Nucleus-Dependent Valence-Space Approach to Nuclear Structure

S. R. Stroberg,[1,*] A. Calci,[1] H. Hergert,[2] J. D. Holt,[1] S. K. Bogner,[2] R. Roth,[3] and A. Schwenk[3,4,5]
[1]TRIUMF 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada
[2]Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48844, USA
[3]Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany
[4]ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany
[5]Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany
(Received 11 July 2016; revised manuscript received 26 September 2016; published 20 January 2017)

We present a nucleus-dependent valence-space approach for calculating ground and excited states of nuclei, which generalizes the shell-model in-medium similarity renormalization group to an ensemble reference with fractionally filled orbitals. Because the ensemble is used only as a reference, and not to represent physical states, no symmetry restoration is required. This allows us to capture three-nucleon ($3N$) forces among valence nucleons with a valence-space Hamiltonian specifically targeted to each nucleus of interest. Predicted ground-state energies from carbon through nickel agree with results of other large-space *ab initio* methods, generally to the 1% level. In addition, we show that this new approach is required in order to obtain convergence for nuclei in the upper p and sd shells. Finally, we address the $1^+/3^+$ inversion problem in ^{22}Na and ^{46}V. This approach extends the reach of *ab initio* nuclear structure calculations to essentially all light- and medium-mass nuclei.

DOI: 10.1103/PhysRevLett.118.032502

The development of a first-principles, or *ab initio*, theoretical description of atomic nuclei is a central challenge in nuclear physics. This task is complicated by the combined difficulties of not having an exact form for nuclear interactions and the great complexity in solving the nuclear many-body problem. Regardless, controlled predictions with uncertainty estimates are vital to guide efforts of rare-isotope beam facilities [1,2], to constrain nucleosynthesis models predicting the origin of heavy elements in the Universe [3,4], and to quantify nuclear structure effects in searches for beyond-standard-model physics such as neutrinoless double-beta decay [5], dark matter [6,7], and superallowed beta decay [8]. Developments in chiral effective field theory [9,10], similarity renormalization group (SRG) [11], and *ab initio* many-body techniques [12–17] provide a unified picture for these efforts, while three-nucleon ($3N$) forces have emerged as an essential component of nuclear forces [2,18–29]. In this Letter, we present a powerful many-body development which significantly extends the range of systems in which nuclear forces may be tested.

One promising approach to the many-body problem is offered by the shell-model paradigm, where a valence-space Hamiltonian of tractable dimension is decoupled from the much larger Hilbert space and diagonalized. This allows the treatment of excited states, deformation, and transitions in open-shell systems within a single framework. Building upon earlier perturbative approaches [30–32], *ab initio* methods now provide shell-model Hamiltonians in a nonperturbative manner [33–39], similar to recent work for chemical systems, see, e.g., Ref. [40]. However, the inclusion of residual $3N$ forces [41] among valence particles [42,43] remains problematic in nonperturbative methods and leads to a loss in accuracy compared to large-space *ab initio* calculations [38].

A first attempt to address this shortcoming within the in-medium similarity renormalization group (IM-SRG) framework [38] used normal ordering with respect to closed subshells in the valence space, but gave no clear prescription for systems far from closed shells. In this Letter, we generalize our approach to a reference with fractionally occupied orbits, capturing the dominant effects of neglected $3N$ forces among valence nucleons. Since these effects scale nontrivially with mass number A, the standard shell-model approach of constructing one Hamiltonian for an entire region [44,45] appears to be insufficient from an *ab initio* standpoint. Therefore, we adopt a new strategy and decouple a targeted valence-space Hamiltonian for each nucleus with the IM-SRG, using a specialized reference for the normal ordering. The resulting ground-state energies agree well with large-space *ab initio* methods, generally to the 1% level. We highlight the improvement for systems far from closed shells in ^{22}Na and ^{46}V, where the $1^+_1/3^+_1$ level-inversion problem is addressed for the first time in an *ab initio* framework.

