PTEP

Prog. Theor. Exp. Phys. **2019**, 073D02 (8 pages)
DOI: 10.1093/ptep/ptz073

Ab initio no-core shell model study of neutron-rich nitrogen isotopes

Archana Saxena and Praveen C. Srivastava*

Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247 667, India
*E-mail: chandrapraveen1@gmail.com

Received April 16, 2019; Revised June 12, 2019; Accepted June 15, 2019; Published July 29, 2019

We have calculated the energy spectra for neutron-rich $^{18-22}$N isotopes using the no-core shell model. To calculate the energy spectrum we have used three different *NN* potentials: inside non-local outside Yukawa (INOY), next-to-next-to-next-leading order (N3LO) from chiral effective field theory, and charge-dependent Bonn 2000 (CDB2K). The INOY potential is a two-body interaction but also has the effect of three-body forces at short range and a non-local character present in it. The calculations have been done at $\hbar\Omega = 20$ MeV, 14 MeV, and 12 MeV using INOY, N3LO, and CDB2K potentials, respectively. We have also performed shell model calculations with the YSOX interaction. The results with the INOY interaction show good agreement with the experimental data in comparison to the other three interactions. We have also shown the occupancy of different orbitals involved corresponding to the largest model space ($N_{\max} = 4$) in the calculations.

Subject Index D00, D10

1. Introduction

In nuclear physics, solving many-body problems from first principles is computationally hard. Recent advancements in computational facilities have made it possible, however. There are many *ab initio* methods available to study nuclear properties; the no-core shell model (NCSM) [1–4] is one of them. It is a well-established technique used in nuclear physics to calculate nuclear properties. Here, we solve the A-body Schrödinger equation for particles treated non-relativistically and interacted with by realistic two-body forces. With the NCSM, a detailed study has been done for carbon isotopes where the ground state energy, the quadrupole moment of the 2_1^+ state, some $B(E2)$ transitions, and occupancies of 0_1^+ and 2_1^+ have been calculated [5] using inside non-local outside Yukawa (INOY) [6,7] and charge-dependent Bonn 2000 (CDB2K) [8] interactions.

In the present work we will study the nitrogen isotopes, mainly focused on the neutron-rich side. The structure of the neutron-rich nuclei of $^{19-22}$N has been studied by in-beam γ-ray spectroscopy, and spectra and other properties have been compared with shell model calculations using the WBT and WBTM interactions, where the $N = 14$ closed subshell has been discussed [9]. ^{22}N has a halo structure in its ground state [10,11]. Recently, the point proton radii of neutron-rich $^{17-22}$N isotopes have been measured from the charge changing cross section in Ref. [12]. More recently, Yuan et al. have performed a systematic study of B to O isotopes with the YSOX interaction which included $(0–3)\hbar\Omega$ excitations [13] in the full *psd* model space. To the best of our knowledge for the first time we have done systematic NCSM calculations for nitrogen isotopes.

The present paper is organized as follows: In Sect. 2, the theory and formalism of NCSM is given. In Sects. 3 and 4, we have discussed the effective interactions used in the calculations and details of the

calculations, respectively. The results and discussions are presented in Sect. 5, and the conclusions summarized in Sect. 6.

2. No-core shell model formalism

The starting A-body Hamiltonian is given by

$$H_A = T_{\rm rel} + V = \frac{1}{A}\sum_{i<j}^{A}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{NN,ij}. \tag{1}$$

$T_{\rm rel}$ is the relative kinetic energy. The momenta of the individual nucleons are given by p_i ($i = 1,\ldots,A$). The nucleon mass is given by m. In the present work we have dealt with the two-body part only. $V_{NN,ij}$ is the NN interaction having with both nuclear and Coulomb parts. Next, we divide the A-nucleon infinite harmonic oscillator (HO) basis space into a finite active space (P) having all states of up to $N_{\rm max}$ HO excitations above the unperturbed ground state and an excluded space ($Q = 1-P$).

