Study of Shell Evolution in Neutron-Rich Boron, Carbon, and Nitrogen Isotopes with In-Medium Similarity Renormalization Group Calculations

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Date: 2025-07-04T11:08:46+00:00

Abstract

Neutron-rich boron, carbon, and nitrogen isotopes have garnered extensive experimental and theoretical interest. In the present work, we conducted a comprehensive study for these nuclei utilizing ab initio valence-space in-medium similarity renormalization group calculations with chiral nucleon-nucleon and three-nucleon interactions.

Full Text

Study of Shell Evolution in Neutron-Rich Boron, Carbon, and Nitrogen Isotopes with In-Medium Similarity Renormalization Group Calculations

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Neutron-rich boron, carbon, and nitrogen isotopes have garnered extensive experimental and theoretical interest. In the present work, we conducted a comprehensive study for these nuclei utilizing ab initio valence-space in-medium similarity renormalization group calculations with chiral nucleon-nucleon and three-nucleon interactions. First, we systematically calculated the spectra of these nuclei. Our results align well with the available experimental data, which are comparable with phenomenological shell model calculations. Subsequently, the evolution of the N = 14 and N = 16 shell gaps is discussed based on the calculated spectra and effective single-particle energies. Our calculations suggest that the N = 14 neutron sub-shell is present in the oxygen isotopes but disappears in the boron, carbon, and nitrogen isotopic chains. Moreover, the N = 16 sub-shell is present in all those isotopes but gradually decreases from ^{24}O to ^{21}B. The results provide valuable information for future experiments.

Keywords: Ab initio calculations, chiral nuclear forces, shell evolution, low-lying spectra

INTRODUCTION

The shell structure of nuclei is a fundamental framework in nuclear physics. However, for neutron-rich nuclei far from the valley of stability, the traditional magic numbers N = 8, 20, 28, and 40 vanish [1–10] and new magic numbers, such as N = 14, 16, 32, and 34 emerge [11–14]. The evolution of shell structure in exotic nuclei has significantly deepened our understanding of nuclear quantum many-body systems and the underlying nuclear forces. Light neutron-rich nuclei are particularly intriguing, as the development of radioactive beam facilities has facilitated unprecedented exploration of isotopic chains extending to the dripline region [15].

The neutron-rich oxygen isotopes ^{22}O and ^{24}O are doubly magic nuclei, with the high excitation energy of the first 2^+ excited state providing clear evidence for the emergence of the N = 14 and 16 sub-shell closures [14, 16–18]. However, the comparison of the systematic behavior of the 2^+ energy levels in the oxygen and carbon isotopic chains suggests that the N = 14 shell gap disappears in carbon isotopes [19, 20]. In ^{15}C, the ground state and the first excited state are $1/2^+$ and $5/2^+$, respectively, indicating an inversion of the neutron $1s_1/_2$ and $0d_5/_2$ orbits in ^{15}C compared to ^{17}O [21, 22]. A similar inversion is anticipated as neutrons are added to ^{20}C [19, 20]. As the transition region between oxygen and carbon isotopes, nitrogen isotopes also signal the erosion of the N = 14 shell gap [23–26]. Moreover, the evolution of the N = 16 shell gap in the neutron-rich boron, carbon, nitrogen, and oxygen isotopic chains remains an intriguing question. Further experimental and theoretical studies are required to fully understand the origin and evolution of the N = 14 and N = 16 shell gaps.

Neutron-rich boron, carbon, and nitrogen isotopes exhibit many exotic phenomena. For instance, two-neutron halo structures were observed in ^{17}B [27], ^{19}B [28], and ^{22}C [29], while one-neutron halo structures were found in ^{15}C [30] and ^{19}C [31]. Additionally, the observation of the most neutron-rich unbound nuclei, ^{20}B and ^{21}B, was recently reported in Ref. [32]. Furthermore, a thick neutron skin has been detected in $^{17-22}$N [26]. These light neutron-rich systems, which straddle the neutron dripline, have accumulated a wealth of experimental data, providing an ideal testing ground for theoretical models [33–36]. They have inspired extensive theoretical studies, including shell model (SM) [21, 37–40], Gamow shell model (GSM) [41–43], antisymmetrized molecular dynamics (AMD) [44, 45], and ab initio no-core shell model (NCSM) calculations [46–48].

