ADVANCES IN THE SHELL-MODEL DESCRIPTION OF WEAKLY BOUND AND UNBOUND NUCLEAR STATES*

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We report on recent advances in the description of weakly bound and unbound nuclear states using either a real ensemble representing (quasi-)bound single-particle states and non-resonant continuum states (the so-called Shell Model Embedded in the Continuum) or a complex Berggren ensemble representing bound single-particle states, decaying resonant states, and non-resonant continuum states (the so-called Gamow Shell Model). These two different strategies in formulating the multiconfigurational Continuum Shell Model are illustrated by showing how the non-resonant continuum impacts the mechanism of nuclear binding.

1. Introduction

The major thoretical challenge in the microscopic description of weakly bound nuclei is the rigorous treatment of both the many-body correla-

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tions and the continuum of positive-energy states and decay channels. A fully symmetric description of the interplay between scattering states, resonances and bound states in the many-body wave function requires a close interplay between methods of nuclear structure and nuclear theory. This mutual cross-fertilization, which cannot be accomplished without overcoming a traditional separation between nuclear structure and nuclear reaction methods, is a splendid opportunity for opening a new era in the nuclear theory of loosely bound systems. Many traditional approaches of nuclear theory, including the standard shell model and the pairing theory, must be modified to include an explicit coupling between bound states and continuum. Weakly bound states or resonances cannot be described within the closed quantum system formalism. For bound states, there appears a virtual scattering into the continuum phase space involving intermediate scattering states. Continuum coupling of this kind affects also the effective nucleon-nucleon interaction. For unbound states, the continuum structure appears explicitly in the properties of those states.

The impact of the particle continuum was discussed in the early days of the multiconfigurational SM in the middle of the last century. However, thanks to the success of the 'standard' SM in terms of interacting nucleons assumed to be *perfectly isolated* from an *external environment* of scattering states, the continuum-related matters had been swept under the rug. An example of a problem is the so-called Thomas-Ehrman shift [1] appearing in, e.g., the mirror nuclei ^{13}C, ^{13}N, which is a salient effect of a coupling to the continuum depending on the position of the respective particle emission thresholds. The mathematical formulation of the problem of nuclear states embedded in the continuum of decay channels goes back to Feshbach [2], who introduced the two subspaces containing the discrete (Q subspace) and scattering (P subspace) states. Feshbach succeeded in formulating a unified description of nuclear reactions for both direct processes in the short-time scale and compound nucleus processes in the long-time scale. A unified description of nuclear structure and nuclear reaction aspects is much more complicated and became possible in realistic situations only at the end of the last century (see Ref. [3] for a recent review).

In the recently developed Shell Model Embedded in the Continuum (SMEC), all coupling matrix elements between different discrete states, different scattering states, as well as between discrete and scattering states, are calculated using the realistic effective SM interaction. The many-body system is described by an effective non-hermitian Hamiltonian $\mathcal{H}$ that cosists of two terms: (i) the Hamiltonian matrix of the closed system with discrete eigenstates, and (ii) the coupling matrix between the system and its environment[a]. The eigenvalues of $\mathcal{H}$ are complex and correspond to the poles of the scattering (S) matrix.

