Gamow Shell Model Description of Neutron-Rich Nuclei

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This work presents the first continuum shell-model study of weakly bound neutron-rich nuclei involving multiconfiguration mixing. For the single-particle basis, the complex-energy Berggren ensemble representing the bound single-particle states, narrow resonances, and the nonresonant continuum background is taken. Our shell-model Hamiltonian consists of a one-body finite potential and a zero-range residual two-body interaction. It is demonstrated that the residual interaction coupling to the particle continuum is important; in some cases, it can give rise to the binding of a nucleus.

The microscopic structure of exotic nuclei near the particle drip lines is a topic of great current interest in low-energy nuclear physics. Apart from theoretical and experimental nuclear structure interest, calculations for nuclei far from stability have astrophysical implications, especially in the context of stellar nucleosynthesis. What makes this subject particularly challenging is the weak binding, hence the closeness of the particle continuum.

There are many factors which make the coupling to the particle continuum important. First, even for a bound nucleus, there appears a virtual scattering into the phase space of unbound states. Although this process involves intermediate scattering states, the correlated bound states must be particle stable; i.e., they have zero width. Second, the properties of unbound states, i.e., above the particle (or cluster) threshold directly reflect the continuum structure. In addition, continuum coupling directly affects the effective nucleon-nucleon interaction.

The treatment of continuum states is an old problem which, in the context of excited states near or above the decay threshold, has been a playground of the continuum shell model (CSM) [1]. In the CSM, including the recently developed shell model embedded in the continuum (SMEC) [2], the scattering states and the bound states are treated on an equal footing. So far, most applications of the CSM, including SMEC, have been used to describe situations in which there is coupling to one-nucleon decay channels. However, by allowing only one particle to be present in the continuum, it is impossible to apply the CSM to "Borromean systems" for which A- and $(A-2)$-nucleon systems are particle stable but the intermediate $A-1$ system is not.

The reason for limiting oneself to only one particle in the continuum in the CSM has been twofold. First, the number of scattering states needed to properly describe the underlying dynamics can easily go beyond the limit of what present computers can handle. Second, treating the continuum-continuum coupling, which is always present

when two or more particles are scattered to unbound levels, is difficult. There have been only a few attempts to treat the multiparticle case [3] and, unfortunately, the proposed numerical schemes, due to their complexity, have never been adopted in microscopic calculations involving multiconfiguration mixing. Consequently, an entirely different approach is called for. In this work, we formulate and test the multiconfigurational shell model in the complete Berggren basis. The resulting Gamow shell model (GSM) is then applied to systems with two valence neutrons.

The Gamow states (sometimes called Siegert or resonant states) [4] are generalized eigenstates of the time-independent Schrödinger equation with complex energy eigenvalues $E = E_0 - i\Gamma/2$, where Γ stands for the decay width (which is zero for bound states). These states correspond to the poles of the S matrix in the complex energy plane lying on or below the positive real axis; they are regular at the origin and satisfy a purely outgoing asymptotics. In the following, we consider the Gamow states of a one-body spherical finite potential. The single-particle (s.p.) basis of Gamow states must be completed by means of a set of nonresonant continuum states. This completeness relation, introduced by Berggren [5], reads

$$\sum_n |\phi_{nj}\rangle\langle\tilde{\phi}_{nj}| + \frac{1}{\pi} \int_{L_+} |\phi_j(k)\rangle\langle\phi_j(k^*)| \, dk = 1, \quad (1)$$

where ϕ_{nj} are the Gamow states carrying the s.p. angular momentum j, n stands for all the remaining quantum numbers labeling Gamow states, $\phi_j(k)$ are the modified scattering Gamow states, and the contour L_+ in the complex k plane has to be chosen in such a way that all the poles in the discrete sum in Eq. (1) are contained in the domain between L_+ and the real energy axis. If $u_{nj}(r)$ stands for the radial part of ϕ_{nj}, then $\tilde{u}_{nj}(r) = u_{nj}(r)^*$ and $\tilde{\phi}_{nj} = \phi_{nj}(u \rightarrow \tilde{u})$. If the contour L_+ is chosen reasonably close to the real energy axis, the first term in (1) represents the contribution from bound states and narrow

resonances while the integral part accounts for the nonresonant continuum. A number of completeness relations similar to (1) were studied by Lind [6].