However, the traditional SM calculations, which employ phenomenological interactions, have limited predictive power as nuclei approach the dripline. In contrast, ab initio calculations, based on high-resolution interactions derived from the chiral effective field theory (EFT) of quantum chromodynamics, have made great progress over the past decades [49–56], offering a more robust framework for understanding and predicting the properties of neutron-rich nuclei.

Systematic calculations of neutron-rich boron, carbon, and nitrogen isotopes enable us to gain a more comprehensive understanding of their exotic structures and shell evolution, while simultaneously testing our ab initio methods and nuclear forces. Therefore, in this work, we performed systematic calculations of neutron-rich boron, carbon, and nitrogen isotopes using the ab initio valence-space in-medium similarity renormalization group (VS-IMSRG) [57–63], based on nucleon-nucleon (NN) and three-nucleon (3N) interactions derived from EFT. The paper is organized as follows: First, we give a brief introduction to the VS-IMSRG framework. Next, we present the systematic calculations of the spectra for the neutron-rich boron, carbon, and nitrogen isotopes. Subsequently, we discuss the shell evolution of the N = 14 and N = 16 shell gaps in these isotopes, utilizing the calculated effective single-particle energies (ESPE). Finally, we conclude with a summary of the present work.

METHOD

The intrinsic Hamiltonian of an A-nucleon system can be written as:

$$H = T + V = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}$$

where p is the nucleon momentum in the laboratory, m refers to the nucleon mass, v_{NN} and v_{3N} are the NN and 3N interactions, respectively. In this paper, we use three different EFT NN + 3N interactions: EM1.8/2.0 [64, 65], N3LO+3N(lnl) [9, 66], and N4LO+3N(lnl) [67]. The EM1.8/2.0 interaction, consisted of a next-to-next-to-next-to-leading order (N3LO) NN interaction softened by the similarity renormalization group (SRG) evolution with momentum resolution scale $\lambda = 1.8$ fm^{-1} and a next-to-next-to-leading order (N2LO) 3N interaction with momentum cut-off $\Lambda = 2.0$ fm^{-1}, can well reproduce ground-state energies up to ^{132}Sn [64, 65]. The N3LO+3N(lnl) interaction, which presents good description of ground-state energies up to nickel isotopes, is composed of a N3LO NN interaction and a N2LO 3N interaction, adopting a large SRG scale of $\lambda = 2.6$ fm^{-1} for the NN interaction without including the induced 3N force [9, 66]. The N4LO+3N(lnl) interaction, composed of a next-to-next-to-next-to-next-to-leading order (N4LO) NN interaction and a N2LO 3N interaction, also adopts a large SRG scale of $\lambda = 2.6$ fm^{-1} for the NN interaction without including the induced 3N force [67].

In this work, we taking harmonic-oscillator basis at $\hbar\omega = 16$ MeV with $e_{max} =$

$2n+l = 14$ and $E_{3max} = 14$, which is large enough for convergence. In practical calculations, Hamiltonian (1) is rewritten as normal-order operators with respect to the Hartree-Fock reference state:

$$H = E_0 + \sum_{ij} f_{ij} : a_i^\dagger a_j : + \sum_{ijkl} \Gamma_{ijkl} : a_j^\dagger a_i^\dagger a_k a_l : + \sum_{ijklmn} W_{ijklmn} : a_i^\dagger a_j^\dagger a_k^\dagger a_m a_l a_n :$$

where E_0, f, Γ, W refer to the normal-ordered zero-, one-, two- and three-body terms respectively. As the contribution of 3N force can be well captured at the normal-ordered two-body level [68], the residual normal-ordered three-body term W is neglected.

