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Ab initio* study of $Z(N) = 6$ magicity

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Abstract: The existence of magic numbers of protons and neutrons in nuclei is essential for understanding the nuclear structure and fundamental nuclear forces. Over decades, researchers have conducted theoretical and experimental studies on a new magic number, $Z(N)=6$, focusing on observables such as radii, binding energy, electromagnetic transition, and nucleon separation energies. We performed *ab initio* no-core shell model calculations for the occupation numbers of the lowest single particle states in the ground states of $Z(N)=6$ and $Z(N)=8$ isotopes (isotones). The results of our calculations do not support $Z(N)=6$ as a magic number over a range of atomic numbers. However, ^{14}C and ^{14}O exhibit the characteristics of double-magic nuclei.

Keywords: *Ab-initio* calculations, magic number, $Z(N)=6$ and $Z(N)=8$ isotopes (isotones), occupation number

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The nuclear shell structure arises from the independent motion of nucleons in an average mean-field, serving as a valuable framework for comprehending the nuclear structure and fundamental nuclear potential. The most notable characteristic of the shell structure is the presence of the so-called magic numbers of protons and neutrons, which are associated with enhanced stability. The occupation of nuclear shells results in the formation of nuclei with magic numbers. The introduction of the phenomenological strong nuclear force, which relies on the inherent spin and orbital angular momentum of a nucleon,

along with the total angular momentum (orbital plus spin) coupling scheme [1, 2], played a crucial role in fully explaining the magic numbers. This breakthrough led to Goeppert-Mayer and Jensen receiving the Nobel Prize.

Evidence from a multitude of experimental and theoretical studies indicates the existence of nuclear shell structures. These findings have also revealed new magic numbers, the absence of previously recognized magic numbers in different regions of the periodic chart, and the so-called local magic numbers [3]. A limited number of studies proposed non-traditional magicities such as $N =$

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14 [4–6], $N = 16$ [7–9], $Z = 16$ [10], $N = 32$ [11–13], and $N = 34$ [14].

In the realm of light nuclei, Kanungo *et al.* [7] comprehensively studied the sub-shell closure at $N = 6$ for neutron-rich isotopes based on the analysis of separation energy systematics, beta decay Q -values, and the first excited states of nuclei. In addition, Otsuka *et al.* [15] examined the magicity of $N = 6$ in relation to the spin-isospin dependent component of the nucleon-nucleon interaction. Furthermore, studies utilizing the extension of the Bethe–Weizscker mass formula [16], potential energy surfaces within the cluster-core model [17], and relativistic mean-field theory [18] have demonstrated that $N = 6$ and $Z = 6$ exhibit traits similar to those of the shell closures. A persistent $Z = 6$ magicity in $^{13-20}\text{C}$ was proposed [19] based on systematic analyses of radii, electromagnetic transition rates, and nuclear masses in carbon and neighboring isotopes using published data. New experimental data were reported along with results from the shell model and *ab initio* coupled-cluster calculations with inter-nucleon interactions based on the modern chiral effective field theory; these results were obtained by these authors and those of Ref. [20].

In this study, we examined the $Z = 6$ magicity of carbon isotopes and the magicity of their mirror $N = 6$ isotones using *ab initio* no-core shell model (NCSM) [21–23] calculations of occupation numbers in the lowest oscillator single-particle states of these nuclei. While oscillator states are less preferred than natural or Hartree-Fock orbitals, we consider them sufficient for our purposes. In fact, we set the $0s_{1/2} + 0p_{3/2}$ occupancies near their maxima and compared the $0p_{1/2}$ occupancies with those of $0d_{5/2}$ in the nuclei with the well-established magic numbers $Z = 8$ and $N = 8$. Our NCSM results were obtained with the Daejeon16 [24] NN interaction. This interaction is based on the Entem–Machleidt $N^3\text{LO}$ chiral effective field theory interaction [25], softened via a similarity renormalization group transformation [26] to provide a faster convergence, and then adjusted via phase-shift equivalent transformations (PETs) to provide a good description of nuclei with $A \leq 16$ without using $3N$ forces, whose effects were mimicked by the PET modification of the off-shell properties of the NN interaction. Using the MFDn code [27, 28], we diagonalized the Hamiltonian of the nuclear system in a many-body harmonic oscillator basis characterized by basis energy scale $\hbar\Omega$ and basis truncation parameter N_{max} , which is the maximum number of oscillator excitation quanta allowed in the many-body space relative to the lowest Pauli-allowed configuration.