A key feature of the IM-SRG is the use of operators that are normal ordered with respect to a particular reference state $|\Phi_0\rangle$. The Hamiltonian, which in free space has one-, two-, and three-body pieces, is rewritten exactly as [21]

$$H = E_0 + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}, \quad (1)$$

where the braces indicate normal ordering with respect to the reference for any string of creation or annihilation operators such that $\langle\Phi_0|\{a_1^\dagger \ldots a_N\}|\Phi_0\rangle = 0$. To make the calculation tractable, the residual $3N$ interaction W_{ijklmn} is neglected, leading to the normal-ordered two-body approximation [18,46,47]. Naively, the quality of this approximation depends on how well $|\Phi_0\rangle$ approximates the eigenstate of the full Hamiltonian.

In the original implementation of the IM-SRG [15,48,49], $|\Phi_0\rangle$ was taken to be a single Slater determinant, limiting its applicability to ground states of closed-shell nuclei such as ^{16}O. The multireference formulation [21,26,50] extended the reach to general open-shell nuclei, although current implementations are limited to ground states of even-even nuclei. The shell-model variant [34,35,38] of the IM-SRG uses the core of the valence space as the reference—e.g., ^{16}O for an *sd* valence space—enabling the treatment of open-shell nuclei and excited states.

Comparing the results of the above approaches provides a test of the validity of their respective approximations. As discussed in Refs. [35,38], the shell-model IM-SRG gives good agreement for few valence particles, but as more are added, the results become overbound relative to large-space methods. This may be understood by considering that, for the choice of interaction used in those studies, the initial $3N$ forces combined with those induced by SRG and IM-SRG transformations produce a net repulsion [51]. The bulk of this repulsive $3N$ force is captured by the normal-ordered two-body approximation. However, if the normal ordering is performed with respect to the core, the repulsive $3N$ interaction among valence nucleons is neglected, leading to overbinding that grows with the number of valence particles.

A first attempt to address this issue, illustrated schematically in Fig. 1(a), is to normal order with respect to the nearest closed shell (e.g., using a ^{22}O reference to calculate ^{23}F), while still decoupling the core [38]. At the end of the decoupling, the interaction is re-normal ordered with respect to the core for use in a standard shell-model code.

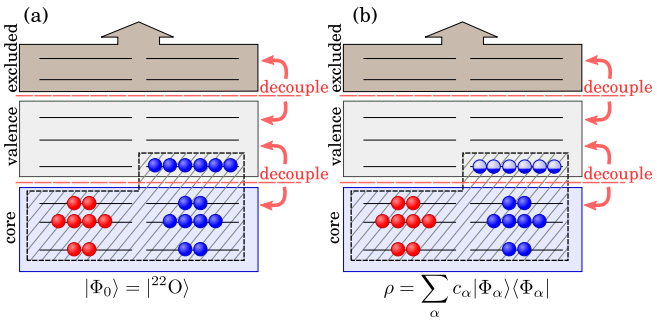

FIG. 1. Examples of (a) a reference which is different from the core, here ^{22}O, and (b) an ensemble reference with fractional filling, here approximating ^{18}O. Note that in both cases the valence space is identical.

This final transformation, carried out at the two-body level, is unitary and preserves the decoupling. This approach, referred to as targeted normal ordering (TNO), largely corrects the discrepancy between the shell-model results and other large-space methods for the oxygen and fluorine chains.

One caveat is that some doubly open-shell nuclei (e.g., ^{22}Na) are far from a closed shell. A physically intuitive next step, illustrated in Fig. 1(b), would be to "interpolate" between closed shells with a fractional occupation of the last shell (e.g., a $0d_{5/2}$ occupation fraction of 0.5 for ^{22}Na), ideally without the additional computational effort associated with the multireference formulation. As discussed in Refs. [52,53], this so-called equal-filling approximation formally amounts to employing an ensemble or mixed-state reference defined by a density matrix $\rho = \sum_\alpha c_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha|$, with normal ordering defined using a trace: $\mathrm{Tr}(\rho\{a_1^\dagger \ldots a_N\}) = 0$ [54,55]. The coefficients c_α are chosen such that the desired occupations are achieved (see the Supplemental Material for details [56]). Note that, for our present purposes, we merely require the existence of such an ensemble so that we are formally justified in using fractional occupation numbers. For closed shells, this ensemble normal ordering (ENO) reduces to the TNO described above.