Next, using continuous unitary transformation $U(s)$, Hamiltonian (2) is decoupled from large Hilbert space to a small valence space by VS-IMSRG. This is achieved by solving the flow equation:

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

with an anti-Hermitian generator, $\eta(s) \equiv \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$. In the present work, we adopted protons in the p shell and neutrons in the sd shell as the valence space. In practical calculations, the Magnus formalism is employed with all operators truncated at the two-body level [69]. The effective Hamiltonians for this model space are derived consistently by VS-IMSRG with ensemble normal ordering (ENO) [59]. Then, we use the large-scale shell model code, KSHELL [70], to diagonalize the effective Hamiltonians.

RESULTS

A. Energy Spectra

The nuclear spectra provide invaluable insights into nuclear structure. In the present paper, the spectra of neutron-rich boron, carbon, and nitrogen isotopes are systematically calculated by ab initio VS-IMSRG with three sets of EFT NN + 3N interactions: EM1.8/2.0 [64, 65], N3LO+3N(lnl) [9, 66], and N4LO+3N(lnl) [67]. For comparison, we also performed phenomenological SM calculations using the YSOX interaction within the full psd valence space, which well reproduce the properties of boron, carbon, nitrogen, and oxygen isotopes [37]. The results are compared with the available experimental data, as illustrated in Fig. 1 [Figure 1: see original paper], Fig. 2 [Figure 2: see original paper], and Fig. 3 [Figure 3: see original paper].

Nitrogen isotopes have abundant experimental data, which provides a valuable test ground for our ab initio calculations. Besides, nitrogen nuclei lie between the oxygen and carbon isotopes, offering essential insights into shell evolution. For ^{16}N, the ordering of the first four states has been experimentally determined as 2^-, 0^-, 3^-, and 1^- [71]. Our VS-IMSRG calculations with the EM1.8/2.0 and N3LO+3N(lnl) interactions show good agreement with the experimental results, whereas the SM calculations using the YSOX interaction failed to reproduce the spectra of ^{16}N. For ^{17}N, the VS-IMSRG calculations with the three NN + 3N interactions, as well as the SM calculations using the YSOX interaction, well reproduce the lowest three states. In the case of ^{18}N, the ground state is correctly reproduced by the VS-IMSRG calculations with the EM1.8/2.0 interaction and the SM calculations using the YSOX interaction. However, the VS-IMSRG calculations with the N3LO+3N(lnl) and N4LO+3N(lnl) interactions give 2^- as the ground state. For ^{19,21}N, all calculations correctly give the ground state as $1/2^-$ and predict the first excited state to be $3/2^-$, with the excited states yet to be experimentally confirmed. For ^{20}N, the ground state is 2^- given by all the calculations.

In the case of ^{22}N, the VS-IMSRG calculations with the N3LO+3N(lnl) and N4LO+3N(lnl) interactions predict a 0^- ground state, while the VS-IMSRG calculations with the EM1.8/2.0 interaction and the SM calculations using the YSOX interaction give the ground state to be 2^- and 1^-, respectively. The size of the N = 16 shell gap in ^{23}N remains an open question [72]. All calculations predict the ground state of ^{23}N to be $1/2^-$. However, the SM calculations with the YSOX interaction yield higher excitation spectra compared to the VS-IMSRG results, indicating an overly large N = 16 shell gap in the SM calculations using the YSOX interaction. This behavior has also been observed in ^{21}B, ^{22}C, and ^{24}O, as discussed above. For ^{24}N, all the calculations give the ground state to be 2^- and predict the first excited state as 1^-.