The NCSM calculations with the Daejeon16 NN interaction were performed wherever possible in model spaces $N_{\text{max}} = 4, 6, 8$, and 10. However, because of the fast growth of the model space dimension and hence the computational cost, we first dropped the calculations for

$N_{\text{max}} = 10$ as number of nucleons A increased, and next additionally for $N_{\text{max}} = 8$ after a further increase in A . Fig. 1 shows the results for occupation numbers in low-lying harmonic oscillator single-particle states obtained for oscillator energy $\hbar\Omega = 17.5$ MeV. This $\hbar\Omega$ value corresponds to the minimum of the ground state energy obtained with the largest N_{max} for nearly all nuclei discussed here; we used a grid with 2.5 MeV increments in $\hbar\Omega$. The only exception is ^{13}O ; however, the $\hbar\Omega$ dependence of the occupation numbers is weak and in ^{13}O , they differ by less than 2% at $\hbar\Omega = 15$ MeV corresponding to the minimum ground state energy in this nucleus. To visualize the $\hbar\Omega$ dependence for the results at the largest model space, we present 'error bars' where the lowest (highest) point indicates the minimal (maximal) occupation number value in the range from $\hbar\Omega = 15$ to 20 MeV.

In the "naive shell model" with non-interacting nucleons moving in the mean field, the proton or neutron orbitals above the closed shells associated with respective magic Z or N numbers are completely unoccupied. Conversely, orbitals at or below closed shells are occupied at their maximum occupation number of $2j + 1$.

Concerning the NCSM calculations with the Daejeon16 NN interaction, the occupation numbers of protons and neutrons in the $0d_{5/2}$ single-particle state, the first single-particle state above the $Z = 8$ and $N = 8$ shell closures in oxygen ($Z = 8$) isotopes and $N = 8$ isotones, respectively, range from approximately 0.1 in the smallest presented model space with $N_{\text{max}} = 4$ to approximately 0.27 in the largest presented model space with $N_{\text{max}} = 10$, as shown in Figs. 1(a), (b). Based on the results of the $0d_{5/2}$ occupations in $Z = 8$ isotopes and $N = 8$ isotones, we suggest to set a proton (neutron) occupation number value of approximately 0.27 for the $0p_{1/2}$ orbital at $N_{\text{max}} = 10$ as an approximate border of magicity in $Z(N)=6$ isotopes (isotones).

Let us now suppose that $Z = 6$ is a "good" magic number in carbon isotopes. Thus, we should expect that the $0p_{3/2}$ orbital is nearly completely occupied while the occupation numbers in the $0p_{1/2}$ orbital are similar to those of protons and neutrons in the $0d_{5/2}$ single-particle states in the oxygen isotopes and $N = 8$ isotones. The $0p_{1/2}$ proton occupation numbers in $^{10-20}\text{C}$ isotopes are presented in Fig. 1(c). There is an increasing trend with A observed between ^{10}C and ^{12}C , where the $0p_{1/2}$ occupation numbers are approximately 0.4–0.6, i. e., much larger than those expected for the closed $0p_{3/2}$ subshell. For further increase in A , we observe a sharp decline of the $0p_{1/2}$ occupation number. In particular, the one in ^{14}C falls into the range of 0.2–0.25, as expected for "good" magic numbers. Beyond ^{14}C , we see a gradual rise of the $0p_{1/2}$ occupation number, and in ^{20}C , it presents approximately the same value as in ^{12}C .

From our results, it follows that the ^{14}C nucleus with $Z = 6$ and $N = 8$ exhibits features of a double-magic nuc-