Different continuum shell model approaches, including SMEC, are based on the completeness of an one-particle basis consisting of bound orbits and a *real* continuum. After removing the scattering tails, the single-particle (s.p.) resonances are included in Q whereas their tails are fully incorporated in P [5]. Hence, in corresponding configuration-mixing calculations, the resonances resemble bound orbits. On the other hand, in certain situations (e.g., $0p_{3/2}$, $0p_{1/2}$ s.p. orbits outside of the ^{4}He core, or the $0d_{3/2}$ orbit outside of the ^{16}O core) one wants to use broad resonances as physical building blocks in the configuration-mixing calculations. Here, the original two-subspace approach of Feshbach is not very useful and another strategy is needed. Recently, the multiconfigurational SM in the complete Berggren basis, the so-called Gamow Shell Model (GSM), has been formulated [6]. The s.p. basis of GSM is given by the Berggren ensemble [7] which contains Gamow states (or resonant states[b]) and the (complex) non-resonant continuum. One may see here a two-subspace concept of Feshbach reappearing, with the subspace Q_B consisting of the Gamow states in the complex energy plane, and the subspace P_B containing the non-resonant continuum. In the GSM framework, the number of particles in the scattering continuum is not predetermined, but it results from a variational calculation in the Hilbert space spanned by all Slater determinants in Q_B and P_B subspaces. Hence, GSM can also be applied to Borromean systems for which A- and $(A-2)$-nucleon systems are particle-stable but the intermediate $(A-1)$-system is not. GSM is a natural generalization of the SM concept for the open quantum systems. And, as such, it is a tool *par excellence* for nuclear structure studies. A description of many-body wave functions at large distances, as needed in nuclear reaction studies, even though feasible within the GSM formalism, may be rather cumbersome. For that purpose, the coupled-channel method used in SMEC to describe the asymptotic channels is far more accurate.

[a] In SMEC, the description of the environment is simplified and includes one-nucleon decay channels only. A more complete description is technically cumbersome, though it has been developed for the purpose of two-proton decay studies [4].

[b] The resonant states are the generalized eigenstates of the time-independent Schrödinger equation which are regular at the origin and satisfy purely outgoing boundary conditions. They correspond to the poles of the S matrix in the complex energy plane lying on or below the positive real axis.

2. SMEC and Binding Energy Systematics in Oxygen and Fluorine Isotopes

As one approaches the particle drip lines, the amount of spectroscopic information concerning bound states becomes very scarce. Hence, to extract nuclear structure data, one relies on the analysis of decaying states and reaction dynamics. For that purpose, SMEC - which gives a unified description of the energy spectra, including nucleon emission widths and electromagnetic transition probabilities, as well as the reactions involving one nucleon in the continuum [8] - provides an adequate theoretical framework. Below, we shall discuss the generic features of the coupling to the particle continuum on the example of binding energy systematics.

The detailed description of the SMEC formalism has been given elsewhere [8,3]. Localized many-body states in Q are obtained by solving the standard SM problem for the Hamiltonian H_{QQ}. P contains asymptotic channels made of $(A-1)$-particle localized states and one nucleon in the scattering state. The residual coupling H_{PQ} between states in Q and P is given by the zero-range interaction $V_{12} = -V_0^{(12)}[\alpha + \beta P_{12}^{\sigma}]\delta(\mathbf{r}_1 - \mathbf{r}_2)$, where $\alpha + \beta = 1$ and P_{12}^{σ} is the spin exchange operator. An effective SM Hamiltonian including the coupling to the continuum is energy-dependent:

$$\mathcal{H}(E) = H_{QQ} + H_{QP}G_P^{(+)}(E)H_{PQ} \quad , \tag{1}$$

where $G_P^{(+)}(E)$ is a Green function for the motion of a single nucleon in the P subspace. The energy scale is settled by the one-nucleon emission threshold $E^{(\mathrm{thr})}$ [3]. For $E > E^{(\mathrm{thr})}$, $\mathcal{H}$ is a complex-symmetric matrix, while it is hermitian for $E < E^{(\mathrm{thr})}$. In the present studies, we use the full sd valence space for $N < 20$ and the full pf space for $N > 20$. For H_{QQ}, we take the USD interaction in the sd shell [9] and the KB$'$ interaction in the pf shell [10]. The cross-shell interaction is given by the G-matrix [11]. The ground state (g.s.) continuum coupling correction to the binding energy is calculated in SMEC as [12] :

$$E_{\mathrm{corr}} = \langle \Phi_{\mathrm{g.s.}} | \mathcal{H} - H_{QQ} | \Phi_{\mathrm{g.s.}} \rangle. \tag{2}$$

The g.s. wave function in the parent nucleus (N, Z) is coupled to different channel wave functions, which are determined by the motion of an unbound neutron relative to the daughter nucleus $(N-1, Z)$ in a certain SM state $\Phi_i^{(N-1)}$. *All* asymptotic channels composed of SM states are included in our calculations.