Neutron-rich carbon isotopes have also attracted significant experimental and theoretical attention. The ground state and the first excited state of ^{15}C are $1/2^+$ and $5/2^+$, respectively, indicating an inversion of the neutron $1s_{1/2}$ and $0d_{5/2}$ orbits in carbon isotopes [21, 22]. Our VS-IMSRG calculations, along with the SM calculations, reproduce the spectra of ^{15}C well. The VS-IMSRG calculations with the N3LO+3N(lnl) interaction for ^{16,17}C did not converge, so we only present the results for ^{16,17}C using the EM1.8/2.0 and N4LO+3N(lnl) interactions in Fig. 2. For ^{16,18,20}C, the first 2^+ excited states obtained from our VS-IMSRG calculations are in good agreement with the experimental data, while the SM calculations using the YSOX interaction generally give higher energies for the first 2^+ excited states of these nuclei. In particular, for ^{22}C, the energy of the first 2^+ excited state calculated by SM using the YSOX interaction is significantly higher than the energy predicted by VS-IMSRG. Notably, the first 2^+ excited state of ^{24}O, calculated by SM with the YSOX interaction, is 5.41 MeV, which is higher than the experimental value of 4.76 MeV. In contrast, our VS-IMSRG calculations with the EM1.8/2.0, N3LO+3N(lnl), and N4LO+3N(lnl) interactions give the first 2^+ excited state of ^{24}O to be 4.87, 5.26, and 4.39 MeV, respectively, which are in better agreement with the experimental value. Moreover, the first 2^+ excited state of ^{22}C calculated by VS-IMSRG is significantly higher than that of neighboring carbon isotopes, implying the presence of the N = 16 shell gap in ^{22}C. However, the calculated first 2^+ excited state of ^{22}C is lower than that of ^{24}O, suggesting a reduction of the N = 16 shell gap in ^{22}C compared to ^{24}O. Additionally, the low energy of the first 2^+ excited state in ^{20}C indicates the disappearance of the N = 14 shell gap in ^{20}C [19]. For ^{17}C and ^{19}C, our VS-IMSRG calculations failed to reproduce the experimental spectra due to the absence of continuum coupling in our current method, as discussed in Ref. [41, 73].

In the case of neutron-rich boron isotopes, experimental data are quite limited. For ^{14}B, the ordering of the first five states has been experimentally assigned as 2^-, 1^-, 3^-, 2^-, and 4^- [71]. Our ab initio VS-IMSRG calculations with the three NN + 3N interactions, as well as the SM calculations using the YSOX interaction, are all in good agreement with the experimental results. The spin and parity of the ground state for isotopes heavier than ^{14}B have not yet been experimentally confirmed. For ^{15,17,19,21}B, our VS-IMSRG calculations with the three NN + 3N interactions predict that the ground states of these isotopes are all $3/2^-$, consistent with the SM calculations using the YSOX interaction. For ^{16}B, the VS-IMSRG calculations with the N3LO+3N(lnl) and N4LO+3N(lnl) interactions predict the ground state to be 2^-, while the VS-IMSRG calculations with the EM1.8/2.0 interaction predict a ground state of 0^-, with a 2^- excited state that is nearly degenerate with it. Additionally, the ground state of ^{16}B obtained from SM calculations using the YSOX interaction is also 0^-. For the unbound nucleus ^{18}B, SM calculations using the YSOX and WBP [74] interactions predict the ground state to be 2^-. Our VS-IMSRG calculations with the EM1.8/2.0 and N4LO+3N(lnl) interactions also predict the ground state of ^{18}B to be 2^-, but the VS-IMSRG calculations with the N3LO+3N(lnl) interaction give the ground state of ^{18}B to be 3^-. Both ^{20}B and ^{21}B are unbound nuclei that exist as resonances and decay by one or two neutron emissions [32]. For ^{20}B, our VS-IMSRG calculations with the three NN + 3N interactions predict the ground state to be 1^-, while SM calculations using the YSOX interaction give the ground state to be 2^-. For ^{21}B, our VS-IMSRG calculations with the three NN + 3N interactions predict a significantly lower energy for the first excited state $1/2^-$ compared to the SM calculations using the YSOX interaction, a situation similar to that observed in ^{22}C and ^{24}O above. The $1/2^-$ state of ^{21}B calculated with VS-IMSRG has larger neutron excitation components than in the SM calculations. However, subsequent analysis of the ESPE calculated by VS-IMSRG suggests that the N = 16 subshell still exists in ^{21}B.