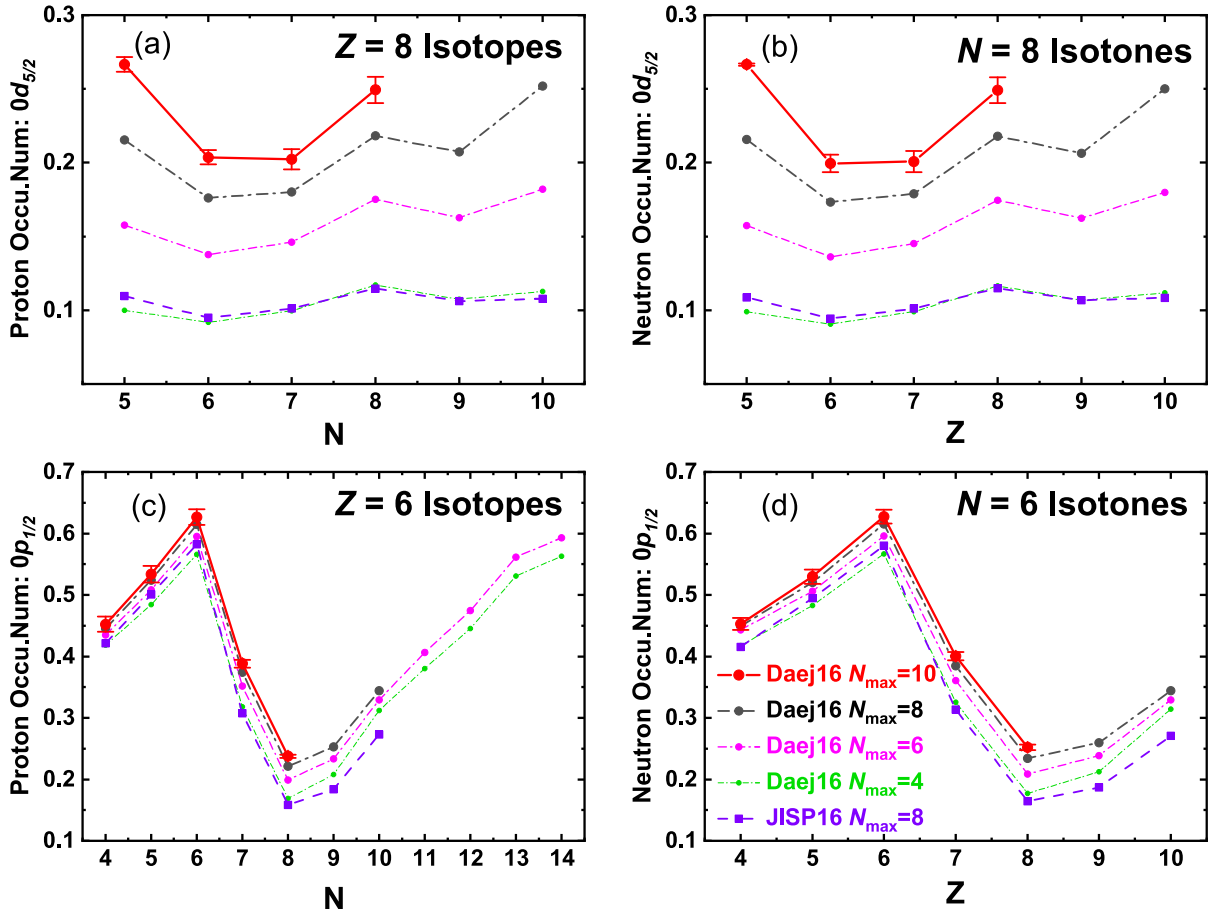


Fig. 1. (color online) Ground state occupation numbers of (a) protons in the $0d_{5/2}$ state in oxygen isotopes, (b) neutrons in the $0d_{5/2}$ state in $N = 8$ isotones, (c) protons in the $0p_{1/2}$ state in carbon isotopes, and (d) neutrons in the $0p_{1/2}$ state in $N = 6$ isotones. The NC-SM calculations were performed in a harmonic oscillator basis using the Daejeon16 (Daej16) NN interaction with N_{\max} ranging from 4 to 10 and $\hbar\Omega = 17.5$ MeV. The 'error bars' for the results in the largest model space present an estimation of the uncertainty of occupation numbers owing to their $\hbar\Omega$ dependence; see the text for details. The results obtained with the JISP16 NN interaction at $N_{\max} = 8$ are shown for comparison.

leus, supporting the same proposition based on the analysis of various data reported in Ref. [19]. However, the $Z = 6$ magicity is weakened in carbon isotopes with $N < 8$ and $N > 9$. From the analysis of the occupation numbers in the $0p_{1/2}$ orbital in carbon isotopes, we can conclude that $Z = 6$ is a *local magic number* that exhibits marked magic features when the number of neutrons lies in interval $8 \lesssim N \lesssim 9$.

Regarding the carbon isotopes, ^{12}C is well-known to have a three-alpha structure associated with a deformed oblate shape manifested in a rotational band including the ground and first 2^+ states of ^{12}C as members [29]. The double-magic nuclei are known to maintain a spherical shape, and a switch from deformation to sphericity results in a strong drop-off of $0p_{1/2}$ proton occupation between ^{12}C and ^{14}C , as shown in Fig. 1(c). As the number of neutrons increases in the $N > 8$ carbon isotopes, the deformation slowly increases, which results in the disappearance of magicity.