Figure 1 shows the neutron number dependence of E_{corr} in oxygen isotopes for (i) $E_n^{(\mathrm{thr})}$ of SMEC (solid line), and for (ii) $E_n^{(\mathrm{thr})}$ fixed arbi-

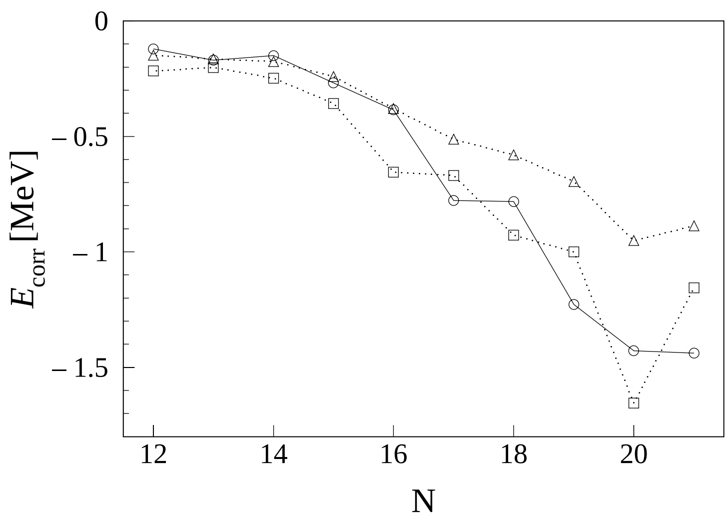

Figure 1. Neutron number dependence of the SMEC energy correction (2) to the SM g.s. energy. The solid line is obtained for one-neutron emission threshold $E_n^{(\rm thr)}$ calculated in SMEC for each nucleus. The dotted line with squares and triangles is obtained for $E_n^{(\rm thr)}$ which is fixed arbitrarily at 0 and 4 MeV, respectively (from Ref. [12]).

trarily at 0 or 4 MeV [c]. The N-dependence of $E_{\rm corr}$ exhibits approximately quadratic behavior with the number of valence neutrons; this is characteristic of a monopole Hamiltonian. Deviations from this dependence reflect the continuum coupling. For $E_n^{(\rm thr)} = 0$ (a one-neutron drip-line limit), there appears an odd-even staggering (OES) around an average N-dependence. A blocking of the virtual scattering to the particle continuum by an odd nucleon diminishes the continuum correction to the binding energy of odd-N nuclei. This "drip-line effect" is restricted to a narrow range of excitation energies around $E_n^{(\rm thr)} = 0$ and vanishes for $E_n^{(\rm thr)} = 4$ MeV. For the values of $E_n^{(\rm thr)}$ calculated in SMEC, one finds an inverted OES with enhanced $E_{\rm corr}$ for odd-N isotopes. This is because $E_n^{(\rm thr)}$ in an odd-N nucleus is smaller than in the even-N neighbors. This continuum coupling effect leads to an attenuation of OES of one-neutron separation energies S_n in nuclei close to the neutron dripline [12].

Figure 2 shows the neutron number dependence of $E_{\rm corr}$ for fluorine

[c] In our model space for the oxygens, the continuum coupling contains the neutron-neutron ($T = 1$) part only. The strength $V_0^{(nn)} = 414$ MeV·fm^3 yields a good overall agreement with the spectra of oxygen isotopes.