There have been several applications of resonant states to problems involving continuum [7], but in most cases the so-called *pole expansion,* neglecting the contour integral in Eq. (1), was used [8]. The importance of the contour contribution was investigated in Refs. [9,10] in the context of the continuum RPA with separable particle-hole interactions where it was concluded that the nonresonant part must be accounted for if one aims at a quantitative description. This can be achieved by discretizing the integral in Eq. (1) [11]. In our work we use the quadrature based on the four-point interpolation.

In our study, Gamow states are determined using the generalized shooting method for bound states which requires an exterior complex scaling [7]. The numerical algorithm for finding Gamow states for any finite-depth potential $U(r)$ has been tested on the example of the Pöschl-Teller-Ginocchio (PTG) potential [12], for which the resonance energies and wave functions are known analytically. Energies of all PTG resonances with a width of up to 90 MeV are reproduced with a precision of at least 10^{-6} MeV. The antisymmetric two-particle wave functions $|\phi_{i_1}^{(1)} \phi_{i_2}^{(2)}\rangle_J$ are obtained in the usual way by coupling the s.p. wave functions of the considered bound, resonance, and scattering Gamow states labeled by subscripts i_1, i_2 to the total angular momentum J. The completeness relation for two-particle states,

$$\sum_{i_1,i_2} |\phi_{i_1}^{(1)} \phi_{i_2}^{(2)}\rangle_J \, _J\langle\phi_{i_1}^{(1)} \phi_{i_2}^{(2)}| \simeq 1 \qquad (2)$$

can be used to calculate the two-body matrix elements. The radial integrals entering the Hamiltonian matrix elements were regularized separately by an appropriate choice of the angle of the external complex scaling. The resulting (complex symmetrix) Hamiltonian matrix can be diagonalized using standard methods.

In most applications, one is interested in bound or resonance N-body states but not in nonresonant continuum. Bound states can be clearly identified, because the imaginary part of their energy must be zero. No equally simple criterion exists for resonance or scattering states. On the other hand, the coupling between scattering states and resonant states is usually weak, so one can determine the resonances using the following two-step procedure. In the first step, the shell-model Hamiltonian is diagonalized in both (i) the full space including the contour and (ii) the subspace of Gamow states (pole expansion). In the second step, one identifies the eigenstates of (i) which have the largest overlap with those of the second diagonalization. For the case of two valence particles discussed in this work, one can include in the basis up to 50 states in the nonresonant scattering continuum.

In the following exploratory GSM calculations, we consider two cases: (i) ^{18}O with the inert ^{16}O core and two

active neutrons in the sd shell and (ii) ^{6}He with the inert ^{4}He core and two active neutrons in the p shell. Our aim is not to give the precise description of ^{18}O and ^{6}He (for this, one would need a realistic Hamiltonian and a larger configuration space) but rather to illustrate the method, its basic ingredients, and underlying features.

The "^{18}O" *case.*—The s.p. basis was generated by a Woods-Saxon (WS) potential with the radius $R_0 = 3.05$ fm, the surface diffuseness $d = 0.65$ fm, the potential depth $U_0 = -55.8$ MeV, and the strength of the spin-orbit term $U_{so} = 6.06$ MeV. With this choice of parameters, the single-particle $0d_{5/2}$ and $1s_{1/2}$ states are bound, with s.p. energies -4.14 MeV and -3.27 MeV, respectively, and $0d_{3/2}$ is a resonance with the s.p. energy $0.9 - i0.97$ MeV. Energies of these s.p. states are close to the s.p. states of ^{17}O.

