Non-Hermitian effective Hamiltonian and continuum shell model

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The intrinsic dynamics of a system with open decay channels is described by a non-Hermitian effective Hamiltonian which at the same time allows one to find the external dynamics—reaction cross sections. We discuss ways of incorporating this approach into the shell model context. The approach is capable of describing a multitude of phenomena in a unified way combining physics of structure and reactions. Self-consistency of calculations for a chain of nuclides and threshold energy dependence of the continuum coupling are crucial for the description of loosely bound states. Schematic and realistic examples of open many-body systems where internal configuration mixing is generated by pairing are presented.

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I. INTRODUCTION

The center of interest in nuclear physics has recently moved toward nuclei far from the region of stability. Weakly bound nuclei cannot be fully described in the limited framework of the shell model with a discrete energy spectrum. Even the properties of their bound states reflect the proximity of the continuum. Loosely bound nucleons create an extended spatial structure that determines the results of possible reactions so that nearly all excitation mechanisms break up the nucleus. The standard approaches to many-body theory, such as the Hartree-Fock-Bogoliubov mean field and random phase approximation, necessarily include virtual and real excitations to the continuum. The Borromean cases of ⁶He, ⁹Be, and ¹¹Li, when the system can be considered to be made of three clusters with all two-body subsystems being unbound, are very sensitive to the continuum physics. This is the area where the conventional division of nuclear physics into "structure" and "reactions" becomes inappropriate, and the two views of the process, from the inside (structure and properties of bound states) and from the outside (cross sections of reactions), should be recombined.

The broad success of the nuclear shell model with effective interactions urges one to look for ways to incorporate the rich experience accumulated in the shell model into a more general context that would properly include the continuum part. The description with the aid of an effective non-Hermitian Hamiltonian is well known going back to the classical Weisskopf-Wigner damping theory [1], works in atomic physics by Rice [2] and Fano [3], and projection formalism by Feshbach [4]. The consistent formulation of the approach was given in the book by Mahaux and Weidenmüller [5] in application to processes with one particle in the continuum. This gave rise to the shell model embedded in the continuum [6,7] recently revived [8–10] for the description of loosely bound nuclei. Another direction of development was related to the shell model description of nuclear reactions [11-13].

The key challenges associated with the continuum shell model approach are similar to the case of the traditional shell model and can be identified as construction of the effective interaction and practical solution. In the continuum shell model the effective Hamiltonian becomes non-Hermitian and energy dependent. In this work we will not discuss the most complicated task in this treatment, namely, the problem of the effective interaction. It is virtually unknown what should be an effective interaction of quasiparticles in the restricted shell model space which includes the continuum. For our limited purpose below we assume that the Hermitian part of the effective interaction of the traditional shell model [14] can be simply readjusted to the new problem. The new non-Hermitian and energy-dependent terms associated with the coupling to continuum at this stage can be determined phenomenologically assuming the energy dependence appropriate to the relevant kinematics and adjusting the remaining parameters to the experimental data. Our goal here is to address the second part of the problem, namely, to develop methods for a consistent and reliable treatment of open many-body systems assuming a given effective Hamiltonian.

Perhaps it is worth identifying the main new features that emerge in the continuum shell model in contrast to its traditional analog. The non-Hermiticity of the effective Hamiltonian was extensively studied in various branches of physics during past several decades. At certain strength of the continuum coupling, the system undergoes restructuring revealing new collective phenomena ("super-radiance" [15]), associated with the coherence of manybody states in the process of decay or radiation [16–18], with bright manifestations in nuclear physics of low [19,20] and intermediate [21,22] energies, atomic physics [23,24], molecular physics [25], quantum chemistry [26], and condensed matter physics [27–29]. The energy dependence of the manybody effective Hamiltonian is a poorly explored area, although simple analytical models have been discussed. In the present work we

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incorporate the realistic energy-dependent and non-Hermitian Hamiltonian into the shell model context.

The continuum shell model is expected to naturally combine the physics of structure and reactions. Therefore it is impossible to consider each nucleus separately, as it is done traditionally for spectroscopic studies. The true solution, as we show below, treats together all nuclear systems within the selected valence space. The nuclear reactions are the linking mechanisms for a chain of nuclides. Properties such as open channels, Q values, threshold behavior, symmetries, and spectroscopic factors for all allowed reactions and various intrinsic eigenstates must enter the overall scheme so that the resulting solution creates a fully consistent picture uniting nuclear structure with reaction mechanisms.

Having set these goals, we conduct the discussion as follows. In Sec. II we briefly recall the underlying theory that leads to the energy-dependent and non-Hermitian effective Hamiltonian, with an emphasis on the points particularly relevant to this work. In Sec. IV we present a two-state model that elucidates the generic features of the problem including coupling of states to common decay channels, near-threshold behavior, dynamics of resonances in the complex plane, and reaction-structure relations. Sections V and VI are devoted to realistic systems, including the chain of oxygen isotopes, where, in general, a large number of states is involved and the self-consistency requirements appear as inalienable ingredients of the approach. The summary and conclusions are presented in Sec. VII.

II. EFFECTIVE HAMILTONIAN

We will not repeat here the derivation of the non-Hermitian effective Hamiltonian that can be achieved by separating the Hilbert space into the intrinsic part and the continua and eliminating the continuum part with the aid of projection operators. This procedure was reviewed by many authors; see, for example, Refs. [7,31]. We label intrinsic states by 1, 2, ..., and the continuum channels by a, b, c, ... The matrix elements of the effective intrinsic Hamiltonian can be written as

$$\mathcal{H}_{12} = H_{12} + \Delta_{12} - \frac{i}{2} W_{12}, \qquad (1)$$

where H is an internal, for example, a standard shell-model part, and the last two terms (which in general are functions of running total energy E) are generated by the exclusion of the continuum.

