasis which diagonalizes the $S$-matrix. We argued that the eigenchannel representation has the most direct connection to a multi-channel resonance state. Using this representation, we have derived a formula which relates the wave functions at different energies around a resonance state, and studied its applicability. For an isolated resonance, we have observed a nice agreement between the approximate and exact wave functions inside the potential radius at energies $|E - E_R| \lesssim \Gamma$.

In many-body problems, one often takes the single-particle states as a good building block to start with. This is the case, for instance, in the BCS calculation for a pairing Hamiltonian. If one includes unbound states in the calculation, one then has to deal with integrals over a wide range of energies in order to compute matrix elements. In the vicinity of a narrow resonance, the energy interval has to be taken small, which may be quite time consuming. This difficulty is substantially lessened if one uses the factorization formula derived in this article. Work is now in progress which uses this formula for resonance contributions in a Hartree-Fock plus BCS calculation for deformed nuclei. We will report the results in a separate paper.
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APPENDIX A: COUPLED-CHANNELS EQUATIONS WITH A DEFORMED SPIN-ORBIT POTENTIAL

In this Appendix, we present an explicit form of the coupling matrix elements in the coupled-channels equations, Eq. (4), for a Hamiltonian with a deformed spin-orbit interaction in the form of Eq.(10). We first perform the multipole decomposition for the potentials:

\[ V_{\text{cent}}(r) = \sum_{\lambda,\mu} V_{\text{cent}}^{(\lambda\mu)}(r) Y_{\lambda\mu}(\hat{r}), \quad (A1) \]
\[ V_{\text{ls}}(r) = \sum_{\lambda,\mu} V_{\text{ls}}^{(\lambda\mu)}(r) Y_{\lambda\mu}(\hat{r}). \quad (A2) \]

We use the Wigner-Eckart theorem [50] to evaluate the matrix elements. For the central potential \( V_{\text{cent}} \), this yields [51]

\[ r \langle Y_{lm} | \hat{V}_{\text{cent}} | Y_{l'm'} \rangle = \sum_{\lambda,\mu} \left( -j - m \right) (j \lambda j' - m \mu m') \langle Y_{ljm} || Y_{\lambda} || Y_{j'l'm'} \rangle V_{\text{cent}}^{(\lambda\mu)}(r), \quad (A3) \]

where \( \hat{l} \) is defined by \( \sqrt{2l + 1} \).

For the spin-orbit part, we first decompose it as [50]

\[ \nabla(V_{\text{ls}}(r)) \cdot (-i \nabla \times \sigma) = \sum_{\lambda,\mu} \left\{ -\sqrt{\frac{\lambda + 1}{2\lambda + 1}} \left( \frac{dV_{\text{ls}}^{(\lambda\mu)}}{dr} - \frac{\lambda}{r} V_{\text{ls}}^{(\lambda\mu)}(r) \right) [Y_{\lambda+1}(-i \nabla \times \sigma)]^{(\lambda\mu)} + \sqrt{\frac{\lambda}{2\lambda + 1}} \left( \frac{dV_{\text{ls}}^{(\lambda\mu)}}{dr} + \frac{\lambda + 1}{r} V_{\text{ls}}^{(\lambda\mu)}(r) \right) [Y_{\lambda-1}(-i \nabla \times \sigma)]^{(\lambda\mu)} \right\}, \quad (A5) \]

and use the Wigner-Eckart theorem for the operators \([Y_{\lambda\pm1}(-i \nabla \times \sigma)]^{(\lambda\mu)}\). That is,

\[ r \langle Y_{l'm'} | \nabla(V_{\text{ls}}(r)) \cdot (-i \nabla \times \sigma) | Y_{ljm} \rangle = \sum_{\lambda,\mu} \left( -j - m \right) (j \lambda j' - m \mu m') \langle Y_{ljm} || \nabla(V_{\text{ls}}(r)) \cdot (-i \nabla \times \sigma) || Y_{l'm'} \rangle \]

\[ = \sum_{\lambda,\mu} (-j - m) (j \lambda j' - m \mu m') \langle Y_{ljm} || Y_{l'm'} \rangle, \quad (A4) \]
\[
\times \left\{ -\sqrt{\frac{\lambda + 1}{2\lambda + 1}} \left( \frac{dV_{ls}^{(\lambda \mu)}}{dr} - \frac{\lambda}{r} V_{ls}^{(\lambda \mu)}(r) \right) + \sqrt{\frac{\lambda}{2\lambda + 1}} \left( \frac{dV_{ls}^{(\lambda \mu)}}{dr} + \frac{\lambda + 1}{r} V_{ls}^{(\lambda \mu)}(r) \right) \right\} r \langle \mathcal{Y}_{jl} | [Y_{\lambda+1}(-i \nabla \times \sigma)]^{(\lambda)} | \mathcal{Y}_{j'l'} \rangle \frac{u_{j'l'm'}(r)}{r} \right) \right\}. 
\] (A6)