Such a reference is problematic for ground-state methods (e.g., single- or multireference IM-SRG, coupled cluster, Hartree-Fock-Bogoliubov) because they are designed to decouple a pure eigenstate of the Hamiltonian. However, in the valence-space approach, the reference merely provides a convenient way to arrange operators (also see [60]). Even if the ensemble is not an eigenstate of angular momentum or particle number, the Hamiltonian conserves these quantities throughout the calculation. While the ensemble does not accurately represent any particular state in the targeted system, it is reasonable (and results confirm) that having the right number of particles in roughly the right configuration is a sufficiently good approximation. Indeed, the exact eigenstate of the full Hamiltonian is not necessarily the optimal reference for making the normal-ordered two-body approximation [40]. Reference [61] demonstrated that little is gained by improving the reference beyond a low-order approximation, and similar observations have been made in nuclear matter [62].

Technical details of the calculation are presented as Supplemental Material [56]. However, we summarize the essential points here. As in Ref. [38], we use a chiral *NN* interaction at N^{3}LO [10,63], and a chiral $3N$ interaction at N^{2}LO [64], SRG evolved in a harmonic oscillator basis [65]. We transform this interaction to the Hartree-Fock basis of the ENO reference, at which point the normal-ordered three-body part is discarded. The valence space is decoupled from the full Hilbert space using the IM-SRG, and finally, the resulting interaction is diagonalized with a standard shell-model code [66]. For comparison, in a few