The imaginary part W(E) originates from the real processes of decay to channels that are open at a given energy. It is represented by the residues of the on-shell terms corresponding to the δ functions coming from the energy conservation and causality requirement imposed on the energy denominators, $E \rightarrow E^{(+)} = E + i0$. The quantity W has a factorized form,

$$W_{12} = \sum_{c;\text{open}} A_1^c A_2^{c*}, \qquad (2)$$

where the decay amplitudes $A_1^c(E)$ are the matrix elements of the original total Hermitian Hamiltonian between the states $|1\rangle$ and $|c;E\rangle$ of different subspaces; the normalization coefficients are included in the definition of A_1^c . The second term of Eq. (1), $\Delta_{12}(E)$, originates from the principal value of the same expression and corresponds to the virtual offshell processes taking place via the continuum. Therefore it includes contributions from all, open and closed, channels. For the system invariant under time reversal, one can use a basis, where the matrix elements H_{12} , Δ_{12} , and A_1^c can be taken as real.

The same effective Hamiltonian (1) determines the scattering amplitude and the reaction cross sections. The relation between the inside and outside views was studied in Refs. [5,16,17,19,20,32]. The scattering matrix in the channel space describing the $b \rightarrow a$ process is given by

$$S^{ab} = (s^{a})^{1/2} (\delta^{ab} - T^{ab}) (s^{b})^{1/2},$$
(3)

$$T^{ab} = \sum_{12} A_1^{a*} \left(\frac{1}{E - \mathcal{H}} \right)_{12} A_2^b.$$
(4)

Here $s^a = \exp(2i\delta_a)$ stands for the smooth scattering phase coming from remote resonances not accounted for explicitly. The propagator $(E - \mathcal{H})^{-1}$ in the scattering amplitude T^{ab} does not depend on a specific reaction and contains the full effective Hamiltonian (1) with the same amplitudes A_1^c as those determining the entrance and exit channels in Eq. (4). This guarantees the unitarity of the *S* matrix since the virtual processes of evolution of the open system to and from the continuum channels are included in all orders in the propagator.

The diagonalization of the non-Hermitian Hamiltonian (1) produces the complex eigenvalues

$$\mathcal{E}_{\alpha}(E) = \tilde{E}_{\alpha}(E) - \frac{i}{2}\Gamma_{\alpha}(E), \qquad (5)$$

where the real (\tilde{E}_{α}) and imaginary (Γ_{α}) parts are functions of running real energy *E*. Without explicit energy dependence of the effective Hamiltonian, these eigenvalues would provide the unstable states with a pure exponential decay law $\exp(-\Gamma_{\alpha}t)$. The presence of energy dependence violates the exponential decay, and the actual quasistationary states are found at real energies E_{α} determined by the self-consistency condition

$$\tilde{E}_{\alpha}(E_{\alpha}) = E_{\alpha}.$$
(6)

The line shape is not of Breit-Wigner type, but we still call $\Gamma_{\alpha}(E_{\alpha})$ the width of the resonance α . In what follows, we omit the tilde sign for E_{α} if it does not lead to a confusion.

In the region of interest for loosely bound systems, the main energy dependence comes from the proximity of thresholds as was stressed in Refs. [17,33]. The channel *c* is open only if the total energy *E* is above threshold energy $E^{(c)}$ for this channel. The decay amplitudes associated with the channel *c* contain therefore the step factor $\Theta(E - E^{(c)})$ and can be written as

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$$A_1^c = a_1^c(E)\Theta(E - E^{(c)}), (7)$$

where $a_1^c(E)$ is a smooth function of energy that falls off to zero when energy decreases to the threshold value. For a single-particle decay channel, it can be parametrized [17,33] as proportional to the square root of the penetrability in this channel.

The real part Δ of the effective potential can be written as the principal value integral,

$$\Delta_{12}(E) = \frac{\mathcal{P}}{\pi} \sum_{c} \int_{E^{(c)}} \frac{dE'}{E - E'} a_1^c(E') a_2^{c*}(E').$$
(8)

Under the same assumption of a nonsingular character of a_1^c , matrix elements (8) also have a smooth energy dependence with no singularities near threshold and usually can be approximated by energy-independent quantities as in Refs. [17,33].

One formal conclusion concerning the existence of bound and unbound states can be reached just from the way the theory is constructed. If the conventional shell model with a purely discrete spectrum (no coupling to the continuum) predicts a state with energy below all decay thresholds, this state will remain bound in the full calculation with the decay amplitudes included. Indeed, all widths depend on the total energy and vanish below thresholds so that the old solution is still valid. However, this statement is formal since it assumes that the reaction thresholds are known beforehand. In fact, they have to be determined consistently for the chain of nuclides relevant to the reactions under consideration.

Certainly, there are limitations in the applicability of the method in the form outlined in the present paper. As energy increases, a rapid growth of a number of interfering open channels makes this approach impractical. We also deliberately limit ourselves here by taking into account only the energy dependence associated with threshold and resonance phenomena although the smooth "potential" scattering part could be included without significant difficulties via the entrance and exit scattering phases hidden in the factors s^a and s^{b} of Eq. (3). The full energy dependence was discussed, in particular, in Refs. [34,35]. The main physical assumption made here is that the states under consideration are close to threshold and, at relatively low energy, only few open channels are really essential. For the purpose of this paper, namely, for the development of shell-model methods intended for the description of low-lying states near the border of stability, the presumed conditions are typically fulfilled to within a sufficient accuracy.

III. SHELL-MODEL APPROXIMATION

We view Hamiltonian (1) as a sum of three terms,

$$\mathcal{H} = H^0 + V - \frac{i}{2}W,\tag{9}$$

where we assume that the intrinsic Hermitian part $H^0 + V$ consists of independent particle energies,

$$H^0 = \sum \epsilon_{\nu} a^{\dagger}_{\nu} a_{\nu}, \qquad (10)$$

and the effective Hermitian interaction V. As a renormalization of the standard shell-model interaction, the Hermitian matrix elements Δ_{12} , Eq. (8), generated by the virtual coupling through continuum, can be incorporated into the operator V. The approximation of energy independence of the operator Δ and, as a result, energy independence of V (also used in previous works [17,33]) can be easily removed.

