Shell Model Embedded in the Continuum for Binding Systematics in Neutron-Rich Isotopes of Oxygen and Fluor

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Continuum coupling correction to binding energies in the neutron rich oxygen and fluorine isotopes is studied using the Shell Model Embedded in the Continuum. We discuss the importance of different effects, such as the position of one-neutron emission threshold, the effective interaction or the number of valence particles on the magnitude of this correction.

PACS number(s): 21.60.Cs, 23.40.-s, 23.40.Hc, 25.40.Lw

Nuclear structure of light neutron-rich nuclei has attracted much attention because of unusual spatial features of these nuclei and the isospin effects in the magic numbers. In this respect, the systematics of neutron separation energies \( S_n \) and interaction cross-section in \( sd \) shell region seem to indicate the disappearance of \( N = 20 \) closure and the appearance of new shell closure at \( N = 16 \) in neutron-rich nuclei with \( T_Z \geq 3 \) close to the drip-line. Another astonishing property is a large change of the neutron drip-line by adding one proton to the oxygen core, as indicate the instability of oxygen isotopes for \( N = 16, 17 \) and the stability of \( ^{31}\text{F} \) with \( N = 22 \). Theoretical description of the low-lying states properties in these nuclei requires taking into account the coupling between discrete and continuum correlated states. This aspect is particularly important near drip-line where one has to use both structure and reaction data to understand basic shell structure and dynamics of these nuclei. In weakly bound light nuclei, not only coupling of bound states to continuum is strong but also many-body correlations should be treated rigorously. Both the continuum coupling and the realistic configuration mixing can be taken into account in the Shell Model Embedded in the Continuum (SMEC). This approach provides a unified description of diverse nuclear characteristics such as the energy spectra, including nucleon emission widths and electromagnetic transition probabilities, and the reactions involving one nucleon in the continuum. In this work, we analyze in the Shell Model (SM) framework the continuum correlation to binding energies and neutron separation energies.

The detailed description of SMEC formalism has been given elsewhere. Separation of (quasi-) bound \((Q\) subspace) and scattering \((P\) subspace) states is achieved using the projection operator technique. \( P \) contains asymptotic channels made of \((A - 1)\)-particle localized states and one nucleon in the scattering state. Localized many-body states which are build up by the bound and resonance single-particle \((s.p.)\) wave functions, are included in \( Q \). They are obtained by solving standard multiconfigurational SM problem for the Hamiltonian \( H_{QQ} \). The residual coupling \( H_{PQ} \) between states in \( Q \) and \( P \) is given by \[ V_{12} = -V_{12}^{(0)}[\alpha + \beta P_{12}^{(s)}]\delta(\mathbf{r}_1 - \mathbf{r}_2), \]
where \( \alpha + \beta = 1 \) and \( P_{12}^{(s)} \) is the spin exchange operator. The effective SM Hamiltonian including the coupling to the continuum is energy-dependent: \[ H_{eff}^{QQ}(E) = H_{QQ} + H_{QP}G_P^{(E)}(E)H_{PQ}, \]
where \( G_P^{(E)}(E) \) is a Green function for the motion of single nucleon in the \( P \) subspace. \( H_{eff}^{QQ} \) is a complex-symmetric matrix above \( E_{thr} \) and Hermitian below it. The energy scale is settled by the one-nucleon emission threshold \( E_{thr} \). Radial s.p. wave functions in \( Q \) and the scattering wave functions in \( P \) are generated in a self-consistent procedure, starting with the average potential of Woods-Saxon type with the spin-orbit and Coulomb parts included, and taking into account the residual coupling. This procedure yields new orthonormalized wave functions in \( Q \) and \( P \) and new self-consistent potentials for each many-body state in \( Q \).

In the present studies we use the full \( sd \) valence space for \( N < 20 \) and the full \( pf \) shell for \( N > 20 \). For the effective interaction in \( H_{QQ} \) we take USD Hamiltonian for the \( sd \) shell and the KB interaction for the \( pf \) shell. The cross-shell interaction is the \( G \)-matrix. In the calculation of binding energies from the nuclear energies in SMEC and SM, we proceed as in Refs.