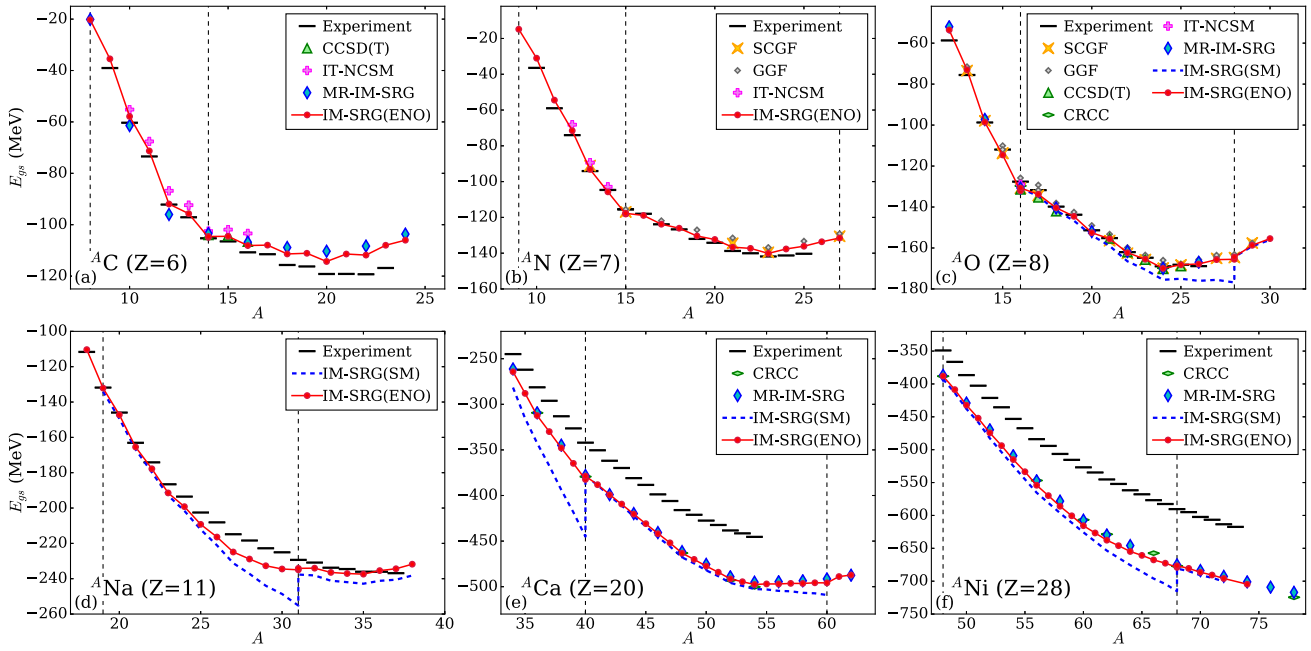

FIG. 2. Ground-state energies of (a) carbon (b) nitrogen, (c) oxygen, (d) sodium, (e) calcium, and (f) nickel isotopic chains, calculated with multireference IM-SRG (MR-IM-SRG) [21,26], coupled cluster (CCSD(T)) [36], completely renormalized coupled cluster (CRCC) [67], importance-truncated no-core shell model (IT-NCSM, see text), self-consistent Green's function (SCGF), and Gor'kov Green's function (GGF) [68], compared to experiment [69]. The IM-SRG (SM) curves use a core reference, while the curves labeled IM-SRG (ENO) use an ensemble reference. Dashed vertical lines indicate neutron harmonic-oscillator shell closures. Calcium isotopes are calculated with $e_{\max} = 14$, consistent with the MR-IM-SRG calculations.

cases, we also perform importance-truncated no-core shell model (IT-NCSM) [17] calculations, fully including 3*N* forces and extrapolating to an infinite model space.

As a first test of this new approach, we investigate ground-state energies of medium-mass isotopic chains. We note here that the development of chiral interactions is still in progress and that all currently available interactions, including the one used here, have known systematic deficiencies [26,27,67]. Consequently, the target for success is not experimental data, but other many-body methods employing the same interaction, *in cases where those methods are reliable.* It is useful to benchmark in the oxygen isotopic chain, where published results from several different many-body methods are available, and no complications from deformation arise. As illustrated in Fig. 2(c), the shell-model IM-SRG approach, with a core reference state (dashed line), leads to increasing error as valence particles are added. At harmonic-oscillator shell closures, changing the core leads to a large change in the ground-state energy. ENO corrects this deficiency, yielding energies that agree well with other methods throughout the chain. Similar improvement is seen in the calcium and nickel isotopic chains with a few notable discrepancies. An analogous pattern was seen in deformed neon isotopes [38,50], where the multireference IM-SRG appeared to decouple an intrinsically spherical excited state. For the nickel isotopes, we stop at ^{74}Ni because the valence-space diagonalization becomes expensive (though not unfeasible). Techniques such as importance truncation [70] provide a clear path forward for such nuclei.

The valence-space approach is not restricted to the vicinity of shell closures; to demonstrate this versatility, we present the carbon, nitrogen, and sodium isotopic chains in Figs. 2(a), 2(b), and 2(d), respectively. The resulting ground-state energies agree well with those obtained by other many-body methods [36,68,71,72], though the binding energy of ^{12}C differs significantly from those obtained with IT-NCSM and multireference IM-SRG. While some discrepancy should be due to the normal-ordering approximation, we leave a more thorough investigation for future work. No previous *ab initio* results exist for sodium isotopes.

