Daejeon 16 NN Interaction

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Abstract

We have developed a realistic nucleon-nucleon (NN) interaction, dubbed Daejeon16. We start from a SRG (similarity renormalization group) evolved chiral N3LO interaction. We then apply PETs (phase-equivalent transformations) to the SRG-evolved interaction. It turned out that the obtained in such a way Daejeon16 NN interaction provides a good description of various observables in light nuclei without NNN forces. In this contribution, we present our new results for some selected nuclei using the *ab initio* no-core shell model (NCSM) with the Daejeon16 interaction. One of the interesting results is that the *ab initio* NCSM with Daejeon16 clearly demonstrates the phenomenon of parity inversion in ¹¹Be, i. e., the ground state in ¹¹Be has the spin-parity $1/2^+$ in experiments contrary to the expectation from the conventional shell model.

Keywords: No-core shell model; NN interaction; parity inversion

1 Introduction

As the advent of new rare isotope (RI) facilities such as FAIR, FRIB, HIRFL, NICA, RAON, etc., we have much more opportunities to resolve big questions in science. Nuclear theory for rare isotopes should be timely developed to face new precise observables from the forthcoming RI facilities which can produce exotic nuclei near the nuclear drip line. Thanks to the rapid developments of high performance supercomputers, we have a good chance to conduct a rigorous study of nuclear structures and reactions using fundamental (or realistic) nuclear interactions based on quantum chromodynamics (QCD). Several promising *ab initio* methods have been developed for nuclear structure and reactions [1–5].

The *ab initio* theory requires a high-quality realistic inter-nucleon interaction to provide predictions for binding energies, spectra and other observables in nuclei with

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mass up to A \sim 20 and selected heavier nuclear systems around closed shells. Therefore, it is important to develop realistic nucleon-nucleon (NN) interactions with better convergence that require less computational resources. In Ref. [6], we developed a realistic NN interaction, dubbed Daejeon16, starting from a chiral N3LO interaction which is SRG (similarity renormalization group) evolved. Then, we apply PETs (phase-equivalent transformations) to the SRG-evolved interaction. It turned out that Daejeon16 provides a good description of various observables in light nuclei without NNN forces and also generates rapid convergence in ab initio calculations.

In this short write-up, after a brief description of Daejeon16, we present some recent results from *ab initio* nuclear studies using the Daejeon16 NN interaction, with an emphasis on the ground-state parity inversion in 11 Be.

2 Daejeon16 and applications

Nuclei are composed of nucleons (protons and neutrons) and their properties such as the binding energy and radius are largely governed by the nuclear force, i. e., the strong interaction. Therefore, nuclear forces are at the core of the nuclear structure studies. Meson exchange theory has been successfully applied to obtain realistic nuclear potentials such as CD-Bonn, Argonne V18, etc. A bit more down to the mother theory of the nuclear force, i. e., QCD, nuclear interactions from the chiral effective field have been developed: N2LO, N3LO, etc. For ab initio nuclear studies, the JISP16 interaction [7], which is phenomenological, has been widely used. Here, JISP stands for J-matrix Inverse Scattering Potential. Recently, a new nuclear force dubbed 'Daejeon16' has been developed from a N3LO NN interaction. Daejeon is a city in Korea where a next generation RI facility called RAON will be built and 16 is from ¹⁶O which is the heaviest nucleus used in fitting process. In Ref. [6], the authors start from Idaho N3LO NN interaction and apply to it PETs which preserve scattering phase shifts and bound state energy of the two-nucleon system (deuteron). The optimal set of PET parameters is determined to describe the binding energies of ³H, ⁴He, ⁶Li, ⁸He, ¹⁰B, ¹²C and ¹⁶O nuclei and excitation energies of a few narrow excited states: the two lowest excited states with $(J^{\pi}, T) = (3^+, 0)$ and $(0^+, 1)$ in ⁶Li and the first excited states $(1^+, 0)$ in 10 B and $(2^+, 0)$ in 12 C. For a sketch about the procedure to obtain JISP16 and Daejeon16, we refer to Fig. 1.