The completeness relation requires taking the $s_{1/2}$, $d_{5/2}$, and $d_{3/2}$ nonresonant continuums. For the $1s_{1/2}$ and $0d_{5/2}$ bound states, their nonresonant continuums can be chosen along the real momentum axis. Since, to the first order, the inclusion of these continuums should result only in the renormalization of the effective interaction, they are ignored for the purpose of the present exercise whose main focus is the neutron emission. On the contrary, $0d_{3/2}$ is a resonance state, so the associated contour has to be complex to produce the correct energy width. The contour L_+ representing the $d_{3/2}$ continuum was chosen to consist of three straight segments connecting the points $k_1 = 0 - i0$, $k_2 = 0.3 - 0.2i$, $k_3 = 0.5 - i0$, and $k_4 = 2.0 - i0$ (all in fm^{-1}). The strength of the δ force was taken to be $V_0 = -350$ MeV fm^3.

The completeness of the Gamow basis depends on the number of discretized scattering basis states considered. Table I illustrates this dependence. The real part of energy represents the binding energy of a state with respect to the ^{16}O core, i.e., the two-neutron separation energy. For the resonance states, the real and imaginary parts of energy do not change much by increasing the number of scattering states. On the other hand, bound states acquire a very small *negative* width which does not exceed several keV. This spurious negative width depends strongly on the basis size, and the convergence to zero is both slow and nonmonotonic. The presence of a small and negative width is a feature of particle-bound states obtained in the GSM. The results displayed in Table I show that only about 10–20 vectors in the scattering continuum are sufficient to keep the error of calculated energies and widths at the acceptable level. It is also clear that the "pole approximation" (inclusion of no scattering states) gives a rather poor description of bound and near-threshold states, while it works fairly well for high-lying states carrying a sizable width. In this respect, this result is consistent with the conclusions of Refs. [9,10].

In the considered example, the calculated one-neutron threshold is -4.142 MeV ($0d_{5/2}$ energy) while the two-neutron threshold is at zero (the binding energy of the core). Consequently, few states shown in Table I are

TABLE I. Dependence of energies (left number, in MeV) and neutron widths (right number, in keV) of calculated states in ^{18}O on the number of discretized scattering basis states along the contour L_+.

J_π	0 states	10 states	30 states	50 states
		Bound states		
0_1^+	$-11.73, -131$	$-12.11, -2.91$	$-12.12, 0.27$	$-12.12, 0.21$
2_1^+	$-9.20, -26.37$	$-9.24, -0.51$	$-9.24, -0.031$	$-9.24, -0.032$
4_1^+	$-8.64, -13.51$	$-8.64, -0.25$	$-8.64, -0.004$	$-8.64, -4 \times 10^{-4}$
0_2^+	$-7.66, -1.08$	$-7.66, -0.324$	$-7.66, -0.264$	$-7.66, -0.260$
2_2^+	$-7.85, -4.64$	$-7.86, -0.167$	$-7.86, -0.066$	$-7.86, -0.049$
		Resonances		
4_2^+	$-4.00, -89.8$	$-4.03, -8.15$	$-4.04, 0.54$	$-4.04, 0.54$
2_3^+	$-3.48, 29.08$	$-3.48, 43.08$	$-3.49, 44.65$	$-3.49, 44.65$
2_4^+	$-2.60, 46.45$	$-2.61, 55.82$	$-2.61, 57.02$	$-2.61, 57.04$
0_3^+	$1.05, -172$	$0.94, -18.64$	$0.94, 0.82$	$0.94, 0.76$
2_5^+	$1.63, 112.4$	$1.64, 111.9$	$1.63, 117.5$	$1.63, 118.5$

two-neutron bound but one-neutron unstable, e.g., the calculated width, 57 keV, of the $J^\pi = 2_4^+$ state at $E_0 = -2.61$ MeV characterizes single neutron emission from this state. The higher-lying states shown in Table I are unstable with respect to both one- and two-neutron emission.