We add the center-of-mass (cm) HO Hamiltonian $H_{\rm cm}$ ($= T_{\rm cm} + U_{\rm cm}$, where $U_{\rm cm} = \frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = (\frac{1}{A})\sum_{i=1}^{A}\vec{r}_i$) to Eq. 1. As we use the Slater determinant basis, the Lawson projection term [14] is added to shift the spurious states (arising from the incorrect treatment of the centre-of-mass motion) to Eq. 1. The Hamiltonian used in the final calculations is given by

$$H^{\Omega}_{A,\rm eff} = P\left\{\sum_{i=1}^{A}\left[\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2 + V^{\Omega,A}_{ij,\rm eff}\right] + \beta\left(H_{\rm cm} - \frac{3}{2}\hbar\Omega\right)\right\}P, \tag{2}$$

where β is a parameter which is equal to 10.0 in the present calculations. Equation 2 is the Hamiltonian we get after applying unitary transformation because we are not using soft interactions (to soften the potential with the purpose of simplifying many-body calculations, these interactions are obtained by applying the unitary transformation to the two-nucleon system in momentum space with a regulator). So, we need a renormalization scheme to soften the interactions. Here, we use Okubo–Lee–Suzuki (OLS) scheme [15–17], and we now get an effective Hamiltonian which is in A-body space. We have performed NCSM calculations with the renormalized interactions keeping up to the two-body cluster terms.

For the NCSM calculations we have used the pAntoine [18,19] shell model code which has been adapted to NCSM [20]. In the case of ^{22}N, for the largest model space $N_{\rm max} = 4$, the corresponding dimension is $\sim 6.4 \times 10^7$. We have compared the NCSM results with shell model calculations using the YSOX interaction, performed using the KSHELL code [21].

3. Effective *NN* interaction

In the present work we have studied neutron-rich nitrogen isotopes with three different NN interactions: INOY, CDB2K, and next-to-next-to-next-leading order (N3LO) [22,23] (R. Machleidt, private communication). The magnitude of higher body forces decreases as we go from two-body to higher numbers, but still they are important in studying some properties of nuclei, e.g. the drip-line in oxygen isotopes can be explained only with the inclusion of three-body forces [24]. In the INOY potential, a non-local potential in coordinate space is a mixture of local and non-local parts. The behaviour of INOY is a local Yukawa tail at longer ranges ($>$ 3 fm) and non-local at short range. The form of the INOY NN interaction is given in Refs. [6,7]. This interaction reproduces the ^{3}H and ^{3}He binding energy accurately, and the results are in agreement with the experimental data without adding 3N forces. The CDB2K interaction is also a non-local interaction and charge dependent. The

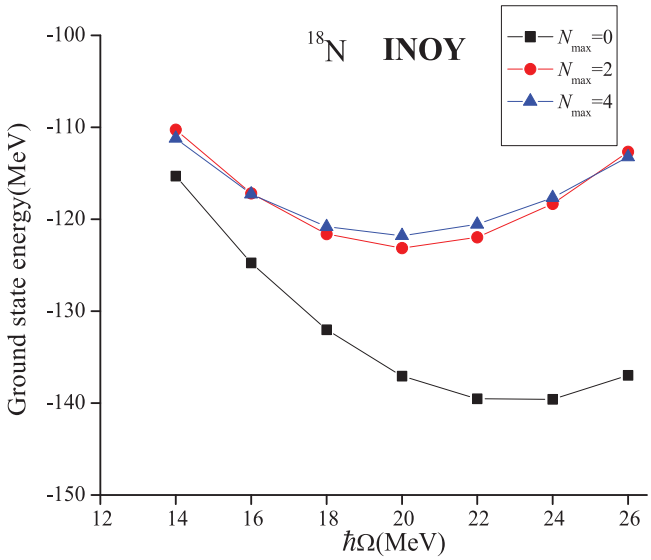

Fig. 1. The variation of ground state energy with different frequencies and different model space sizes

charge dependency is introduced due to pion mass splitting. This potential fits the p–p data below 350 MeV that was available in the year 2000. The N3LO interaction is from chiral effective field theory. Here, we use only the NN part.