For an open system defined by Hamiltonian (9) there are two types of states that can be selected as a starting point for the diagonalization. In the spirit of the conventional shell model, it is convenient to start from the basis states $|\Phi\rangle$, the eigenstates of H^0 , that are Slater determinants of the m scheme or their linear combinations projected onto correct values of total spin J and isospin T. The coupling to continuum makes the choice of doorway states, the eigenstates of W, another good possibility. As analyzed in detail in Ref. [17], the doorway states correspond to simplest configurations participating directly in reactions. Because the number of channels may be limited, the associated reactions generally cannot explore the full complexity of internal structure. Being related to the factorizable nature of the operator W and degeneracy of its spectrum, this leaves some freedom in the selection of basis states.

Although in general the two choices are different, there are cases where the operators H^0 and W commute, and one can identify the doorway states with specific intrinsic configurations. The most common and transparent example of this is single-particle decay into continuum. For an isolated single-particle level $|\nu\rangle$ embedded in the continuum, the unperturbed real energy is $E_{\rm core} + \epsilon_{\nu}$. If the only open channel, $c \Rightarrow \nu$, is associated with the emission of the particle ν , the imaginary part W leads to the width

$$\gamma_{\nu} = |A_{\nu}^{\nu}|^2 \tag{11}$$

for any configuration that consists of the particle on the level $|\nu\rangle$ and an arbitrary state of the stable core (no interaction between them at this stage). Threshold energy is determined by the core configuration. This extends directly to the case of several different single-particle levels embedded in the continuum.

If there are several single-particle configurations with the same exact quantum numbers, the situation is more complicated, and in general H^0 and W cannot be simultaneously diagonalized. This implies that, apart from the particle emission from a given single-particle state, we now also have the interaction of close intrinsic states through continuum given by the off-diagonal elements of W_{12} . Similarly, interaction via the continuum is almost certainly present in cases where two-particle emission is possible from different initial configurations. In the case of pairing, for example, a zero-spin Cooper pair can be emitted from a few *j* levels leading to the same final state, and therefore into the same decay channel. Here the coupling through the continuum may be very important; this situation is discussed in Sec. IV.

The presence of continuum coupling W distorts the internal states. Depending on the strength of W, one observes different regimes. In the weak coupling regime, W can be treated perturbatively. Within the single-particle decay picture, this leads to the shell model, where spectroscopic factors are usually used to determine widths of the resonances. Once the decay widths of manybody states start to overlap, the standard shell model fails and one enters the domain of a crossover behavior [18], where the alignment of states along doorway configurations competes with the intrinsic configuration mixing. At strong continuum coupling the term W dominates, and the eigenstates reorient along doorway configurations. This limit can be juxtaposed to the collective effect of super-radiance [15] where the internal states are coherently coupled through the common decay channel [16,36]. The limits of this paper do not allow us to fully illustrate the richness and nontrivial character of the complicated interplay of internal and external dynamics, and we refer the reader to Refs. [16,36,7,18,37] for subjects such as the phase transition to super-radiance, role of symmetries, redistribution of the widths, segregation of direct and compound nucleus processes, interference between the intrinsic residual interaction and the interaction mediated by the excursion into open decay channels, dynamics of the poles in the complex energy plane with unusual crossings and anticrossings.

Finally, the energy dependence of the amplitudes A_1^c makes the problem highly nonlinear since the positions of the quasistationary eigenstates of \mathcal{H} in the complex plane should be determined consistently with special care taken to avoid false solutions that can appear due to the possible nonanalytic energy dependence at thresholds. Another new feature is that threshold energies are not known *a priori*. They are to be calculated self-consistently comparing total energies of the parent and daughter nuclei found in the same approximation. The treatment of these consistency issues is presented in Secs. V and VI.

IV. DYNAMICS OF TWO STATES COUPLED TO A COMMON DECAY CHANNEL

Here we consider a model that shows how the attractive pairing-type interaction generates the binding of originally unstable states competing with the coupling through continuum. We consider two single-particle levels in the continuum; their unperturbed energies are positive if the continuum threshold is put at zero energy. (A special case with only one initial nonzero decay amplitude was discussed in Ref. [33].) This is a prototype of the three-body Borromean model for ¹¹Li with the inert core of ⁹Li and particleunstable ¹⁰Li. The two active orbitals $s_{1/2}$ and $p_{1/2}$ are those for a pair of halo neutrons, $\epsilon_1 = 2\epsilon(p), \epsilon_2 = 2\epsilon(s)$. They are quasistationary, and their decay amplitudes A_{12} characterize the only open channel with the core nucleus in the ground state and the neutron pair in the state $J^{\pi}=0^+$ in the continuum. At this point the exact form of the energy dependence is not fixed, except for the fact that when the total energy approaches zero, the decay becomes forbidden so that, as in Eq. (7), the amplitudes $A_{1,2}$ contain the step function $\Theta(E)$. Because of the Cooper pair in the continuum, the non-Hermitian operator *W* is not of a single-particle nature, and the model is more complicated than that of two Gamow resonances. The novel aspects here include interference between internal and external interactions, violation of width sum rules, and possible appearance of bound state in the continuum. Here we also show the calculation of the reaction cross section, a necessary step to the unified description of structure and reactions. The problem of two-body decay, especially relevant for Borromean systems, was recently approached with the use of different shell-model formalisms in Refs. [9,10]. Two-proton radioactivity [38] is another example requiring a similar consideration. Many features of two-level unstable systems with other physical applications were discussed in Refs. [39,40].

A. General features of the model

According to Sec. II, the effective non-Hermitian Hamiltonian in the 2×2 space is

$$\mathcal{H} = \begin{pmatrix} \epsilon_1 - \frac{i}{2}\gamma_1 & v - \frac{i}{2}A_1A_2 \\ v - \frac{i}{2}A_1A_2 & \epsilon_2 - \frac{i}{2}\gamma_2 \end{pmatrix}.$$
 (12)

Here $V_{12} \equiv v$ is the real mixing matrix element, $\gamma_{1,2} = A_{1,2}^2$, and the amplitudes $A_{1,2}$ are also real. One should be careful with the phases. For a pure internal interaction, the sign of the mixing matrix element V_{12} is irrelevant, it always can be changed by the redefinition of the phase of one of the states, 1 or 2. But, with the coupling to continuum present, this change must be accompanied by the corresponding phase change in the decay amplitude; therefore we cannot simply put $A_{1,2} = \sqrt{\gamma_{1,2}}$.