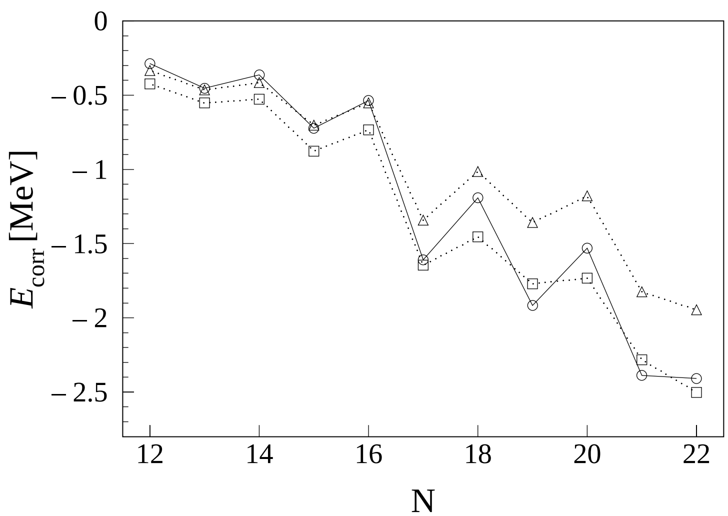

Figure 2. The same as in Fig. 1 except for the fluorine isotopes.

isotopes. The neutron-proton residual coupling strength has been taken as $V_0^{(np)} = (1/2)V_0^{(nn)}$. (In fluorine isotopes, both neutron-neutron ($T = 1$) and neutron-proton ($T = 0, 1$) couplings between states in Q and P are present. The nn-coupling has been adjusted to the oxygen isotope chain.) The value of $E_{\rm corr}$ depends both on $|N_p - N_n|$ and $(N_p + N_n)$ (cf. Figs. 1 and 2), where N_p and N_n is the number of valence protons and neutrons, respectively. The three cases displayed in Fig. 2 can be directly compared with those of Fig. 1. For $E_n^{(\rm thr)} = 4$ MeV, one can see the OES which is absent in the oxygen chain. This is an effect of the np-coupling. $E_{\rm corr}$ in odd-odd isotopes is increased as compared to the neighboring odd-even ones. The size of $E_{\rm corr}$ in this case depends weakly on $E_n^{(\rm thr)}$. Qualitatively, a similar effect can also be seen at the neutron drip line ($E_n^{(\rm thr)} = 0$ in Fig. 2), but the OES due to the np-coupling is now attenuated by the nn-coupling (cf. Fig. 1) which gives rise to the opposite OES. For the values of $E_n^{(\rm thr)}$ calculated in SMEC, the OES is enhanced due to the combined effects of the np-continuum coupling (which weakly depends on $E_n^{(\rm thr)}$) and the nn-continuum coupling (which closely follows the OES of $E_n^{(\rm thr)}$). These two effects act 'in phase', enhancing the binding of odd-N nuclei and strongly attenuating the OES of S_n.

2.1. *Threshold dependence of the continuum energy correction*

In this section, we shall analyze the generic features of the SMEC energy correction to an SM eigenstate. If one neglects external and channel-channel couplings, then the continuum correction to the (closed system) eigenenergy E_i has the form [3]:

$$E_{\mathrm{corr}}^{(i)} = \sum_c \int_0^\infty \mathrm{d}r\, {\omega_i}^{c\,(+)}(r) \cdot w_i(r) \quad , \tag{3}$$

where ${\omega_i}^{c\,(+)}(r)$ is the solution of the inhomogeneous radial equation:

$$(E - H_{cc})\, {\omega_i}^{c\,(+)}(r) = w_i(r) \quad . \tag{4}$$

Boundary conditions for ${\omega_i}^{c\,(+)}(r)$ require that it is regular at $r = 0$ and has only outgoing waves in all open channels, or it is exponentially decreasing in closed ones. In the case of one channel only, Eq. (4) has the following form :

$$\left[E + \left(\frac{\mathrm{d}^2}{\mathrm{d}\,r^2} - \frac{l\,(l+1)}{r^2}\right) - V(r)\right] {\omega_l}^{(+)}(r) = w(r) \quad . \tag{5}$$