4. Details of the calculations

In the present work we perform calculations for nitrogen isotopes. As we know, NCSM calculations are variational, depending on the HO frequency $\hbar\Omega$ and the size of the model space $N_{\max}$. To see this dependence, we have calculated the ground state energy for different $N_{\max}$ and $\hbar\Omega$—see Fig. 1. We are interested to see the region in which the dependence of the ground state energy on frequency is a minimum (for the largest model space). We select that frequency for our NCSM calculations. This procedure is called optimization of frequency. When we use this frequency, we get faster convergence (the computational time will be smaller). So, we have performed our calculations with the frequency $\hbar\Omega = 20$ MeV. For the other interactions we have chosen a the frequency from the literature which is suitable in this mass region. We chose $\hbar\Omega = 20$ MeV for INOY and $\hbar\Omega = 14$ MeV for N3LO interactions [2]. In the case of CDB2K, we have taken $\hbar\Omega = 12$ MeV [5].

5. Results and discussions

We performed calculations using INOY at $\hbar\Omega = 20$ MeV, and CDB2K and N3LO interactions at 12 and 14 MeV, respectively. We have also compared our INOY results at $\hbar\Omega = 22$ MeV. The energy spectra are shown in Figs. 2 and 3. In the case of ^{18}N, the ground state is correctly reproduced by the INOY NN and YSOX interactions, while the other two interactions give 2^- as a ground state. The order of the energy states is correct with INOY ($\hbar\Omega = 20$ MeV) and YSOX only. The calculated 1^-_2 state is at a higher energy (> 2.5 MeV) with the INOY interaction (except for $N_{\max} = 0$). The NCSM results for $N_{\max} = 4$ with INOY ($\hbar\Omega = 22$ MeV) are compressed in comparison to the CDB2K interaction.

For ^{20}N, the results with the INOY ($\hbar\Omega = 22$ MeV) interaction are better than the other interactions. Although the ground state is correctly reproduced by all three interactions, the higher states are not in