A formal diagonalization of the effective Hamiltonian gives the complex energies of the quasistationary states,

$$\mathcal{E}_{\pm} = \frac{1}{2} \left[\epsilon_{1} + \epsilon_{2} - \frac{i}{2} (\gamma_{1} + \gamma_{2}) \right] \pm \frac{1}{2} \left\{ (\epsilon_{1} - \epsilon_{2})^{2} + 4v^{2} - \frac{1}{4} (\gamma_{1} + \gamma_{2})^{2} - i [(\epsilon_{1} - \epsilon_{2})(\gamma_{1} - \gamma_{2}) + 4vA_{1}A_{2}] \right\}^{1/2}.$$
(13)

For the case of stable states, $A_{1,2}=0$, we come to the standard two-level repulsion,

$$\mathcal{E}_{\pm} = E_{\pm} = \frac{1}{2} [\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4v^2}].$$
(14)

The lower level reaches zero energy under the condition

$$v^2 = \epsilon_1 \epsilon_2. \tag{15}$$

In the case of degenerate resonances ($\epsilon_1 = \epsilon_2 \equiv \epsilon$) with different widths γ_1 and γ_2 , in the absence of intrinsic mixing (v=0) we obtain

$$\mathcal{E}_{\pm} = \epsilon - \frac{i}{4} (\gamma_1 + \gamma_2) \pm \frac{i}{4} (\gamma_1 + \gamma_2)$$
$$\Rightarrow \begin{cases} E = \epsilon, & \Gamma = 0\\ E = \epsilon - \frac{i}{2} \Gamma, & \Gamma = \gamma_1 + \gamma_2. \end{cases}$$
(16)

In this case the Hamiltonian consists of the unit matrix ϵ and the matrix W of a factorized type (rank r=1) so that the correct linear combinations are the eigenvectors of W; one of them, the analog of the Dicke coherent state [15,16], accumulates the total width, whereas the second one is stable.

The crossing and anticrossing of unstable levels were considered in Refs. [23,31,40-42] and experimentally studied with microwave cavities [43]. In contrast to the avoided crossing (14) of stable levels, the coincidence of two complex eigenvalues is possible, see Ref. [44] and references therein. In our case it requires that two conditions should be fulfilled,

$$(\boldsymbol{\epsilon}_1 - \boldsymbol{\epsilon}_2)^2 = \boldsymbol{\gamma}_1 \boldsymbol{\gamma}_2 \tag{17}$$

and

$$(\gamma_1 - \gamma_2)^2 = 16v^2.$$
 (18)

The coinciding complex energies \mathcal{E}_{\pm} , Eq. (13), evenly divide the trace of the Hamiltonian. There is a difference between our case and the energy-independent two-level Hamiltonian discussed in Ref. [41], where the crossing condition

$$(\boldsymbol{\epsilon}_1 - \boldsymbol{\epsilon}_2)(\boldsymbol{\gamma}_1 - \boldsymbol{\gamma}_2) + 4\boldsymbol{v}\boldsymbol{A}_1\boldsymbol{A}_2 = 0 \tag{19}$$

leads to crossing of either real energies, $E_+ = E_-$, or widths, $\Gamma_+ = \Gamma_-$, for the negative or positive sign of

$$X = (\epsilon_1 - \epsilon_2)^2 + 4v^2 - \frac{1}{4}(\gamma_1 + \gamma_2)^2, \qquad (20)$$

respectively. In the energy-dependent case the same condition remains true for the crossing of energies, however, not for the crossing of the widths because generally $\mathcal{H}(E_+) \neq \mathcal{H}(E_-)$.

The secular equation for the eigenvalues can be also written in a form explicitly separating the real, \tilde{E} , and imaginary, $\tilde{\Gamma}$, parts of complex roots (here we again restore the tilde sign in order to distinguish the roots from the running energy value E). The real part of this equation gives

$$\tilde{E}^2 - \tilde{E}(\epsilon_1 + \epsilon_2) - \frac{\tilde{\Gamma}}{4}(\tilde{\Gamma} - \gamma_1 - \gamma_2) + \epsilon_1\epsilon_2 - v^2 = 0,$$
(21a)

while from the imaginary part we obtain

$$\widetilde{\Gamma} = \frac{\widetilde{E}(\gamma_1 + \gamma_2) - \gamma_1 \epsilon_2 - \gamma_2 \epsilon_1 + 2vA_1A_2}{2\widetilde{E} - \epsilon_1 - \epsilon_2}.$$
 (21b)

The coupled equations (21a) and (21b) determine \tilde{E} and $\tilde{\Gamma}$. For an arbitrary energy dependence of the amplitudes $A_{1,2}(E)$ that are to be taken in these equations at $E = \tilde{E}$, this is still an implicit solution; even the number of roots can change.

For a sufficiently strong interaction v, the repulsion of real energies can bring the lower eigenvalue E_{-} to zero (a threshold value). Then both amplitudes $A_{1,2}$ disappear together with the eigenwidth Γ_{-} , Eq. (21b). This means that the lowest quasistationary state becomes bound under the same condition (15). If the mixing increases further, the binding energy of the lower state is going down,

$$E_{-} \approx -\frac{v^2 - \epsilon_1 \epsilon_2}{\epsilon_1 + \epsilon_2}.$$
 (22)

As was mentioned in Ref. [33] for a similar model with only one nonvanishing γ , this is a prototype of the dynamics leading to the binding of nuclei as ¹¹Li, where the residual interaction among the valence neutrons is of pairing type. The higher level, in the point of bifurcation (15), has the energy

$$E_{+} = \frac{1}{2} \left[\epsilon_{1} + \epsilon_{2} + \sqrt{(\epsilon_{1} + \epsilon_{2})^{2} + \Gamma_{+}(\Gamma_{+} - \gamma_{1} - \gamma_{2})} \right],$$
(23)

where $\gamma_{1,2}$ are to be taken at energy $E = E_+$.

