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

He Li (李贺)[1,2,3,4] H. J. Ong[1,3,4,5,6,7] Dong-Liang Fang (房栋梁)[1,3] I. A. Mazur[8] I. J. Shin[9]
A. M. Shirokov[10] J. P. Vary[11] Peng Yin (尹鹏)[12,4†] Xing-Bo Zhao (赵行波)[1,3,4] Wei Zuo (左维)[1,3,4]

[1]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China
[2]School of Nuclear Science and Technology, Lanzhou University, Lanzhou 730000, China
[3]School of Nuclear Physics, University of Chinese Academy of Sciences, Beijing 100049, China
[4]CAS Key Laboratory of High Precision Nuclear Spectroscopy, Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China
[5]Joint Department for Nuclear Physics, Lanzhou University and Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China
[6]Research Center for Nuclear Physics, Osaka University, Ibaraki, Osaka 5670047, Japan
[7]RIKEN Nishina Center, Wako, Saitama 3510198, Japan
[8]Center for Exotic Nuclear Studies, Institute for Basic Science, Daejeon 34126, Republic of Korea
[9]Institute for Rare Isotope Science, Institute for Basic Science, Daejeon 34000, Republic of Korea
[10]Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia
[11]Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA
[12]College of Physics and Engineering, Henan University of Science and Technology, Luoyang 471023, China

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

DOI: 10.1088/1674-1137/ad766e

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 =

Received 17 July 2024; Accepted 2 September 2024; Published online 3 September 2024

* This work is partially supported by the National Natural Science Foundation of China (Grant Nos. 12175280, 12250610193, 12375143, 11975282, 11705240, 11435014), the Natural Science Foundation of Gansu Province, China (Grant Nos. 20JR10RA067, 23JRRA675), the Chinese Academy of Sciences "Light of West China" Program, the Key Research Program of the Chinese Academy of Sciences (Grant Nos. ZDB-SLY-7020, XDPB15), the Foundation for Key Talents of Gansu Province by the Central Funds Guiding the Local Science and Technology Development of Gansu Province, China (Grant No. 22ZY1QA006), the International Partnership Program of the Chinese Academy of Sciences (Grant No. 016GJHZ2022103FN), the National Key R&D Program of China (Grant No. 2023YFA1606903), the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB34000000), the Gansu International Collaboration and Talents Recruitment Base of Particle Physics (2023–2027), the US Department of Energy (Grant No. DE-SC0023692), the National Research Foundation of Korea (2013M7A1A1075764). The Chinese Academy of Sciences President's International Fellowship Initiative (Grant Nos. 2023VMA0013) provides financing for A. M. Shirokov's trip to China to participate in this work. I. A. Mazur is supported by the Institute for Basic Science (IBS-R031-D1). A portion of the computational resources were provided by Gansu Computing Center, Sugon Computing Center in Xi'an. Computational resources including technical support were also partly provided by the National Supercomputing Center of Korea (KSC-2024-CHA- 0001)

† E-mail: pengyin@iastate.edu

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 $^{13\text{-}20}$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}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 $N_{\max} = 4$, 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 $N_{\max} = 10$ as number of nucleons A increased, and next additionally for $N_{\max} = 8$ 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 $N_{\max} = 4$ to approximately 0.27 in the largest presented model space with $N_{\max} = 10$, 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 $N_{\max} = 10$ 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 $^{10\text{-}20}$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-