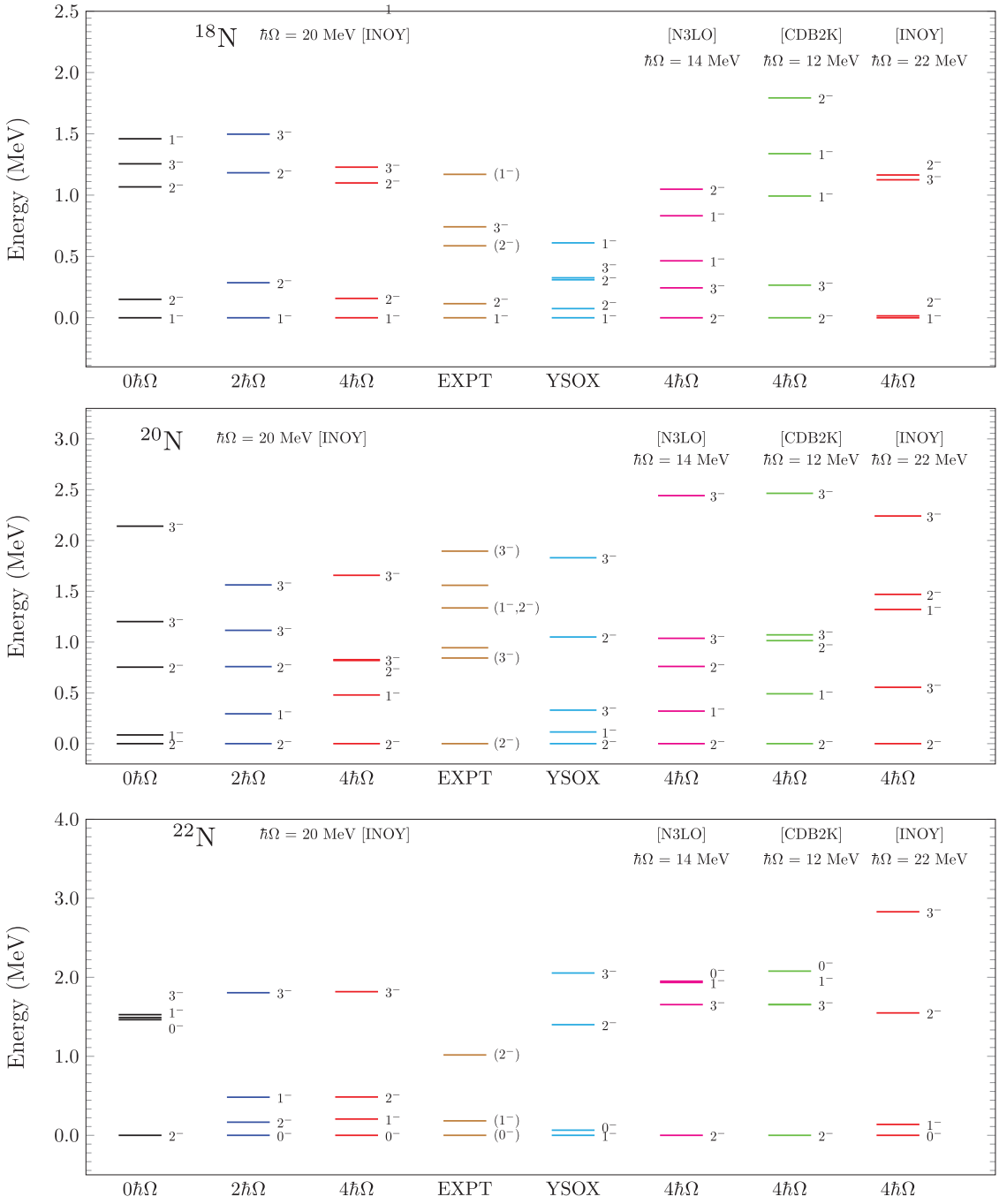

Fig. 2. The energy spectra of ^{18,20,22}N with different model space sizes. The experimental data is taken from Refs. [25,26]

agreement with the N3LO and CDB2K interactions. The first 3^- state is close to the experimental data with INOY ($\hbar\Omega = 20$ MeV) and 1^- is close to the experimental data with INOY ($\hbar\Omega = 22$ MeV).

In the case of ^{22}N, only the INOY interaction can reproduce the correct ground state 0^- and level ordering with both the frequencies. All the other interactions are unable to produce the correct ground state and level ordering of the energy states.

In the case of ^{19}N, INOY ($\hbar\Omega = 20$ MeV) and the other interactions reproduce the correct ground state $1/2^-$, though not all the states have yet been confirmed experimentally. The ground and first two