The violation of Wigner sum rules [13] associated with the widths of resonances is a critical feature of the physics near driplines. If the effective Hamiltonian were energy independent, both the real and imaginary parts of its trace would be separately preserved by the complex orthogonal transformation to the eigenvectors. This means that we would always have

$$\Gamma_{+} + \Gamma_{-} = \operatorname{tr} W = \gamma_{1} + \gamma_{2} \tag{24}$$

and

$$E_{+} + E_{-} = \operatorname{tr} \boldsymbol{\epsilon} = \boldsymbol{\epsilon}_{1} + \boldsymbol{\epsilon}_{2} \,. \tag{25}$$

At the bifurcation point, $E_{-} = \Gamma_{-} = 0$, we would have

$$\Gamma_{+} = \gamma_{1} + \gamma_{2}, \quad E_{+} = \epsilon_{1} + \epsilon_{2}, \quad (26)$$

while it follows from Eqs. (15) and (21b) that

$$\Gamma_{+}(E_{+}) = \frac{[A_{1}(E_{+})\sqrt{\epsilon_{1}} + A_{2}(E_{+})\sqrt{\epsilon_{2}}]^{2}}{\epsilon_{1} + \epsilon_{2}}$$
(27)

and

$$\Gamma_{+}(E_{+}) - \gamma_{1}(E_{+}) - \gamma_{2}(E_{+})$$

$$= -\frac{[A_{1}(E_{+})\sqrt{\epsilon_{2}} - A_{2}(E_{+})\sqrt{\epsilon_{1}}]^{2}}{\epsilon_{1} + \epsilon_{2}} < 0, \qquad (28)$$

in contradiction to the first part of Eq. (26). The trace violation occurs because the imaginary parts have their own energy behavior with compulsory zero-energy thresholds. When the levels are repelled by the mixing interaction, their widths are changed by the dynamics outside the 2×2 matrix. But the trace is preserved and Eq. (26) is fulfilled if

$$\frac{A_1(E)}{A_2(E)} = \sqrt{\frac{\epsilon_1}{\epsilon_2}},\tag{29}$$

so that in the entire energy range of interest the two partial widths grow proportionally, an interesting exceptional case.

B. Solutions with energy-dependent widths

To illustrate the dynamics of two states coupled to a common continuum with energy-dependent widths, we show a numerical example. For all figures below we take $\epsilon_1 = 100 \text{ keV}$ and $\epsilon_1 = 200 \text{ keV}$ for the particle pair in *p* and *s* states, respectively. For these parameters the ground state reaches zero energy, and thus becomes bound, at $v \approx 141 \text{ keV}$ by virtue of Eq. (15).

The picture with energy-independent widths is not consistent with the definition of thresholds. As seen from Fig. 1(a), the residual interaction pushes the levels apart, and the lower state crosses zero energy. However, the width Γ_{-} of this state, dashed lines in Figs. 1(b) and 1(c), is still positive. For the calculations shown by solid lines in Figs. 1(b) and 1(c), similar to Ref. [33], we assume in the low energy region the square root energy dependence for the *s* wave, and $\sim E^{3/2}$ for the *p* wave,

$$\gamma_2(E) = \alpha \sqrt{E}, \quad \gamma_1(E) = \beta E^{3/2}. \tag{30}$$

This makes the evolution of complex energies as a function of the residual interaction strength v consistent with the existence of thresholds: at $v^2 = \epsilon_1 \epsilon_2$ the lower state becomes stationary, $E_- = \Gamma_- = 0$. The near-threshold behavior of the width is governed by the *s*-wave component with the infinite slope, $\Gamma \sim \sqrt{E - E^{(c)}}$. However, as α becomes smaller, Fig. 1(c), the singularity is getting confined to a narrow vicinity of threshold, to the limit that at an observable scale the behavior is dominated by the *p* wave.

Besides the trivial situation, when the width of a particular state vanishes due to energy conservation, blocking of the decay via dynamical mixing at a single point corresponding to a certain strength v is also possible. This effect of the bound state in the continuum is seen in Fig. 1(b), where a conspiracy of the parameters leads to the vanishing width Γ_{-} of the lower state at energy E_{-} still in the continuum, Fig. 1(a). Equations (21a) and (21b) with $\Gamma_{-}=0$ show that this happens at the interaction strength

$$v = A_1 A_2 \frac{\epsilon_1 - \epsilon_2}{\gamma_1 - \gamma_2}.$$
(31)

Here $A_{1,2}$ and $\gamma_{1,2}=A_{1,2}^2$ are to be taken at the energy E_{-} found from Eq. (21a). For the model in Fig. 1(b), this happens at $v \approx 63$ keV.

The energy dependence of the amplitudes complicates the trajectories of the eigenvalues in the complex plane. Unlike in a stable system or a system with energy-independent parameters, here the solutions for \mathcal{E}_+ and \mathcal{E}_- involve a diago-



FIG. 1. Panels (b) and (c) show the behavior of the width Γ_{-} of a lower resonance as a function of v for energy-dependent (solid lines) and energy-independent (dashed lines) decay amplitudes. Selected parameters are $A_1 = 8.1$ (keV)^{1/2} and $A_2 = 12.8$ (keV)^{1/2} in the energy-independent case, and $\alpha = 15$ (keV)^{1/2} and β = 0.05 (keV)^{-1/2} in the energy-dependent case [panel (b)]; A_1 = 7.1 (keV)^{1/2} and $A_2 = 3.1$ (keV)^{1/2}, dashed line, and α = 1 (keV)^{1/2} and $\beta = 0.05$ (keV)^{-1/2} [panel (c)]. Parameters are selected in such a way that at v = 0 the two solid and dashed lines agree. The relative phases are such that $v \ge 0$ and $A_1A_2 \ge 0$. In panel (a) energies of the two states are shown, solid lines, for the case relevant to panel (b) with the energy-dependent amplitudes, Eq. (30), and compared to the energies of a nondecaying system, dashed lines. The dotted line in all three plots corresponds to the zero value of the width or energy.