It turned out that the Daejeon16 works well for light p-shell nuclei compared with other established interactions such as JISP16, for instance see Fig. 2.

Now, we move on to some recent results using the Daejeon16 interaction.

2.1 Parity inversion in ¹¹Be

¹¹Be shows an interesting feature which is opposite to the expectation from the conventional shell model. Experimentally, the ground state of ¹¹Be is 1/2⁺ [9], while it was expected to be a 1/2⁻ state in the conventional shell model. To tackle the issue of the parity inversion in ¹¹Be, we evaluate the spectrum of ¹¹Be using the *ab initio* no-core shell model (NCSM) with the Daejeon16 interaction and extrapolate the results to the infinite basis space using the method of Ref. [8]. For the two lowest-lying states, we obtain

$$1/2^+: -65.22(7) \text{ MeV}, \quad 1/2^-: -64.63(2) \text{ MeV}.$$

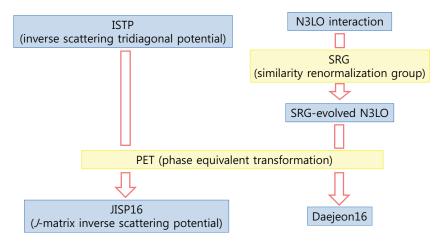


Figure 1: A sketch of the procedure to obtain Daejeon16 compared with JISP16.

The numbers in parenthesis show the uncertainties of the extrapolations of the energies. This result is compared with the experiment and with the one from JISP16 in Fig. 3, which shows that the *ab initio* NCSM with Daejeon16 successfully reproduces the parity inversion in ¹¹Be. Note that the JISP16 is unable to reproduce the

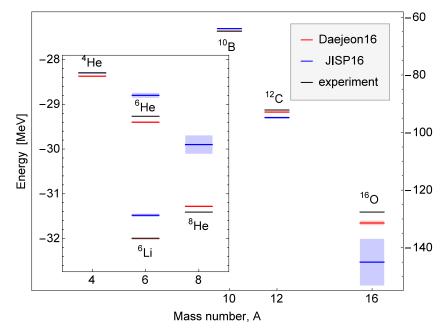


Figure 2: The ground state energies of several p-shell nuclei using Daejeon16 and JISP16 compared with experiment. The calculations were performed within the NCSM and extrapolated to the infinite basis space using the methods of Ref. [8]; the shaded areas show the uncertainties of the extrapolations. It is noted that all shown nuclei were used to PET fitting as mentioned in the text.

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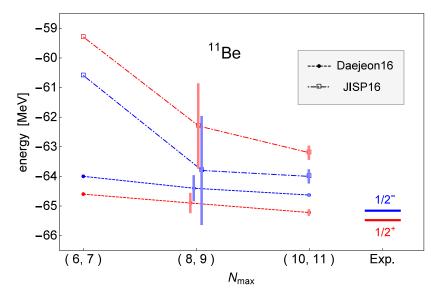


Figure 3: Energies of the ground and first-excited states of 11 Be calculated within the *ab initio* NCSM with Daejeon16 and JISP16. The values are obtained using extrapolation B [8] for each highest $N_{\rm max}$ at the variational minima and the error bars are given as the differences with the previous $N_{\rm max}$ extrapolation. Experimental values are taken from Refs. [9,10].

parity inversion (the current evaluation of the uncertainties of the JISP16 results is yet preliminary).

For an earlier study of the parity inversion in ab initio nuclear theory, we refer to Ref. [11].