Figure 1(d) displays the neutron occupation numbers in the $0p_{1/2}$ orbital for $N = 6$ isotones from $Z = 4$ to $Z = 10$. We calculated fewer $N = 6$ isotones than carbon isotopes because proton-excess nuclei with $N = 6$ and $Z > 8$ are particle-unstable. The results for $N = 6$ isotones exhibit concordance with those for carbon isotopes: increase in the $0p_{1/2}$ neutron occupation numbers from ^{10}Be to ^{12}C , followed by a sharp drop toward ^{14}O , which appears to exhibit double-magic features, and a gradual increase in ^{15}F and ^{16}Ne . Thus, we conclude that $N = 6$ is also a *local magic number* in interval $8 \lesssim Z \lesssim 9$.

To ensure the independence on the NN interaction of our qualitative conclusions about the *local magicity* of $Z = 6$ and $N = 6$, we also performed the NCSM calculations with the JISP16 NN interaction [30]. The origin of the JISP16 interaction is notably different from that of Daejeon16: it was initially developed from the NN scattering data using inverse scattering techniques, and then, as with Daejeon16, adjusted by PETs to $A \leq 16$ nuclei to

avoid the need for the $3N$ forces.

The JISP16 results for the occupation numbers were obtained with $N_{\max} = 8$. Although the minimum binding energy obtained with JISP16 usually appears at higher $\hbar\Omega$ values, we also set $\hbar\Omega = 17.5$ MeV in the JISP16 calculations. The differences between the JISP16 results presented in Fig. 1 (obtained at $\hbar\Omega = 17.5$ MeV) and the occupation numbers calculated at the $\hbar\Omega$ values corresponding to the minima of the ground state energies do not exceed 10%. The results obtained from the JISP16 calculation exhibit modest variations compared to those from Daejeon16; however, the overall pattern of change remains constant.

The occupation numbers obtained with JISP16 clearly follow the same trends. The JISP16 occupations are somewhat smaller than those supported by Daejeon16. For example, the proton $0p_{1/2}$ occupation number in ^{14}C is approximately 0.16, which is approximately 30% smaller than the corresponding Daejeon16 result from the same model space. Note, however, that the JISP16 also predicts much smaller occupation numbers in the $0d_{5/2}$ orbital just above the proton $Z = 8$ and neutron $N = 8$ shell closures than the Daejeon16 NN interaction. Therefore, we obtained approximately the same occupation numbers for the proton $0p_{1/2}$ orbital and neutron $0d_{5/2}$ orbital in ^{14}C . Generally, the JISP16 calculations support our conclusion that the ^{14}C and ^{14}O nuclei have double-magic features. However, both $Z = 6$ and $N = 6$ are *local magic numbers*, whose magicity markedly reveals only in

the intervals of neutron numbers $8 \lesssim N \lesssim 9$ and proton numbers $8 \lesssim Z \lesssim 9$, respectively.

In summary, we examined the *ab initio* NCSM calculations in terms of the proton (neutron) occupation numbers in the $0p_{1/2}$ orbital in carbon isotopes ($N = 6$ isotones) and the $0d_{5/2}$ orbital in oxygen isotopes ($N = 8$ isotones). We checked that the occupancies of the orbitals above $0p_{1/2}$ are significantly smaller than the value of $0p_{1/2}$ in $Z(N)=6$ isotopes (isotones). Correspondingly, we also found nearly complete occupation of the $0s_{1/2} + 0p_{3/2}$ orbitals, which provides a foundation for examining the magicity of $Z(N) = 6$. Our analysis supports the proposition of Ref. [19] that ^{14}C and ^{14}O are double-magic nuclei, and suggests that $Z = 6$ and $N = 6$ are *local magic numbers* whose magicity weakens when the respective neutron numbers are approximately beyond interval $8 \lesssim N \lesssim 9$ and proton numbers are approximately beyond interval $8 \lesssim Z \lesssim 9$. It is interesting to conduct future spectroscopic studies based on proton- or neutron-transfer and/or knockout reactions on the relevant $Z(N)=6$ isotopes (isotones) to investigate the structural evolution. We thank Professor Vladilen Goldberg, Texas A & M University, for pointing out an important experimental paper that extracts proton occupation fractions from (d,t) measurements [31]. We note that the extracted proton occupation fractions of 0.69, 0.36 and 0.29 for the $0p_{1/2}$ shell in ^{12}C , ^{13}C and ^{14}C respectively, compare well with our results of 0.63, 0.39 and 0.24 in our largest basis spaces.

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