nalization of different matrices. The Hamiltonian matrices differ in their imaginary part W(E). The "interaction" between the levels occurs via the common Hermitian part $H^0 + V$. Thus, for a general system it can be expected that bound states and weakly unbound resonances are still strongly correlated although new features related to small imaginary components appear, and the usual level repulsion on the real energy axis is present only up to a spacing of the order of the width of the resonance [16]. For states deeply in the continuum, however, the correlation must rely on the

structure of W(E) that represents features and symmetries of the continuum.

C. Cross sections near threshold

Here we consider the scattering cross section for the case of two intrinsic states coupled to one open channel. Although two neutron scattering is not a feasible reaction from an exprimental point of view, the result of this study is relevant for the excitation processes of a Borromean system. The elastic cross section in the *s* wave for a relative momentum $k \propto \sqrt{E}$ is

$$\sigma(E) = \frac{\pi}{k^2} |S(E) - 1|^2,$$
(32)

where the scattering matrix is defined by Eqs. (4) and (5) in terms of the effective Hamiltonian \mathcal{H} . In our case [Eq. (12)], neglecting the potential scattering \hat{s} , the propagator can be easily found, and we obtain

$$T(E) = \frac{E(\gamma_1 + \gamma_2) - \gamma_1 \epsilon_2 - \gamma_2 \epsilon_1 - 2vA_1A_2}{(E - \mathcal{E}_+)(E - \mathcal{E}_-)}, \quad (33)$$

with the poles $\mathcal{E}_{\pm} = E_{\pm} - (i/2)\Gamma_{\pm}$ given by Eq. (13), or by a pair of coupled equations (21). One can notice that the relative sign of the matrix elements for the direct internal interaction between the mixed states, v, and for their continuum mediated interaction, A_1A_2 , may considerably change the resulting cross section.

In the special case of a pair of degenerate intrinsic levels with no direct interaction, Eq. (16), the general result (33) reduces to the single Breit-Wigner resonance on a Dicke coherent state accumulating the total width,

$$T(E) = \frac{\gamma_1 + \gamma_2}{E - \epsilon + (i/2)(\gamma_1 + \gamma_2)}.$$
(34)

The second root, $\Gamma = 0$, of Eq. (16) is decoupled from the continuum and does not influence the scattering process. We have to stress again that the "widths" $\gamma_{1,2}$ in general depend on running energy *E*.

At the bifurcation point (15), the scattering amplitude becomes

$$T(E) = \frac{E(\gamma_1 + \gamma_2) - (A_1 \sqrt{\epsilon_2} + A_2 \sqrt{\epsilon_1})^2}{E(E - \mathcal{E}_+)},$$
 (35)

where the higher root \mathcal{E}_+ is defined by Eqs. (23) and (27). At low energy $(E \rightarrow 0)$, the behavior of the scattering cross section, as well as photonuclear processes, is determined by the actual energy dependence of decay amplitudes.

At the critical value of v, Eq. (15), and in the low energy region where approximation (30) can be valid, the scattering amplitude (33) is singular, $\sim E^{-1/2}$,

$$T(E) \approx \frac{\alpha \epsilon_1}{\sqrt{E} \{ \epsilon_1 + \epsilon_2 - (i/2) \alpha [\epsilon_2 / (\epsilon_1 + \epsilon_2)] \sqrt{E} \}}.$$
 (36)



FIG. 2. The near-threshold scattering cross section is shown for loosely bound systems with v = 180 and 200 keV in solid and dashed lines, respectively. Due to similarity between the curves, the dashed curve is not shown in panel (b). Other selected parameters are $\alpha = 15$ (keV)^{1/2} and $\beta = 0.05$ (keV)^{-1/2}. Phases are $A_1A_2 > 0$ and $A_1A_2 < 0$ for panels (a) and (b), respectively.

When the interaction is overcritical, $v^2 > \epsilon_1 \epsilon_2$, and at low energies, $E \leq |E_-|$ [Eq. (22)], we obtain

$$T(E) \approx \frac{\alpha \epsilon_1 \sqrt{E}}{\mathcal{E}_+(E-E_-)}.$$
(37)

Therefore the cross section (32) has a constant value at threshold and behaves at low energies as $(E+|E_-|)^{-2}$, revealing "attraction" to the subthreshold region [17,45]. The cross sections shown in Fig. 2(a) for two overcritical values of the interaction strength display a threshold behavior characteristic for loosely bound systems that can be mistaken for resonances. The case $A_1A_2>0$ produces only a very broad peak [not shown on Fig. 2(a)] corresponding to the upper quasistationary state E_+ . Figure 2(b) shows that in the case of $A_1A_2<0$ the interference of the internal and external interactions results in a narrow resonance with a very high cross section at $E=E_+=340$ keV, along with the maximum at zero energy (of course, all numerical values characterize only the model parameters).

V. TWO-LEVEL MODEL WITH PAIRING INTERACTION

Here we make the next step to realistic manybody physics working with a system of two orbitals that can accommodate $\Omega_1 = \Omega_2 = 10$ particles each; both levels can decay to a final state at fixed energy $E_f = 0$. The decay widths γ_1 and γ_2 are different but have the same, $\gamma_{1,2}(E) = \alpha_{1,2}\sqrt{E}$, energy dependence near threshold. It should be noted that synchronous decay with $\gamma_1 = \gamma_2$ would not affect the internal dynamics since W in that case would be proportional to a unit matrix.