The reduced matrix elements are given by [51]

\[
\langle \mathcal{Y}_{jl} | [Y_{\lambda \pm 1}(-i \nabla \times \sigma)]^{(\lambda)} | \mathcal{Y}_{j'l'} \rangle = \sum_{j'' l''} (-)^{\lambda+j+j'+1} \sqrt{36} \hat{\lambda} \hat{j''} \hat{j'} \left\{ \begin{array}{ccc}
\lambda + 1 & 1 & \lambda \\
j' & j & j''
\end{array} \right\} \\
\times \left\{ \begin{array}{ccc}
l'' & l' & 1 \\
1/2 & 1/2 & 1 \\
j'' & j' & 1
\end{array} \right\} \langle \mathcal{Y}_{jl} | Y_\lambda | \mathcal{Y}_{j'l''} \rangle \langle l'' | \nabla | l' \rangle, \quad (A7)
\]

with

\[
\langle l'' | \nabla | l' \rangle = \begin{cases} 
\sqrt{l' + 1} \left( \frac{d}{dr} - \frac{l'}{r} \right) & \text{if } l'' = l' + 1, \\
-\sqrt{l'} \left( \frac{d}{dr} + \frac{l' + 1}{r} \right) & \text{if } l'' = l' - 1.
\end{cases} \quad (A8)
\]

This yields

\[
r \langle \mathcal{Y}_{jl} | [Y_{\lambda \pm 1}(-i \nabla \times \sigma)]^{(\lambda)} | \mathcal{Y}_{j'l'} \rangle \frac{u_{j'l'm'}(r)}{r} = \sum_{j''=l'+1/2}^{l'+3/2} (-)^{\lambda+j+j'+1} \sqrt{36} \hat{\lambda} \hat{j''} \hat{j'} \left\{ \begin{array}{ccc}
\lambda + 1 & 1 & \lambda \\
j' & j & j''
\end{array} \right\} \\
\times \left\{ \begin{array}{ccc}
l'' & l' & 1 \\
1/2 & 1/2 & 1 \\
j'' & j' & 1
\end{array} \right\} \langle \mathcal{Y}_{jl} | Y_\lambda | \mathcal{Y}_{j'l''} \rangle \cdot \sqrt{l' + 1} \left( \frac{d}{dr} - \frac{l' + 1}{r} \right) u_{j'l'm'}(r) \\
+ \sum_{j''=l'-1/2}^{l'-3/2} (-)^{\lambda+j+j'+1} \sqrt{36} \hat{\lambda} \hat{j''} \hat{j'} \left\{ \begin{array}{ccc}
\lambda + 1 & 1 & \lambda \\
j' & j & j''
\end{array} \right\} \\
\times \left\{ \begin{array}{ccc}
l'' & l' & 1 \\
1/2 & 1/2 & 1 \\
j'' & j' & 1
\end{array} \right\} \langle \mathcal{Y}_{jl} | Y_\lambda | \mathcal{Y}_{j'l''} \rangle \cdot (-\sqrt{l'}) \left( \frac{d}{dr} + \frac{l'}{r} \right) u_{j'l'm'}(r). \quad (A9)
\]

The matrix elements of the coupling potential were evaluated in this way in Ref. [30] for the vibrational excitation in the proton decay of spherical nuclei.

Notice that the matrix elements become trivial for the monopole part (\( \lambda = 0 \)), and are given by

\[
r \langle \mathcal{Y}_{ljm} | \hat{V}_{\lambda=0} | \mathcal{Y}_{j'l'm'} \rangle \frac{u_{j'l'm'}(r)}{r} = \left[ \frac{V_{\text{cent}}^{(00)}(r)}{\sqrt{4\pi}} + \frac{1}{\sqrt{4\pi r}} \frac{dV_{\text{ls}}^{(00)}(r)}{dr} \left( j(j + 1) - l(l + 1) - \frac{3}{4} \right) \right] u_{ljm}(r) \delta_{j,j'} \delta_{l,l'} \delta_{m,m'}. \quad (A10)
\]
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FIG. 1. The eigenphase sum (the upper panel) and its energy derivative (the lower panel) as a function of energy for neutron positive energy states of $^{44}$S at $\beta = 0.2$. The spin projection onto the symmetry axis and the parity are taken to be $K^\pi = 5/2^+$. These are denoted by the thick solid line, while the contributions from three main eigenchannels are also shown by the thin dashed, dotted and dot-dashed lines.
FIG. 2. Neutron single-particle energies of \(^{44}S\) obtained with the box discretization method as a function of the box radius \(R_{\text{box}}\). The axial symmetry is assumed, with the deformation parameter \(\beta\) of 0.2. The spin projection onto the symmetry axis and the parity are taken to be \(K^\pi = 5/2^+\). The potential parameters are the same as in fig. 1.
FIG. 3. The channel wave functions around the neutron resonance state of $^{44}$S at $\beta = 0.2$ and for $K^\pi = 5/2^+$. Those are for the eigenchannel basis which dominates the total width. The thick and thin solid lines are the wave functions at the resonance energy, $E_R = 3.44$ MeV and at $E=3.54$ MeV, respectively. The dashed line is obtained by using the factorization formula for a multi-channel resonance state. The potential parameters are the same as in fig. 1.
FIG. 4. The total eigenchannel wave function around the neutron resonance state of $^{44}\text{S}$ at $\beta = 0.2$ and for $K^\pi = 5/2^+$. The spin degree of freedom is eliminated by projecting the wave function onto the upper spin component. The upper and the lower panels are for the wave function along the $(\theta, \phi) = (\pi/4, 0)$ and the $(\theta, \phi) = (\pi/2, 0)$ directions, respectively. The meaning of each line is the same as in fig. 3.
FIG. 5. The energy dependence of the $g_{9/2}$ component of the eigenchannel wave function around the $K^\pi = 5/2^+$ resonance of $^{44}$S. The solid line is the exact wave function, while the dashed line is obtained with the factorization formula for a multi-channel wave function.