An important issue arising in the upper *p* shell, illustrated in Fig. 3(a) for ^{16}O, is that shell-model IM-SRG calculations (using a ^{4}He reference) do not converge with $e_{\max}$, while ENO calculations do. Similar behavior is observed for other upper-*p*-shell nuclei. The most likely reason is that the Hartree-Fock single-particle wave functions for the ^{4}He and ^{16}O reference states are quite different. Since the former are not optimized for ^{16}O, we expect that three- and higher-body operators induced by the IM-SRG flow are necessary for a proper description; their omission leads to the observed lack of

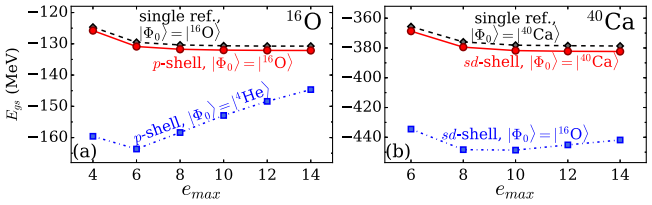

FIG. 3. (a) Convergence of the ^{16}O ground-state energy as a function of $e_{\max}$. The curve labeled "single ref." is obtained by directly decoupling a single Slater determinant representing the ground state. The other curves are obtained by decoupling the valence $0p$ shell, using either a ^{4}He or ^{16}O Slater determinant as the normal-ordering reference $|\Phi_0\rangle$. (b) The analogous case for ^{40}Ca in the sd shell.

convergence. This effect likely arises in other methods deriving shell-model interactions [33,37,39] and, as shown in Fig. 3(b), is also present in the upper sd shell, albeit more weakly.

Calculations of ^{16}O and ^{40}Ca provide a check on a major source of uncertainty in the valence-space approach since they consist of a single Slater determinant in the p and sd shells, respectively. The valence-space results should be identical to those of the single-reference IM-SRG, and any discrepancy must be due to the additional valence-space decoupling. If this decoupling were perfectly unitary, it would not cause any error. Since in practice the IM-SRG flow equations are truncated at the two-body level, unitarity is spoiled and a small error (approximately 1%) arises due to this extra decoupling step.

In Fig. 4, we show the ground-state energy per nucleon for several closed p- and sd-shell nuclei. Clearly, the ENO results agree well with the large-space results. The circles above Fig. 4 indicate the overlap of the reference determinant with the valence-space ground state. The small overlap for ^{28}Si indicates that the reference is a poor approximation of the ground state and suggests that the single-reference calculation selects an excited 0^+ state.

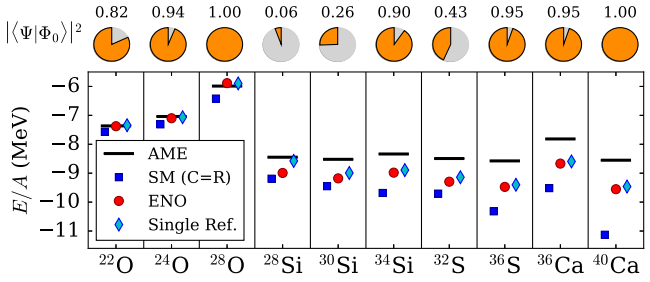

FIG. 4. Ground-state energy per nucleon of closed sd-shell nuclei, calculated with the shell-model IM-SRG using the core as the reference SM(C = R), the ENO approach (here equivalent to TNO), and single-reference IM-SRG. The black bars indicate the experimental values [69], and the orange circles indicate the overlap of the ENO ground-state wave function $|\Psi\rangle$ with the reference determinant $|\Phi_0\rangle$.

Finally, 3N forces are important for spectroscopy. A famous example is ^{10}B, where 3N forces are necessary to reproduce the ordering of ground state and first excited state [73,74]. Figure 5(a) compares results obtained with various references to IT-NCSM results, which include full 3N forces. The variation of the cutoff Λ_{3N} demonstrates the sensitivity of the level ordering to the details of the 3N force. Reference [61] demonstrated that the normal-ordered two-body approximation can capture the relevant physics if an adequate reference is used. Our results show that the ENO reference meets this requirement.

The analogous sd- and pf-shell systems are ^{22}Na and ^{46}V, respectively. Results for the $1^+_1/3^+_1$ energy splittings in these nuclei are shown in Figs. 5(b) and 5(c) for two choices of reference. As these nuclei are not within reach of IT-NCSM or other large-space methods, we compare to experiment, where we observe a similar effect to that in ^{10}B. For ^{46}V, the sizable SRG-induced many-body forces for the $\Lambda_{3N} = 500$ MeV interaction lead to unreliable results [47], so we report only the $\Lambda_{3N} = 400$ MeV result. To our knowledge, these are the first *ab initio* calculations to reproduce the experimental $1^+_1/3^+_1$ ordering in these systems.