Overall, our ab initio VS-IMSRG calculations based on the three EFT NN + 3N interactions, particularly the EM1.8/2.0 interaction, are in good agreement with the available experimental data. These results will provide critical assistance for future experiments.

B. Shell Evolution

In neutron-rich boron, carbon, nitrogen, and oxygen isotopes, the evolution of the N = 14 and N = 16 shell gaps has attracted significant experimental and theoretical attention. The ESPE provides a good reflection of the size of shell gaps, which is defined as [75, 76]:

$$\varepsilon_i = \varepsilon_i^{\text{core}} + \sum_j \bar{V}_{ij} n_j$$

where $\varepsilon_i^{\text{core}}$ is the valence space single particle energy, $\bar{V}_{ij}$ is the monopole interaction, and n_j is the occupation number calculated consistently by SM.

To study the evolution of the N = 14 and N = 16 shell gaps, we calculated the ESPE of the $1s_1/_2$, $0d_5/_2$, and $0d_3/_2$ orbits in these nuclei employing the VS-IMSRG method, based on the EM1.8/2.0, N3LO+3N(lnl), and N4LO+3N(lnl) interactions, compared with the SM calculations using the YSOX interaction. As shown in Fig. 4 [Figure 4: see original paper], for VS-IMSRG calculations, when protons are removed from the oxygen isotopes, the ESPE of the $1s_1/_2$ orbital is gradually lowered relative to the $0d_5/_2$ orbital, and a reversal occurs in boron and carbon isotopes. This indicates that the N = 14 neutron sub-shell is present in the oxygen isotopes but disappears in the boron, carbon, and nitrogen isotopic chains. The SM calculations using the YSOX interaction show the same trend as the VS-IMSRG results, while the N = 14 shell gap in ^{21}N and ^{22}O calculated by SM is significantly larger than that obtained from VS-IMSRG. Notably, the N = 16 sub-shell is present in the boron, carbon, nitrogen, and oxygen isotopic chains, and gradually decreases from ^{24}O to ^{21}B. Moreover, the N = 16 shell gap calculated by SM using YSOX interaction is significantly larger than that calculated by VS-IMSRG. Additionally, the N = 16 shell gap calculated by VS-IMSRG using the N3LO+3N(lnl) interaction is generally larger than that calculated by the EM1.8/2.0 and N4LO+3N(lnl) interactions. Correspondingly, the energy spectra exhibits higher excitation energies, particularly in ^{24}O, as discussed above.

To further understand the contribution of the 3N force to shell evolution, Fig. 5 [Figure 5: see original paper] shows the VS-IMSRG calculations using the full NN + 3N EM1.8/2.0 interaction (solid lines), compared with the VS-IMSRG calculations without the 3N force (dashed lines). As shown in Fig. 5, the 3N force enhances the N = 14 shell gap in oxygen isotopes while reducing the N = 16 shell gap in boron, carbon, nitrogen, and oxygen isotopes. A similar trend is observed for the results using the N3LO+3N(lnl) and N4LO+3N(lnl) interactions.