The ground state \((g.s.)\) continuum coupling correction in SMEC is calculated as: \[ E_{corr} = \Phi_{g.s.} [H_{eff}^{QQ} - H_{QQ}] \Phi_{g.s.}, \]
the g.s. wave function in 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 \( \Phi_{i}^{(N-1)} \). The magnitude of coupling matrix elements vary depending on the structure of SM wave function \( \Phi_{i}^{(N-1)} \) and the value of one-neutron emission threshold \( E_{thr} \). The individual contributions for different channel couplings tend to decrease with increasing excitation energy of a SM state \( \Phi_{i}^{(N-1)} \) due to a growing mismatch of both quantum numbers and radial properties of wave functions in parent and daughter nuclei.

This decrease is exponential on average. In the present studies, we include all asymptotic channels composed of SM states; their number vary from 3 in \(^{28}\text{O} \) to 1837...
in $^{31}$F. Even though in most nuclei these channels are closed, nevertheless the coupling to them modifies the binding energy depending both on $E_{n}^{\text{thr}}$ and the structure of the g.s. wave function.

The choice of the initial average potential follows a procedure described in Ref. [7]. We demand, that the self-consistent potentials yield the energies of s.p. states at the same position as in the average potential with Woods-Saxon central part of radius $R_0 = 1.27 A^{1/3} \text{ fm}$, depth $V_0(N,Z) = -51.1[1 \pm 0.69(N-Z)/(N+Z)] \text{ MeV}$ ($-/+$ stands for neutron/proton potential), diffuseness $a = 0.67 \text{ fm}$. The spin-orbit potential is $V_{so}(2I \cdot s)r^{-1}dr$ with $\lambda_s^2 = 2 \text{ fm}^2$, $V_{so}(N,Z) = 0.131 V_0(N,Z) \text{ MeV}$ and radial formfactor $f(r)$ of the central potential. The Coulomb potential is calculated for the uniformly charged sphere with radius $R_0$.

Fig. 1 shows results for oxygen isotopes. In our $0\hbar\omega$ description, the continuum coupling in these nuclei contains only neutron-neutron ($T = 1$) part. For the strength $V_{12}^{(n,n)}(\alpha - \beta) = 414 \text{ MeV-fm}^3$, one obtains a good overall agreement with the spectra of oxygen isotopes. For example, SMEC calculation in $^{24}$O yields the first excited state $2^+_1$ above the experimental $E_{n}^{\text{thr}}$, in agreement with the data [15]. The $nn$-continuum coupling modifies $T = 1$ monopole terms [14] of the SM interaction. A good agreement for the binding systematics in oxygen chain can be found provided the $T = 1$ part of two-body interaction is modified as follows: $\delta V_{12}^{(1s,1s,1d,1d)} = -0.05 \text{ MeV}, ~\delta V_{12}^{(1s,2d,3d)} = +0.25 \text{ MeV}, ~\delta V_{12}^{(3d,3d)} = -0.35 \text{ MeV}$.

Fig. 1a shows the neutron number dependence of $E_{n}^{\text{corr}}$ for (i) $E_{n}^{\text{thr}}$ of SMEC (solid line), and for (ii) $E_{n}^{\text{thr}}$ fixed arbitrarily at 0 and 4 MeV (the dotted lines with open squares and triangles, respectively). The $N$-dependence of $E_{n}^{\text{corr}}$ in these three cases exhibits approximately quadratic dependence on the number of valence neutrons, which is usual for a monopole Hamiltonian [14]. Deviations from this dependence are characteristic of the continuum coupling. For $E_{n}^{\text{thr}} = 0$ (a limit of one-neutron drip-line), one can see an odd-even staggering (OES) of $E_{n}^{\text{corr}}$ 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 broken-pair g.s. of odd-$N$ nuclei. This “drip-line effect”, which is seen also in the coordinate-space Hartree-Fock-Bogolyubov approach [17], is restricted to a narrow window of excitation energies around $E_{n}^{\text{thr}} = 0$. It vanishes if $E_{n}^{\text{corr}}$ is calculated for $E_{n}^{\text{thr}} = 4 \text{ MeV}$ (see the dotted line with triangles in Fig. 1a).