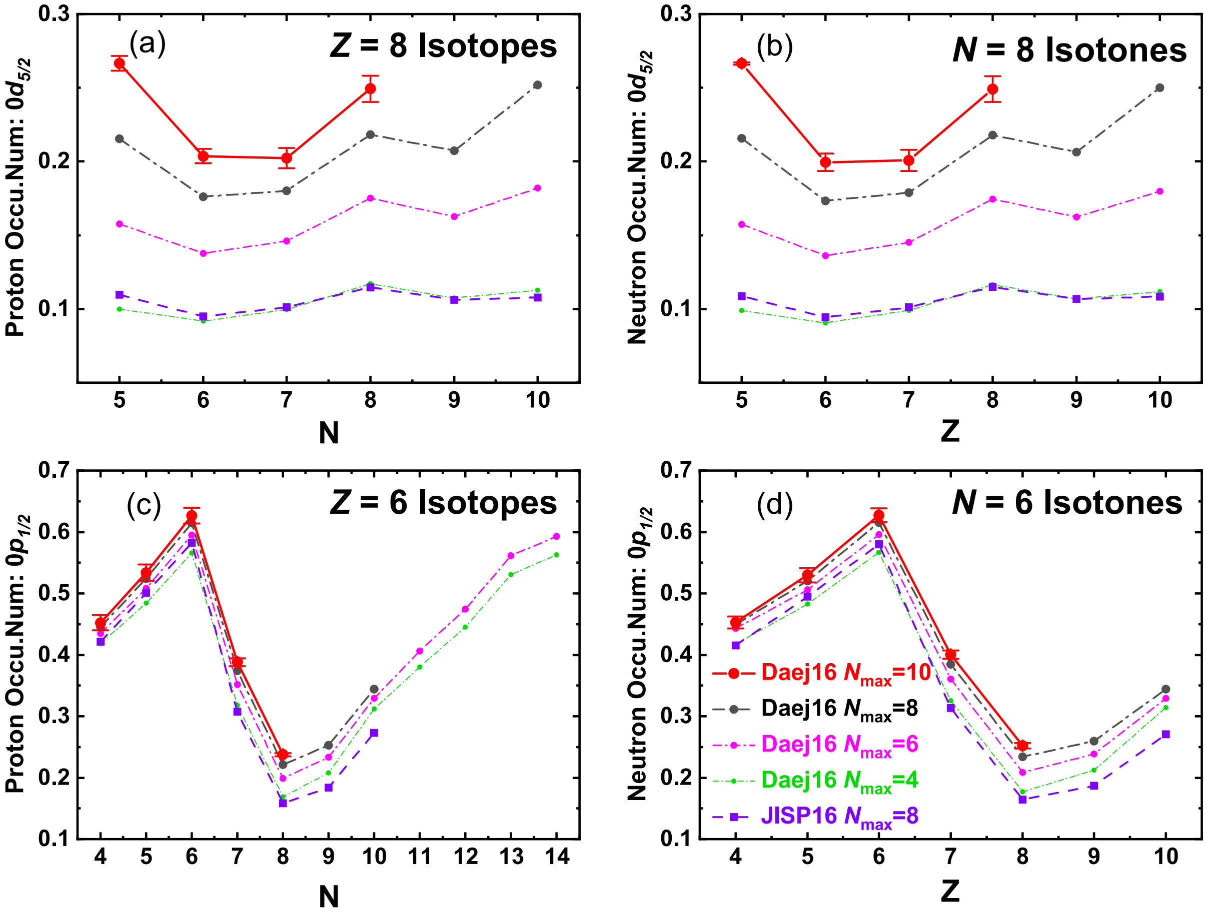

Fig. 1. (color online) Ground state occupation numbers of (a) protons in the $0d_{5/2}$ state in oxygen isotopes, (b) neutrons in the $0d_{5/2}$ state in $N = 8$ isotones, (c) protons in the $0p_{1/2}$ state in carbon isotopes, and (d) neutrons in the $0p_{1/2}$ state in $N = 6$ isotones. The NCSM calculations 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.

References

[1] M. G. Mayer, Phys. Rev. **75**, 1969 (1949)
[2] O. Haxel, J. H. D. Jensen, and H. E. Suess, Phys. Rev. **75**, 1766 (1949)
[3] I. N. Boboshin, Bull. Russ. Acad. Sci. Phys. **87**, 1196 (2023)
[4] M. Stanoiu *et al.*, Phys. Rev. C **69**, 034312 (2004)
[5] B. A. Brown and W. A. Richter, Phys. Rev. C **72**, 057301 (2005)
[6] E. Becheva *et al.*, Phys. Rev. Lett. **96**, 012501 (2006)
[7] R. Kanungo, I. Tanihata, and A. Ozawa, Phys. Lett. B **528**, 58 (2002)
[8] C. R. Hoffman *et al.*, Phys. Lett. B **672**, 17 (2009)
[9] K. Tshoo *et al.*, Phys. Rev. Lett. **109**, 022501 (2012)
[10] Y. Togano *et al.*, Phys. Rev. Lett. **108**, 222501 (2012)
[11] A. Gade *et al.*, Phys. Rev. C **74**, 021302 (2006)
[12] F. Wienholtz *et al.*, Nature **498**, 346 (2013)
[13] M. Rosenbusch *et al.*, Phys. Rev. Lett. **114**, 202501 (2015)
[14] D. Steppenbeck *et al.*, Nature **502**, 207 (2013)
[15] T. Otsuka, R. Fujimoto, Y. Utsuno *et al.*, Phys. Rev. Lett. **87**, 082502 (2001)
[16] C. Samanta and S. Adhikari, Phys. Rev. C **65**, 037301 (2002)
[17] R. K. Gupta, M. Balasubramaniam, S. Kumar *et al.*, J. Phys. G **32**, 565 (2006)
[18] M. Kumawat, G. Saxena, M. Kaushik *et al.*, Can. J. Phys. **96**, 1413 (2018)
[19] D. T. Tran *et al.*, Nature Commun. **9**, 1594 (2018)
[20] C. Forssén, R. Roth, and P. Navrátil, J. Phys. G **40**, 055105 (2013)
[21] B. R. Barrett, P. Navratil, and J. P. Vary, Prog. Part. Nucl. Phys. **69**, 131 (2013)
[22] P. Navratil, J. P. Vary, and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000)
[23] P. Navratil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000)
[24] A. M. Shirokov, I. J. Shin, Y. Kim *et al.*, Phys. Lett. B **761**, 87 (2016)
[25] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001 (2003)
[26] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C **75**, 061001 (2007)
[27] P. Maris, M. Sosonkina, J. P. Vary *et al.*, Procedia Computer Science **1**, 97 (2010)
[28] H. M. Aktulga, C. Yang, E. Ng *et al.*, Concurrency and Computation: Practice and Experience **26**, 2631 (2013)
[29] T. Otsuka, T. Abe, T. Yoshida *et al.*, Nature Commun. **13**(1), 2234 (2022)
[30] A. M. Shirokov, J. P. Vary, A. I. Mazur *et al.*, Phys. Lett. B **644**, 33 (2007)
[31] G. Mairle and G. J. Wagner, Nucl. Phys. A **253**, 253 (1975)