2.2 Deep learning for ab initio nuclear theory

Recently, we proposed a feed-forward artificial neural network (ANN) method as an extrapolation tool for *ab initio* nuclear theory [12,13]. Using the *ab initio* NCSM with Daejeon16 and the feed-forward ANN method, we predicted the ground-state energy and the ground-state point-proton root-mean-square (rms) radius of 6 Li. We observed that our results are nearly converged at $N_{\rm max}=70$ (ground-state energy) and $N_{\rm max}=90$ (ground-state point-proton rms radius). Therefore, we concluded that the designed ANNs are sufficient to produce results for these two very different observables utilizing the NCSM results obtained in small basis spaces that exhibit the independence of basis space parameters in the limit of extremely large matrices [12,13].

Before closing this Section, we refer to Refs. [14,15], where resonance states such as tetraneutron and 5 He were studied in the framework of the single-state harmonic oscillator representation of scattering equations and the *ab initio* NCSM with Daejeon16 and some other modern NN interactions.

3 Summary

In this contribution, we briefly introduced the Daejeon16 NN interaction. We then presented some of interesting results from the *ab initio* NCSM studies with Daejeon16 and some other NN interactions such as JISP16. A remarkable result is that the parity inversion in ¹¹Be is successfully reproduced in our study with Daejeon16.

We will continue to use Daejeon16 and some other modern NN interactions for various *ab initio* nuclear studies to be well-prepared for the forthcoming RI facilities.

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References

- [1] S. C. Pieper and R. B. Wiringa, Annu. Rev. Nucl. Part. Sci. 51, 53 (2001).
- [2] K. Kowalski, D. J. Dean, M. Hjorth-Jensen, T. Papenbrock and P. Piecuch, Phys. Rev. Lett. 92, 132501 (2004).
- [3] B. R. Barrett, P. Navrátil and J. P. Vary, Prog. Part. Nucl. Phys. 69, 131 (2013).
- [4] E. Epelbaum, H. Krebs, D. Lee and U. G. Meißner, Phys. Rev. Lett. 106, 192501 (2011).
- [5] P. Navrátil, S. Quaglioni, I. Stetcu and B. R. Barrett, J. Phys. G 36, 083101 (2009).
- [6] A. M. Shirokov, I. J. Shin, Y. Kim, M. Sosonkina, P. Maris and J. P. Vary, Phys. Lett. B 761, 87 (2016).
- [7] A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, Phys. Lett. B 644, 33 (2007).
- [8] P. Maris, J. P. Vary and A. M. Shirokov, Phys. Rev. C 79, 014308 (2009).
- [9] J. H. Kelley, E. Kwan, J. E. Purcell, C. G. Sheu and H. R. Weller, Nucl. Phys. A 880, 88 (2012).
- [10] M. Wang, G. Audi, F. G. Kondev, W. J. Huang, S. Naimi and X. Xu, Chin. Phys. C 41, 030003 (2017).
- [11] A. Calci, P. Navrátil, R. Roth, J. Dohet-Eraly, S. Quaglioni and G. Hupin, Phys. Rev. Lett. 117, 242501 (2016).

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[12] G. A. Negoita, G. R. Luecke, J. P. Vary, P. Maris, A. M. Shirokov, I. J. Shin, Y. Kim, E. G. Ng and C. Yang, in Proc. Ninth Int. Conf. Comput. Logics, Algebras, Programming, Tools, and Benchmarking COMPUTATION TOOLS 2018, Barcelona, Spain, February 18–22, 2018. IARIA, 2018, p. 20, arXiv:1803.03215 [physics.comp-ph] (2018).

- [13] G. A. Negoita, J. P. Vary, G. R. Luecke, P. Maris, A. M. Shirokov, I. J. Shin, Y. Kim, E. G. Ng, C. Yang, M. Lockner and G. M. Prabhu, Phys. Rev. C 99, 054308 (2019).
- [14] A. M. Shirokov, Y. Kim, A. I. Mazur, I. A. Mazur, I. J. Shin and J. P. Vary, AIP Conf. Proc. 2038, 020038 (2018).
- [15] A. M. Shirokov, A. I. Mazur, I. A. Mazur, E. A. Mazur, I. J. Shin, Y. Kim, L. D. Blokhintsev and J. P. Vary, Phys. Rev. C 98, 044624 (2018).