($h^2/2m \equiv 1$, everywhere.) For simplicity, we assume a square well potential defined as $V(r) = -|V_0|$ for $r < R$ and $V(r) = 0$ otherwise. Similarly, we take the source of the simplest linear form inside the well: $w(r) = w_0\, r$, and vanishing outside. In this case, $E_{\mathrm{corr}}^{(i)}$, Eq. (3), has the upper bound at $r = R$:

$$E_{\mathrm{corr}}^{(l)} = \int_0^R \mathrm{d}r\, {\omega_l}^{(+)}(r) \cdot w_0\, r \quad . \tag{6}$$

The general solution ${\omega_l}^{(+)}(r)$ for $r < R$ can be written as :

$${\omega_l}^{(+)}(r) = A\, r\, j_l(K\, r) + \frac{w_0}{K^2} r \quad , \tag{7}$$

where $K = \sqrt{E + |V_0|}$. The normalization constant $A \equiv A(E)$ can be found by matching the above solution with the outside wave function, which, in this case, is proportional to a spherical Hankel function:

$${\omega_l}^{(+)}(r) = B\, r\, {h_l}^{(+)}(k\, r) \quad (r \geq R) \tag{8}$$

with $k = \sqrt{E}$. The normalization B does not influence the value of the integral (6). The only source of a singular behavior of $E_{\mathrm{corr}}^{(l)}(E)$ at $E \to 0$ is the function $A(E)$, because both $j_l(K\, r)$ and $1/K^2$ are analytic functions of E. This analysis can be easily generalized to the case of an arbitrary

$l \neq 0$. We have found that the $(l+1)$-th derivative of $A(E)$ is discontinuous in both real and imaginary parts. The origin of this discontinuity comes solely from the $k \rightarrow E$ transformation ($A(k)$ is analytic at $k=0$), and in the case of the square well potential, the jump in the $(l+1)$-derivative is even infinite[d].

The threshold phenomenon discussed in this section is a genuine effect of the continuum coupling for neutrons. Strong irregularities are expected in even-N systems for all those states lying close to the one-neutron emission threshold that contain a significant admixture of s- and p-partial waves. For g.s. configurations, this mechanism contributes to the attenuation of OES of S_n in oxygen and fluorine isotopes close to the neutron drip line.

3. Gamow Shell-Model Description

There exist several completeness relations involving resonant states which can be derived from the Mittag-Leffler theory. As said before, in the heart of GSM is the Berggren completeness relation [7] :

$$\sum_n |u_n\rangle\langle\tilde{u}_n| + \int_{L_+} |u_k\rangle\langle\tilde{u}_k| dk = 1, \tag{9}$$

where $|u_n\rangle$ are the Gamow states (both bound states and the decaying resonant states lying between the real k-axis and the complex contour L_+) and $|u_k\rangle$ are the scattering states on L_+. The resonant states are normalized according to the squared radial wave function and not to the modulus of the squared radial wave function. This is a consequence of the analytical continuation which is used to introduce the normalization of Gamow states. In practical applications, one has to discretize the integral in (9). Such a discretized Berggren relation is formally analogous to the standard completness relation in a discrete basis of L^2-functions and, in the same way, leads to the eigenvalue problem $H|\Psi\rangle = E|\Psi\rangle$. However, as the formalism of Gamow states is non-hermitian, the matrix H is complex symmetric. The discretized Berggren basis can be a starting point for establishing the completeness relation in the many-body case in full analogy with the standard SM in a complete (discrete) basis of L^2-functions. One obtains :

$$\sum_n |\Psi_n\rangle\langle\tilde{\Psi_n}| \simeq 1, \tag{10}$$

[d]For diffused potentials, the jump is finite and it vanishes if the Coulomb potential is present, i.e., for protons.

where $|\Psi_n\rangle \equiv |\phi_1 \cdots \phi_N\rangle$ are the N-body Slater determinants, and $|\phi_m\rangle$ are the resonant (bound and decaying) and scattering (contour) s.p. states. The approximate equality in Eq. (10) is a consequence of the continuum discretization. As in the case of s.p. Gamow states, the normalization of Gamow-Slater determinants is given by the squares of SM amplitudes :

$$\sum_n c_n^2 = 1 \tag{11}$$

and not by the squares of their absolute values.