In order to illustrate the configuration mixing induced by the two-body interaction in the GSM, Table II shows the complex squared shell-model amplitudes calculated for the bound (0_1^+ and 2_1^+) and resonance (2_3^+) states in ^{18}O. All eigenstates are normalized according to Berggren [5,6]: $\sum_n c_n^2 = 1$. One should notice that—contrary to the conventional SM case—no modulus square appears in the normalization. This implies that the probabilistic interpretation of c_n must be generalized [5,13]; i.e., when computing expectation values the real part of c_n^2 should be associated with the mean value while the imaginary part represents the uncertainty due to the decaying nature of the state. As seen in Table II, the contribution from the nonresonant continuum plays a different role compared to that from the resonant states. First, it is generally smaller than the leading components involving resonant orbits, though in the example shown in Table II the contribution of the $0d_{3/2}$ resonance is similar in magnitude. Second, according to our calculations, the inclusion of the contour primarily affects the imaginary part. Finally, the

contribution from two particles in the nonresonant continuum, $L_+^{(2)}$, even though smaller than the one-particle contribution, $L_+^{(1)}$, is not negligible.

The "^{6}He" case.— A description of the Borromean nucleus ^{6}He is a challenge for the GSM. ^{4}He is a well-bound system with the one-neutron emission threshold at 20.58 MeV. On the contrary, the nucleus ^{5}He, with one neutron in the p shell, is unstable with respect to the neutron emission. Indeed, the $J^\pi = 3/2_1^-$ ground state of ^{5}He lies 890 keV above the neutron emission threshold and its neutron width is large, $\Gamma = 600$ keV. The first excited state, $1/2_1^-$, is a very broad resonance ($\Gamma = 4$ MeV) that lies 4.89 MeV above the threshold. ^{6}He, on the contrary, is bound with the two-neutron emission threshold at 0.98 MeV and one-neutron emission threshold at 1.87 MeV. The first excited state 2_1^+ at 1.8 MeV in ^{6}He is neutron unstable with a width $\Gamma = 113$ keV. In our GSM calculations, the states in ^{5}He are viewed as one-neutron resonances outside of the ^{4}He core. A good fit to $3/2_1^-$ and $1/2_1^-$ states in ^{5}He is obtained by taking the WS potential with $R_0 = 2.0$ fm, $d = 0.65$ fm, $U_0 = -47.0$ MeV, and $U_{so} = 7.5$ MeV. With this potential, one finds the single-neutron resonances $p_{3/2}$ and $p_{1/2}$ at $E = 0.745 - i0.32$ MeV and $E = 2.13 - i2.94$ MeV, respectively. The s.p. basis has been restricted to the

TABLE II. Squared amplitudes of different configurations in 0_1^+, 2_1^+, and 2_3^+ states of ^{18}O. The sum of squared amplitudes of all Slater determinants including one and two particles in the nonresonant continuum are denoted by $L_+^{(1)}$ and $L_+^{(2)}$, respectively. 50 discretized scattering states were used.

c^2	0_1^+	2_1^+	2_3^+
$1s_{1/2}^2$	$0.05 - i9.1 \times 10^{-6}$	$\cdots$	$\cdots$
$0d_{5/2}^2$	$0.91 - i6.1 \times 10^{-6}$	$0.86 + i1.2 \times 10^{-5}$	$6.9 \times 10^{-3} - i5.3 \times 10^{-4}$
$0d_{3/2}^2$	$0.02 - i5.3 \times 10^{-3}$	$1.9 \times 10^{-3} - i4.4 \times 10^{-4}$	$1.6 \times 10^{-3} - i5.2 \times 10^{-4}$
$1s_{1/2}0d_{5/2}$	$\cdots$	$0.13 - i1.2 \times 10^{-5}$	$4.5 \times 10^{-3} - i3.6 \times 10^{-4}$
$1s_{1/2}0d_{3/2}$	$\cdots$	$4.6 \times 10^{-3} - i5 \times 10^{-4}$	$0.03 - i4.9 \times 10^{-3}$
$0d_{5/2}0d_{3/2}$	$\cdots$	$7.7 \times 10^{-3} - i8.4 \times 10^{-4}$	$0.96 + i4.5 \times 10^{-3}$
$L_+^{(1)}$	$1.3 \times 10^{-2} + i3.8 \times 10^{-3}$	$2.5 \times 10^{-3} + i1.7 \times 10^{-3}$	$-1.2 \times 10^{-3} + i1.7 \times 10^{-3}$
$L_+^{(2)}$	$3.4 \times 10^{-3} + i1.5 \times 10^{-3}$	$1.6 \times 10^{-4} + i9.9 \times 10^{-5}$	$5.5 \times 10^{-5} + i4.3 \times 10^{-5}$