FIG. 3. The level scheme of s=0 states in the two-level, eightparticle system as a function of pairing strength. Solid lines correspond to the system embedded in the continuum with the fixed width values $\alpha_1=0.1$ and $\alpha_2=5$. These curves are compared with a nondecaying situation $\alpha_1=\alpha_2=0$ of the usual shell model, dashed lines. The dotted line at E=0 indicates the threshold location.

The single-particle energies are taken as $\epsilon_1 = 1$ and $\epsilon_2 = 3$. Intrinsic dynamics in this model are generated by the constant pairing $V_{L=0}^{jj'} \equiv G$. In Fig. 3 the spectrum of states with seniority s=0 in a system of eight particles is shown as a function of the pairing strength. The attractive pairing interaction pushes down low-lying levels, forcing some of them to become bound. The ground state becomes bound at $G \approx 0.2$.

Comparison of spectra with and without continuum coupling (solid and dashed lines, respectively) shows generic features. The bound states are not affected by the continuum coupling. The low-lying levels, as compared to highly excited states, are less influenced by the presence of continuum. In contrast to the usual perturbation theory, we see that the ground state and even the first excited state once embedded in the continuum become attracted to the bulk of other states that increases their energy. Such a situation usually leads to an increase of the decay Q value that in turn further increases the decay width.

The following figure, Fig. 4(a), demonstrates the shift ΔE of the ground state energy as a result of decay for various choices of continuum coupling given by parameters α_1 and α_2 . Clearly, $\Delta E = 0$ if there is no configuration mixing at G = 0, or once the state becomes bound. The complex behavior of the decay width for the ground state is shown in Fig. 4(b); at the critical strength the width goes to zero with an infinite slope, $\sim \sqrt{E}$.

VI. REALISTIC PAIRING MODEL

As a demonstration of a realistic self-consistent shellmodel calculation, we consider oxygen isotopes in the mass region A = 16-28. In this study we use a universal *sd*-shell-model description with the semiempirical effective interaction (USD) [46]. The model space includes three single-particle orbitals $1s_{1/2}$, $0d_{5/2}$, and $0d_{3/2}$ with corre-



FIG. 4. The upper panel shows the shift in ground state energy between decaying and nondecaying (usual shell-model) systems, $\Delta E = E(\Psi) - E(\Psi_{sm})$, as a function of pairing strength under various assumptions for the decay rates. In the lower panel the width of the ground state is plotted.

sponding single-particle energies -3.164, -3.948, and 1.647 MeV. The residual interaction in the most general form is defined with a set of 63 reduced two-body matrix elements in pair channels with angular momentum *L* and isospin *t*, $\langle (j_3\tau_3, j_4\tau_4)Lt|V|(j_1\tau_1, j_2\tau_2)Lt \rangle$, which scale with nuclear mass as $(A/18)^{-0.3}$.

Although the full shell-model treatment is possible for such light systems, here we truncate the shell-model space to include only seniority s=0 and s=1 states for even and odd A, respectively. This method, "exact pairing + monopole," is known [30] to work well for shell-model systems involving only one type of nucleons (in the case of the oxygen isotope chain only neutrons are involved). The two important ingredients of nuclear forces are treated exactly by this method: the monopole interaction that governs the mean field evolution and the binding energy behavior throughout the mass region, and pairing that is responsible for the emergence of the pair condensate, renormalization of singleparticle properties, and collective pair vibrations. In our exploratory study, the truncation of the large space to the most important states is a reasonable approach since certainly the inclusion of decay makes the computations numerically more intense.

In the resulting shell-model description, the set of the original 30 two-body matrix elements in the isospin t=1 channel is reduced to 12 most important linear combinations, six two-body matrix elements for pair scattering in the L = 0 channel describing pairing, and the other six corresponding to the monopole force in the particle-hole channel,

$$\bar{V}_{j,j'} \equiv \sum_{L \neq 0} (2L+1) \langle (j,j')L1 | V | (j,j')L1 \rangle, \quad (38)$$

where j and j' refer to one of the three single-particle levels.

TABLE I. States of seniority s=0 and s=1 in oxygen isotopes. Energies and neutron decay widths are shown. Results are compared to the full shell-model calculations and to the known experimental data. Ground state energies relative to the ¹⁶O core are given in bold. The rest of the energies are excitation energies in a given nucleus.

		E	Г	$E_{\rm sm}$	$E_{\rm expt}$	Γ_{expt}
А	J	(MeV)	(keV)	(MeV)	(MeV)	(keV)
16	0	0.00	0	0.00	0.00	0
17	5/2	-3.95	0	-3.95	-4.14	0
17	1/2	0.78	0	0.78	0.87	0
17	3/2	5.59	96	5.59	5.08	96
18	0	-12.17	0	-12.17	-12.19	0
19	5/2	-15.75	0	-16.06	-16.14	0
19	1/2	1.33	0	1.47	1.47	0
19	3/2	5.22	101	5.53	6.12	110
20	0	-23.41	0	-23.83	-23.75	0
21	5/2	-26.67	0	-27.47	-27.55	0
21	1/2	1.38	0	1.33		
21	3/2	4.60	63	4.83		
22	0	- 33.94	0	-34.62	-34.40	0
23	1/2	-35.78	0	-37.07	-37.15	0
23	5/2	2.12	0	2.72		
23	3/2	2.57	13	3.28		
24	0	-40.54	0	-41.05	-40.85	0
25	3/2	- 39.82	14	-40.28		
25	1/2	2.37	0	2.36		
25	5/2	4.98	0	3.96		
26	0	-42.04	0	-42.04		
27	3/2	-40.29	339	-40.29		
27	1/2	3.42	59	3.42		
27	5/2	6.45	223	6.45		
28	0	-41.26	121	-41.26		

We assume that the orbital $0d_{3/2}$ belongs to the continuum and therefore its energy has an imaginary part. In this model we account for two possible decay channels for each initial state $|\Phi\rangle$, a one-body channel (c=1) and a two-body channel (c=2). The one-body decay changes the seniority of the $0d_{3/2}$ orbital by one, from 1 to 0 in the decay of an odd-*A* nucleus and from 0 to 1 for an even-*A* nucleus. The twobody decay removes two paired particles and thus does not change the seniority. The two channels lead to the lowest energy state of allowed seniority in the daughter nucleus, i.e., the possibility of transition to excited pair-vibrational states is ignored. This results in

$$e_{3/2}(\Phi) = \epsilon_{3/2} - \frac{i}{2} \alpha_{3/2} (E_{\Phi} - E^{(1)})^{5/2} - i \alpha_{3/2} (E_{\Phi} - E^{(2)})^{5/2}, \qquad (39)$$

where we assumed that one- and two-body decay parameters $\gamma_j^{(c)}$ are related as $\gamma_{3/2}^{(1)} = \gamma_{3/2}^{(2)}/2 \equiv \gamma_{3/2}$, and the particles are emitted in the *d* wave with $\ell = 2$.