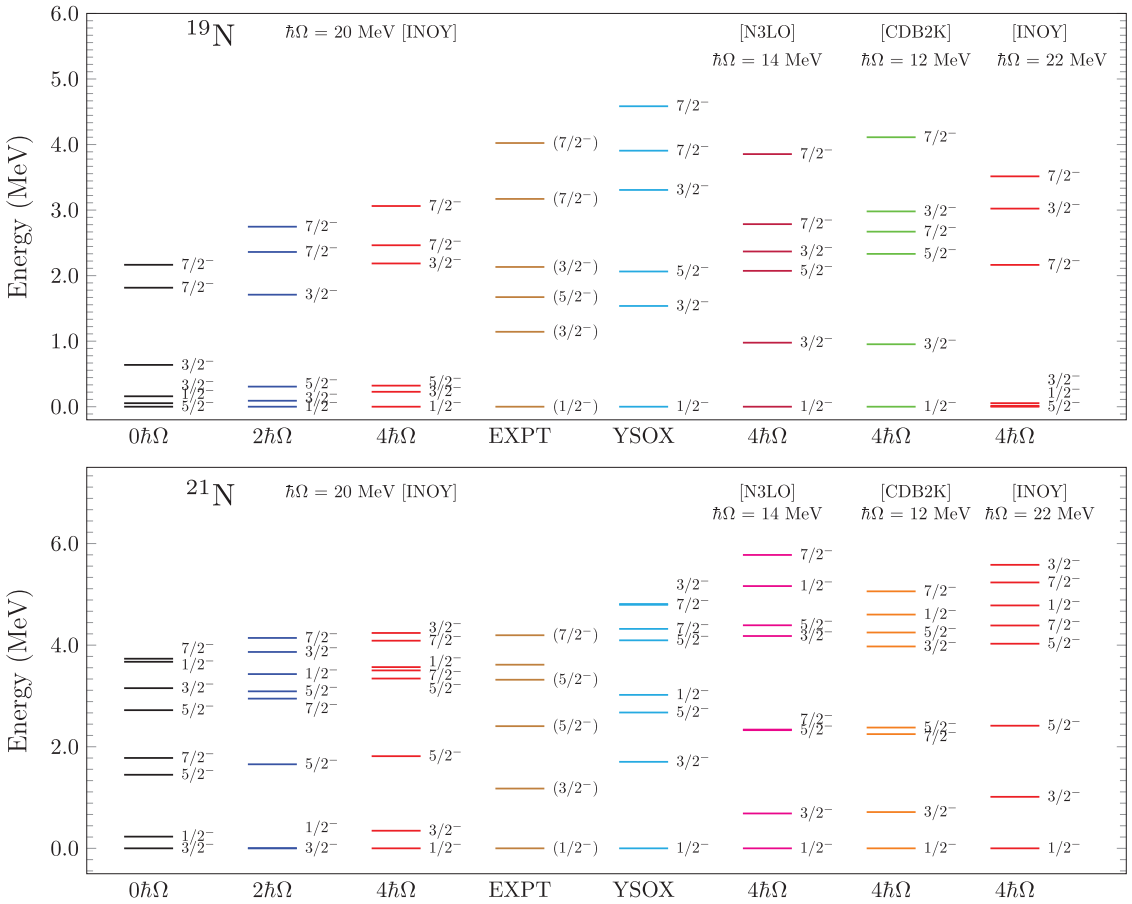

Fig. 3. The energy spectra of ^{19,21}N with different model space sizes. The experimental data is taken from Ref. [25]

excited states are very compressed with INOY at both the frequencies, in comparison with the other interactions. The N3LO interaction gives better results for the energy states and the level ordering is correct compared to the experimental one. Overall the INOY interaction gives compressed energy levels.

For ^{21}N, the ground state is correctly reproduced. Higher states have not yet been confirmed experimentally. All the interactions give the first excited state as $3/2^-$. Similarly, the second excited state seems to be $5/2^-$. For higher states, we are not sure about the spin prediction. So, from our NCSM calculations it is clear that the INOY interaction, which includes the effect of three-body forces, is suitable for studying the neutron-rich nitrogen isotopes. The inclusion of $3N$ forces is important to reproduce correct spectra with the CDB2K and N3LO interactions.

Figure 4 shows the occupancy of the first two states of nitrogen isotopes with the INOY ($\hbar\Omega$ = 20 MeV), CDB2K, and N3LO interactions corresponding to the $N_{\max} = 4$ model space size. For $N_{\max} = 4$ we have taken 28 orbitals. Here, we have shown the occupancy up to *fp* space because the occupancy of higher orbitals is very small to visualize. Although the magnitudes of the occupancies of higher orbitals are very small, they are still important in the calculation. The contribution of neutron occupancy from $0d_{3/2}$ and $1s_{1/2}$ orbitals for the CDB2K and N3LO interactions is larger in comparison to INOY interaction. This larger occupancy is also reflected in the energy spectra. The CDB2K and N3LO results are similar for the ground state spin and first excited state; however, the