TABLE III. Same as in Table II, except for 0_1^+ and 2_1^+ states in ^{6}He.

c^2	0_1^+	2_1^+
$0p_{3/2}^2$	$0.95 - i0.79$	$1.011 + i0.0044$
$L_+^{(1)}$	$0.11 + i0.76$	$-0.011 - i0.0049$
$L_+^{(2)}$	$-0.06 + i0.03$	$-1.3 \times 10^{-4} + i4.8 \times 10^{-4}$

$0p_{3/2}$ resonance state and the $p_{3/2}$ nonresonant continuum. [The $0p_{1/2}$ resonance is very broad and cannot be included in a meaningful way in the discrete sum in Eq. (1). Consequently, following the reasoning applied to the ^{18}O case, the $p_{1/2}$ contour along the real k axis has been ignored.] The L_+ contour for the nonresonant $p_{3/2}$ continuum is chosen to enclose the $0p_{3/2}$ resonance: $k_1 = 0 - i0$, $k_2 = 0.2 - 0.2i$, $k_3 = 0.5 - i0$, and $k_4 = 2.0 - i0$ fm^{-1}. The strength of the δ force was taken to be $V_0 = 650$ MeV fm^3. The number of points used to discretize the scattering continuum is 50, though even with 15 points the results are reasonably stable. With this precision, we reproduce the most important feature of ^{6}He: *the ground state is particle-bound, despite the fact that all the basis states lie in the continuum.* Table III shows the structure of wave functions of 0_1^+ and 2_1^+ states in ^{6}He. The important contribution from the nonresonant continuum is seen, even for the 0_1^+ ground state which is particle stable. In spite of a very crude Hamiltonian, the neglect of the exact three-body asymptotics, etc., the calculated ground state energy $E = -0.951 - i0.01$ MeV reproduces surprisingly well the experimental ground state energy with respect to the two-neutron emission threshold. The excited state 2_1^+ is predicted to lie at 2.25 MeV, slightly above the experimental value, and its width $\Gamma = 700$ keV which depends sensitively on the position of the state with respect to the emission threshold is somewhat too high as well.

In conclusion, the complex-energy Berggren ensemble is applied for the first time in shell-model calculations for two-neutron states near the particle-emission threshold. In addition to the successful inclusion of the continuum-continuum coupling, we succeeded in solving another principal problem of the GSM, i.e., the treatment of the nonresonant part of the continuum. Another problem which has been solved in our work is the selection of physical states. As a result of the GSM diagonalization, one obtains a multitude of states corresponding to the many-body continuum, some being resonances and some representing the nonresonant background. Our Letter gives a simple and workable prescription on how to identify the resonance states.

The results of the calculations are very encouraging. It is seen that the contribution from the nonresonant continuum is important, especially for bound and near-threshold states. For instance, pairing correlations due to the continuum-continuum scattering can bind the ground state

of ^{6}He with a completely unbound basis provided by the s.p. resonances of ^{5}He. This also demonstrates that calculations in the spirit of the pole expansion cannot be applied if one aims at the shell-model accuracy.

The particle-bound states calculated in the GSM are characterized by small and (usually) negative width which show nonmonotonic behavior as a function of the basis size. According to our experience, only about 10–20 vectors in the scattering continuum are sufficient to keep the error of calculated energies and widths at an acceptable level.

Very recently, we succeeded in performing GSM calculations in the many-particle case. For instance, for the sequence of ^{19,20,21}O the predicted S_{1n} values are -4.07, -7.55, and -3.95 MeV, respectively, in reasonable agreement with the data. The calculated neutron emission widths in these isotopes become positive for states above the predicted one-neutron threshold, as expected. Further applications of the GSM are in progress [14].

Noted added.—Recently, Id Betan *et al.* applied Berggren basis to two-particle resonant states; see Ref. [15].

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