If $E_{n}^{\text{thr}}$ is calculated in SMEC (the solid line), one finds an opposite OES effect with enhanced $E_{n}^{\text{corr}}$ for odd-$N$ isotopes. This is due to $E_{n}^{\text{thr}}$ which is lower in odd-$N$ isotopes than in neighbouring even-$N$ isotopes. This threshold induced OES effect leads to the attenuation of OES of binding energies. An enhanced modification of one-neutron separation energies $S_n$ is seen for odd-$N$ oxygen isotopes (see Fig. 1b). In general, the effect of continuum coupling on one- and two-neutron separation energies is seen mainly for $S_n \lesssim 3 \text{ MeV}$, i.e. close to the one-neutron drip-line.

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 in the oxygen isotope chain and its value is kept unchanged. The optimal value of the strength of the $np$-continuum coupling : $V_0^{(np)} = V_{12}^{(0)}(a + \beta)$, varies from a standard value $V_0^{(np)} \simeq 2V_0^{(nn)}$ for well-bound isotopes at the valley of stability to $V_0^{(np)} \simeq (1/2)V_0^{(nn)}$ near the neutron drip-line. This coupling modifies strongly $T = 0$ monopole terms of the SM Hamiltonian. For $V_0^{(np)} \simeq (1/2)V_0^{(nn)}$, good agreement for $S_n$, $S_{2n}$ and OES of binding energies $[\text{E}^{\text{corr}}]$:

$$\Delta^{(3)}(N) = ((-1)^N/2)[E(N+1) - 2E(N) + E(N-1)] \quad (1)$$

is found provided the $T = 0$ two-body interaction is modified as follows : $\delta V_{0d_{5/2}}^{(T=0)} = +0.6 \text{ MeV}, \delta V_{0d_{3/2}}^{(T=0)} = +0.9 \text{ MeV}$.

Fig. 2a shows the neutron number dependence of $E_{\text{corr}}^{(\text{thr})}$ for fluorine isotopes, which is calculated for $V_0^{(np)} = (1/2)V_0^{(nn)}$. $E_{\text{corr}}^{(\text{thr})}$ depends both on $|N_p - N_n|$ and $(N_p + N_n)$ (compare Figs. 1a and 2a), where $N_p, N_n$ are the number of protons and neutrons in the valence space. Three cases shown in Fig. 2a can be directly compared with those shown in Fig. 1a. For $E_n^{(\text{thr})} = 4 \text{ MeV}$, one can see the OES of $E_{\text{corr}}^{(\text{thr})}$ which is absent in the oxygen chain. This is the salient feature of the $np$-coupling. $E_{\text{corr}}^{(\text{thr})}$ in odd-odd isotopes is increased as compared to the neighboring odd-even ones. The size of $E_{\text{corr}}^{(\text{thr})}$ in this case is weakly dependent on the precise value of $E_n^{(\text{thr})}$. Qualitatively similar effect can be seen also at the neutron drip-line (see the results for $E_n^{(\text{thr})} = 0$ in Fig. 2a) but now the OES due to the $np$-coupling is attenuated by an opposite staggering due to the $nn$-coupling (see also Fig. 1a). If $E_n^{(\text{thr})}$ is calculated in SMEC for each nucleus (the solid line), the OES of $E_{\text{corr}}^{(\text{thr})}$ around a smooth $N$-dependence is enhanced due to combined effects of the $np$-continuum coupling, which weakly depends on $E_n^{(\text{thr})}$, and the $nn$-continuum coupling, which closely follows the OES of $E_n^{(\text{thr})}$. These two effects act ’in phase’, hence contributing an additional binding for odd-$N$ nuclei.

A strong sensitivity of $E_{\text{corr}}^{(\text{thr})}$ in fluorine chain to the value of the strength $V_0^{(np)}$ can be seen in Figs. 2b and 2c which show the neutron number dependence of $S_n$ and $S_{2n}$. The dashed line shows the SM results, whereas the solid line gives SMEC results for $V_0^{(np)} = (1/2)V_0^{(nn)}$. The agreement of SMEC results with the experimental data is excellent for neutron-rich nuclei. The dotted line in Figs. 2b and 2c corresponds to SMEC calculation with $V_0^{(np)} = 2V_0^{(nn)}$. For this standard value, one finds a somewhat better agreement with the experimental data for light fluorine isotopes. On the contrary, description of neutron-rich nuclei is poor.