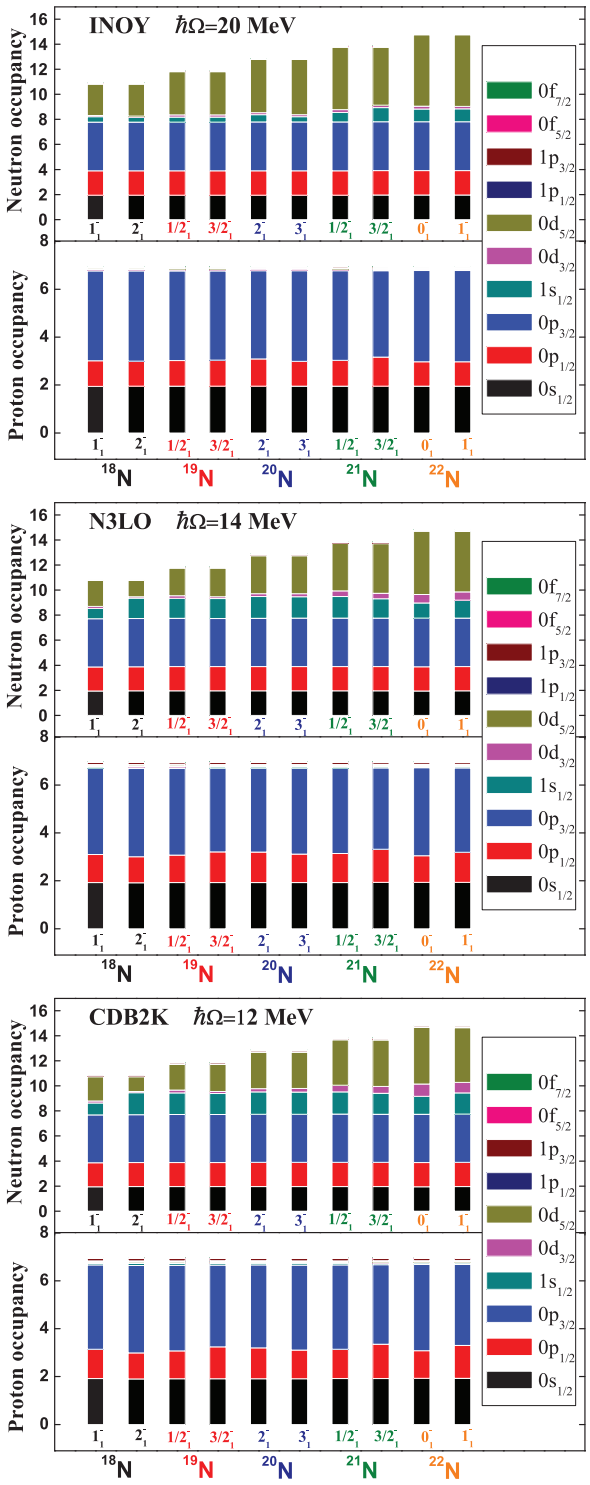

Fig. 4. The occupancy of different orbits for nitrogen isotopes using INOY, N3LO, and CDB2K interactions

occupancies for the INOY interaction are different, and for this interaction we get results which differ from the other two interactions. In Fig. 5, the calculated ground state energy for $^{18-22}$N isotopes using INOY and YSOX interactions follow the same trend as the experimental data. The ground state energy for nitrogen isotopes with the other interactions are given in Table 1, in which the results with

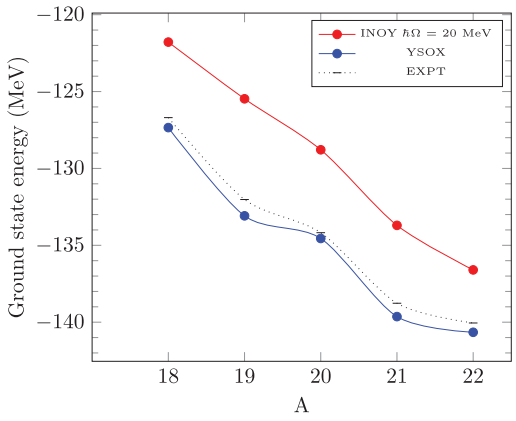

Fig. 5. Comparison of calculated and experimental ground state energies of N isotopes with the INOY and YSOX interactions

Table 1. The ground state energies (in MeV) for nitrogen isotopes using YSOX, INOY ($\hbar\Omega = 20$ MeV), N3LO ($\hbar\Omega = 14$ MeV), and CDB2K ($\hbar\Omega = 12$ MeV) interactions.

Nucleus	EXP	YSOX	INOY	N3LO	CDB2K
^{18}N	−126.695	−127.344	−121.782	−112.036	−102.979
^{19}N	−132.025	−133.083	−125.471	−117.084	−107.616
^{20}N	−134.180	−134.556	−128.788	−119.857	−109.921
^{21}N	−138.768	−139.637	−133.702	−124.769	−114.278
^{22}N	−140.052	−140.657	−136.560	−127.114	−116.052

N3LO and CDB2K are a long way from the experimental data. If we go to higher $N_{\max}$, the results will come closer to the experimental ground state energies.