In order to analyze the roles of different components of the interaction to the shell evolution, we employ the spin-tensor decomposition method [77–79] to decompose the effective interaction derived from VS-IMSRG into central, tensor, and spin-orbit (LS) parts. Firstly, we conducted systematic calculations for boron isotopes and compared the contributions of different components of the interaction derived from VS-IMSRG across the three sets of EFT NN + 3N interactions: N3LO+3N(lnl), N4LO+3N(lnl), and EM1.8/2.0. We also compared the results with the SM calculations using the YSOX interaction. As shown in Fig. 6 [Figure 6: see original paper], the solid lines represent the results with the full interaction, while the dashed lines represent the results without the contribution of the tensor force, and the dot-dashed lines represent the results without the contribution of the two-body LS part. In our VS-IMSRG calculations, we can see that the tensor force slightly lowers the ESPE of the $0d_{3/2}$ orbital relative to the $0d_{5/2}$ orbital, while the two-body LS part raises the ESPE of both the $0d_{3/2}$ and $1s_{1/2}$ orbits relative to the $0d_{5/2}$ orbital. Moreover, the contributions of the tensor force and the two-body LS part are similar across the three sets of NN + 3N forces. Additionally, SM calculations using the YSOX interaction demonstrate the same trend as the VS-IMSRG results, although the strength of the tensor force and the two-body LS force show minor differences.

Next, we further present the contributions of different components of the interaction in various isotopes. For clarity, we only show the results calculated by VS-IMSRG using the EM1.8/2.0 interaction. In Fig. 7 [Figure 7: see original paper], the solid and dashed lines represent the ESPE with and without the contribution of the tensor force, respectively. It can be seen that the tensor force only slightly reduces the N = 16 shell gap for all the isotopes. Fig. 8 [Figure 8: see original paper] compares the results with and without the two-body LS part. The two-body LS part significantly lowers the ESPE of the $0d_{5/2}$ orbital and causes the inversion of the $1s_{1/2}$ and $0d_{5/2}$ orbits in oxygen isotopes compared to the boron and carbon isotopes. This inversion is the origin of the N = 14 shell gap in oxygen isotopes. Additionally, the two-body LS part significantly increases the ESPE of the $0d_{3/2}$ orbital, leading to the appearance of the N = 16 sub-shell.

In Ref. [4], the inversion between the neutron $1s_{1/2}$ and $0d_{5/2}$ orbits in ^{15}C and ^{17}O has been depicted by analyzing the monopole matrix elements of the YSOX interaction, assuming that, from ^{15}C to ^{17}O, the proton $ 0*p{1}*/{2}$ orbit is fully occupied and the last neutron is in either the $1s_{1/2}$ or $0d_{5/2}$ orbital. Similar to the discussion in Ref. [4], we extract the contributions of the monopole matrix elements from various components of the effective interaction derived by VS-IMSRG, including central, tensor, and LS parts, as shown in Fig. 9 [Figure 9: see original paper]. Here, the rest part is due to the A-dependence of our Hamiltonian. We can see that the two-body LS part has a significant contribution to the shift of the $1s_{1/2}$ orbital relative to the $0d_{5/2}$ orbital, even determining the inversion of the $1s_{1/2}$ and $0d_{5/2}$ orbits. In contrast, the contribution from the tensor force is much smaller than that observed in the YSOX interaction in Ref. [4].

CONCLUSIONS

Utilizing three sets of chiral NN + 3N interactions—EM1.8/2.0, N3LO+3N(lnl), and N4LO+3N(lnl)—we present ab initio VS-IMSRG calculations for neutron-rich boron, carbon, and nitrogen isotopes. We systematically calculated and predicted the low-lying spectra of these nuclei. For comparison, we also performed SM calculations using the YSOX interaction. Based on the calculated spectra and effective single-particle energies, we studied the evolution of the N = 14 and N = 16 shell gaps. Our results suggest that the N = 14 neutron sub-shell is present in the oxygen isotopes but collapses in the boron, carbon, and nitrogen isotopic chains. Furthermore, the N = 16 sub-shell is predicted to be present in boron, carbon, nitrogen, and oxygen isotopes, but its size gradually decreases from ^{24}O to ^{21}B. Additionally, we investigated the roles of different components of the interaction in shell evolution by employing the spin-tensor decomposition method. We find that the two-body spin-orbit force plays a significant role in the formation of the N = 14 and N = 16 shell gaps. In general, our ab initio VS-IMSRG calculations agree well with the available experimental data, and the theoretical predictions for these nuclei will be helpful for future experiments.

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