A useful indicator of OES is $\Delta^{(3)}(N)$ (Eq. 1). Fig. 3 compares experimental data for $\Delta^{(3)}(N)$ in fluorine isotopes with those calculated in SMEC and in SM. SMEC results correspond to : $V_0^{(np)} = (1/2)V_0^{(nn)}$ (the solid line) and $V_0^{(np)} = 2V_0^{(nn)}$ (the dotted line). SM results have been obtained using two different SM interactions : (i) with the modified $T = 0, 1$ monopole terms (the dashed line), as discussed above, and (ii) without these modifications (the dashed-dotted line). One can see that the SM calculations overestimate systematically the OES effect, in particular close to the neutron drip-line. The $np$-continuum coupling strongly attenuates the OES and may even wash it out for values of ratio $V_0^{(np)}/V_0^{(nn)}$, close to the accepted value $\geq 2$ in nuclei from the valley of stability.

FIG. 2. The same as in Fig. 1 but for the fluorine isotopes. SMEC calculations shown by the solid line are performed for the strengths of the continuum coupling : $V_0^{(nn)} = 414 \text{ MeV·fm}^3$ and $V_0^{(np)} = (1/2)V_0^{(nn)}$. The dotted lines in (b) and (c) have been obtained for $V_0^{(np)} = 2V_0^{(nn)}$. The closed circles with error bars shows the data [13].
In summary, we have performed first large-scale SM calculations including the coupling to the continuum states which extend from the valley of stability up to the neutron drip-line. Our analysis demonstrates an important renormalization of the effective SM Hamiltonian by the continuum coupling; the principal effects of this renormalization depend on the position of the one-neutron emission threshold $E_{n}^{(thr)}$, on isospin $T$, its projection $T_Z$ and on the number of valence particles. Certain features of this renormalization can be simulated in SM studies by a suitable shifts of the two-body matrix elements. The dependence of $E_{corr}$ on both $E_{n}^{(thr)}$ and the number of valence neutrons $N_n$ and protons $N_p$ implies, however, that the two-body monopoles in SM studies must contain the additional terms depending on $E_{n}^{(thr)}$, $|N_p - N_n|$, and $(N_p + N_n)$, which become important near the drip line.

FIG. 3. The OES of binding energies [7] for SM (the dashed line) and SMEC with different ratios of np- and nn- continuum coupling strengths : $V_0^{(np)} = (1/2)V_0^{(nn)}$ (the solid line) and $V_0^{(np)} = 2V_0^{(nn)}$ (the dotted line). The dashed-dotted line with open diamonds, shows SM results for the USD+KB’ interaction without the modification of $T = 0, 1$ monopole terms discussed in the text. The closed points with error bars shows the data [13].

We have found an important attenuation of the OES of binding energies close to the neutron drip-line by the np-continuum coupling. This attenuation does not mean that the neutron pairing correlations become weaker (see Fig. 1a) but that the np-continuum coupling ‘falsifies’ $\Delta^{(3)}(N)$ indicator of neutron pairing.

The analysis of experimental data in SMEC indicates a significant attenuation of np-continuum coupling in nuclei with large neutron excess. A strong sensitivity of $S_n(N)$ and $\Delta^{(3)}(N)$ to the value of $V_0^{(np)}/V_0^{(nn)}$ allows to estimate this attenuation quantitatively.

The continuum coupling correction to energy of a SM state depends strongly on the position of this state with respect to $E_n^{(thr)}$. This dependence induce downward shifts of excitation energy for SM states close to $E_n^{(thr)}$. The $T_Z$—dependence of these shifts (see Figs. 1a and 2a) implies that these SM states (e.g. intruder states), even for a constant value of one-neutron emission threshold, will be pushed down by an amount which depends on $T_Z$.

The coupling to the two-neutron continuum has not been included in the present analysis. This coupling is expected to be less important if $S_n < S_{2n}$, i.e. for $N < 18$ in O- and F-isotope chains. Since $E_{2n}^{(thr)}$ is a smooth function of $N$ and, moreover, varies slowly near the neutron drip-line, therefore we expect that the coupling to the two-neutron continuum produces a smaller effect on the OES of binding energies than the coupling to the one-neutron continuum. One should keep in mind, however, that additional attractive correlations between nucleons in the scattering continuum are responsible for the appearance of ”Borromean systems” close to the one-neutron drip line [10].

We thank W. Nazarewicz for valuable suggestions and F. Nowacki for useful discussions.

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