6. Conclusions

We have performed NCSM calculations with different interactions (INOY, N3LO, and CDB2K) for neutron-rich nitrogen isotopes. We have also compared our NCSM results with the recently developed YSOX interaction for the *psd* space from the Tokyo group. In ^{18}N, the INOY and YSOX interactions predict the second excited state as 2^-. For ^{20}N, the results of the INOY ($\hbar\Omega = 22$ MeV) interaction are better than the YSOX interaction. For ^{22}N, the INOY results for the ground and first excited states are better than the YSOX interaction. The N3LO and CDB2K interactions are unable to predict the correct ground state. For ^{19}N, the NCSM results with N3LO are much better.

Acknowledgments

AS acknowledges financial support from MHRD (Government of India) for her Ph.D. thesis work. We would like to thank Prof. Petr Navrátil for providing us with his *NN* effective interaction code, and to Prof. Christian Forssén for pAntoine. We would also like to thank Prof. Ruprecht Machleidt for valuable comments on this article, and Prof. Toshio Suzuki for the YSOX interaction. PCS acknowledges the hospitality extended to him during his stay at TRIUMF.

References

[1] P. Navrátil, S. Quaglioni, I. Stetcu, and B. R. Barrett, J. Phys. G: Nucl. Part. Phys. **36**, 083101 (2009).
[2] B. R. Barrett, P. Navrátil, and J. P. Vary, Prog. Part. Nucl. Phys. **69**, 131 (2013).

[3] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).
[4] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000).
[5] C. Forssén, R. Roth, and P. Navrátil, J. Phys. G: Nucl. Part. Phys. **40**, 055105 (2013).
[6] P. Doleschall and I. Borbély, Phys. Rev. C **62**, 054004 (2000).
[7] P. Doleschall, I. Borbély, Z. Papp, and W. Plessas, Phys. Rev. C **67**, 064005 (2003).
[8] R. Machleidt, Phys. Rev. C **63**, 024001 (2001).
[9] D. Sohler et al., Phys. Rev. C **77**, 044303 (2008).
[10] C. S. Sumithrarachchi et al., Phys. Rev. C **81**, 014302 (2010).
[11] C. Rodríguez-Tajes et al., Phys. Rev. C **83**, 064313 (2011).
[12] S. Bagchi et al., Phys. Lett. B **790**, 251 (2019).
[13] C. Yuan, T. Suzuki, T. Otsuka, F. Xu, and N. Tsunoda, Phys. Rev. C **85**, 064324 (2012).
[14] D. H. Gloeckner and R. D. Lawson, Phys. Lett. B **53**, 313 (1974).
[15] K. Suzuki and S. Y. Lee, Prog. Theor. Phys. **64**, 2091 (1980).
[16] K. Suzuki, Prog. Theor. Phys. **68**, 246 (1982).
[17] S. Ôkubo, Progr. Theor. Phys. **12**, 603 (1954).
[18] E. Caurier and F. Nowacki, Acta Phys. Pol. B **30**, 705 (1999).
[19] C. Forssén, B. D. Carlsson, H. T. Johansson, D. Sääf, A. Bansal, G. Hagen, and T. Papenbrock, Phys. Rev. C **97**, 034328 (2018).
[20] E. Caurier, P. Navrátil, W. E. Ormand, and J. P. Vary, Phys. Rev. C **64**, 051301(R) (2001).
[21] N. Shimizu, arXiv:1310.5431v1 [nucl-th] [Search INSPIRE].
[22] D. R. Entem, and R. Machleidt, Phys. Rev. C **68**, 041001(R) (2003).
[23] R. Machleidt and D. R. Entem, Phys. Rep. **503**, 1 (2011).
[24] T. Otsuka, T. Suzuki, J. D. Holt, A. Schwenk, and Y. Akaishi, Phys. Rev. Lett. **105**, 032501 (2010).
[25] National Nuclear Data Center, https://www.nndc.bnl.gov/.
[26] C. R. Hoffman et al., Phys. Rev. C **88**, 044317 (2013).