3.1. *GSM Study of Helium Isotopes*

A description of neutron-rich helium isotopes, including Borromean nuclei ^{6,8}He, is a challenging theoretical problem. The nucleus ^{4}He is a well-bound system with the one-neutron emission threshold at 20.58 MeV. On the contrary, the nucleus ^{5}He is a broad resonance. The nucleus ^{6}He, which consists of two neutrons outside ^{4}He, is bound with the two-neutron emission threshold at 1.87 MeV. The first excited 2_1^+ state in ^{6}He at 1.8 MeV is neutron unstable with a width $\Gamma = 113$ keV. In our GSM calculations, the s.p.

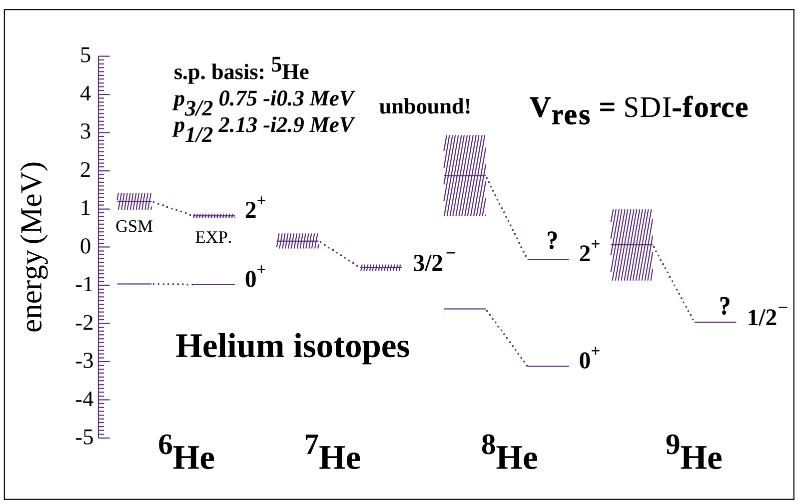

Figure 3. Experimental (EXP) and calculated (GSM) binding energies of $^{6-9}$He as well as energies of $J^\pi = 2^+$ states in ^{6}He and ^{8}He. The resonance widths are indicated by shading. The energies are given with respect to the core of ^{4}He.

configuration space includes both resonances $0p_{3/2}$, $0p_{1/2}$ and the two associated complex continua $p_{3/2}$ and $p_{1/2}$ which are discretized with 5 points each. Figure 3 shows the lowest energy states of helium isotopes calculated with the surface delta interaction with the strength $V_{SDI} = 1670$ MeV·fm^3. The $0p_{3/2}$, $0p_{1/2}$ s.p. resonances are generated by a Woods-Saxon potential with the parameters chosen to reproduce experimental energies and widths of the $3/2^-_1$ and $1/2^-_1$ resonances of ^{5}He.

It is found that the non-resonant continuum contributions are *always essential* and, in some cases (e.g., ^{8,9}He), they dominate the structure of the g.s. wave function. Moreover, the wave function components having many neutrons in the non-resonant continuum give an essential contribution to the binding energy. Without the non-resonant (contour) states, the predicted g.s. energy of ^{8}He is +2.08 MeV. The inclusion of scattering states lowers the binding energy to −1.6 MeV (sic!). GSM calculations reproduce the most important feature of ^{6,8}He: *the ground state is particle bound, despite the fact that all the basis states lie in the continuum.*

The odd-N isotopes of ^{7,9}He are calculated to be wide neutron resonances. The neutron separation energy anomaly, i.e., the *increase* of one-neutron separation energy when going from ^{6}He to ^{8}He, is reproduced. This anomaly is explained in GSM by a large contribution from non-resonant continuum states. This generic mechanism, expected to be present in loosely bound systems, may give rise to the formation of multineutron Borromean systems, changing the *drip line* into a porous *drip zone*.

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