With a simplifying assumption of the single-particle structure of W, one- and two-body decays can be incorporated into the complex single-particle energies. The three singleparticle orbitals can be clearly identified as the 5/2⁺ ground state, and 1/2⁺ and 3/2⁺ excited states in ¹⁷O. Their energies relative to ¹⁶O exactly correspond to the single-particle energies in the USD model. Experimental evidence indicates that the 3/2⁺ state decays via neutron emission with the width $\Gamma(1^{7}O)=96$ keV. This information allows us to determine our parameter $\alpha_{3/2}=\Gamma(1^{7}O)/(\epsilon_{3/2})^{5/2}$ =0.028 (MeV)^{-3/2}. Other two states are particle bound, $\gamma_{1/2}=\gamma_{5/2}=0$. Using the complex single-particle energies, the effective non-Hermitian Hamiltonian for the manybody system is constructed in a regular way.

We treat the chain of isotopes one by one starting from ¹⁶O. Therefore for each A the properties of the possible daughter systems A-1 and A-2 are known. Since the effective Hamiltonian depends on energy and threshold energies have to be determined self-consistently, we solve this extremely nonlinear problem iteratively. We start from the shell-model energies $E_{\rm sm}$ corresponding to a nondecaying system with the Hamiltonian H. Then the diagonalization of $\mathcal{H}(E_{\rm sm})$ allows us to determine the next approximation to the energies. The cycle is repeated until convergence, which is usually achieved in less than ten iterations.

The results of the calculations and comparison with full shell-model results with no seniority truncation and with known data for the chain of oxygen isotopes are shown in Table I. Some words of caution are appropriate for the interpretation of this table. The seniority truncation generally becomes unreliable for the states with excitation energy above twice the pairing gap, i.e., $\sim 2-4$ MeV. This can make the identification of the states of the pairing model in the full shell-model diagonalization difficult. The same problem can emerge in the comparison of theory with experiment. On the other hand, the standard shell model does not include the continuum coupling, and for the stable states our continuum shell model automatically reduces to the standard version. As seen from Table I, for the bound states our seniority restricted calculation is in a good agreement with exact diagonalization. The fact that the pairing-based variational calculation is a good approximation for neutron-rich isotopes is not new and has been discussed earlier [30]. One has to mention also that the seniority truncation introduces an additional quasispin symmetry that prohibits certain decays, and thus sets the corresponding widths to zero.

Despite numerous oversimplifications related to the seniority truncation, limitations on the configuration mixing, and restrictions on possible decay channels and final states, the overall agreement observed in Table I is quite good. The results where experimental data are not available can be considered as predictions. The seniority truncation can be avoided by a full diagonalization that is possible for such a small system. For heavier nuclei one has no possibility of the full diagonalization even within the standard shell model for the discrete spectrum. Then the method of treating only pairing and continuum becomes a valuable starting point. Many physical questions, such as validity of the single-particle assumption for the operator W, possibility of correlated twonucleon emission, or sharp changes in nuclear shape or structure in the reactions, were left outside the scope of this discussion. In the case of spherical oxygen isotopes with only one particle-unstable orbital, the present approach seems to be reasonable. Furthermore, in our view the main merit of this calculation is in demonstrating the fully selfconsistent solution and the power of the method.

VII. CONCLUSIONS

We made an attempt to advance in the development of methods related to the continuum shell model. Although the main ideas of the approach are known for a long time, right now it seems to be an appropriate moment to revive them and convert into a working tool for the solution of numerous practical problems of nuclear, and supposedly more general manybody, theory. In all cases where a quantum system of strongly interacting particles is loosely bound, the interplay of the continuum and intrinsic structure is getting crucial. Therefore the formalism that would allow for a unified description of inter-related structure and reaction aspects is especially needed, and extensive search in this direction made during recent years clearly reveals this need.

Within the discussion presented in this work, we demonstrated some of the features appearing in the loosely bound nuclear systems that undergo one- and two-body decays, and we outlined the path for solving the corresponding manybody problems. The residual interaction we used was limited by the pairing and monopole part. The pairing approximation is known to work well within the traditional shell model [30] for nuclei with one kind of valence nucleons. The restriction to pairing leads to significant simplifications, both for structure and reactions parts of the problem, revealing the generic trends. The inclusion of all interactions is technically possible and should be done in the future. We stressed the importance of the correct account for threshold singularities of the amplitudes at low energies and associated with that behavior of the cross sections. The requirements of selfconsistency are crucial in (i) regular solution for the complex energies of quasistationary states governed by the energydependent Hamiltonian and (ii) determination of bound state energies, open channels, and reaction thresholds for a chain of nuclides connected by those channels. We have shown that all these features can be satisfied in practical calculations. The continuum treatment almost certainly requires new computational efforts and the employed here hybrid of the exact solution for the pairing interaction, with the interaction through the continuum seems to be a promising instrument for future development.

The main theoretical problem that was not discussed above is related to the residual interaction necessary for the very formulation of the shell-model problem in the presence of the continuum. In principle, the effective interaction should be energy dependent and complex; it has to be consistent with the rest of the shell-model input, including the amplitudes of the coupling to closed and open channels. This is a serious challenge for the future, which requires a new insight into the whole physics on the borderline between structure and reactions.

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