In conclusion, we have generalized the IM-SRG framework to ensemble reference states, allowing the approximate inclusion of residual 3N forces in the valence space. Results agree with other large-space *ab initio* methods to the 1% level, but now extend to ground and excited states of essentially all light and medium-mass nuclei, including deformed systems. In the case of the upper p and sd shells, the ENO approach is required to obtain converged results. For the specific cases of ^{10}B, ^{22}Na, and ^{46}V, where residual 3N forces are essential to obtain the correct $1^+_1/3^+_1$ ordering, we have shown that our new approach captures the relevant physics. The unique combination of precision, versatility, and low computational cost establishes the valence-space IM-SRG as a powerful *ab initio* tool for addressing fundamental questions in nuclei.

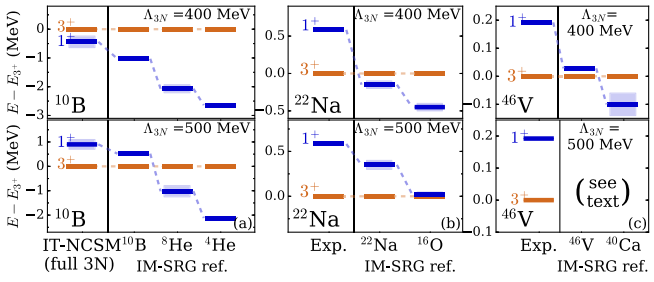

FIG. 5. (a) Energies of the lowest 1^+, 3^+ states of ^{10}B, calculated with two different cutoffs for the 3N force, $\Lambda_{3N} = 400$, 500 MeV, using both IM-SRG and IT-NCSM. The shaded bands indicate the estimated uncertainty due to model space extrapolations. For the IM-SRG calculations, results for different references $|\Phi_0\rangle$ are given. The same is shown for (b) ^{22}Na and (c) ^{46}V, comparing IM-SRG to experiment.

S. R. S. would like to thank T. D. Morris and N. Parzuchowski for enlightening discussions, and K. G. Leach for providing additional computational resources. The IM-SRG code used in this work makes use of the Armadillo C++ library [75]. TRIUMF receives funding via a contribution through the National Research Council Canada. This work was supported in part by NSERC, the NUCLEI SciDAC Collaboration under U.S. Department of Energy Grants No. DE-SC0008533 and No. DE-SC0008511, the National Science Foundation under Grant No. PHY-1404159, the European Research Council Grant No. 307986 STRONGINT, the Deutsche Forschungsgemeinschaft under Grant SFB 1245, and the BMBF under Contract No. 05P15RDFN1. Computations were performed with an allocation of computing resources at the Jülich Supercomputing Center, Ohio Supercomputer Center (OSC), and the Michigan State University High Performance Computing Center (HPCC)/Institute for Cyber-Enabled Research (iCER).

*sstroberg@triumf.ca

[1] A. B. Balantekin, J. Carlson, D. J. Dean, G. M. Fuller, R. J. Furnstahl, M. Hjorth-Jensen, R. V. F. Janssens, B.-A. Li, W. Nazarewicz, F. M. Nunes, W. E. Ormand, S. Reddy, and B. M. Sherrill, Mod. Phys. Lett. A **29**, 1430010 (2014).
[2] K. Hebeler, J. D. Holt, J. Menéndez, and A. Schwenk, Annu. Rev. Nucl. Part. Sci. **65**, 457 (2015).
[3] M. Mumpower, R. Surman, G. McLaughlin, and A. Aprahamian, Prog. Part. Nucl. Phys. **86**, 86 (2016).
[4] D. Martin, A. Arcones, W. Nazarewicz, and E. Olsen, Phys. Rev. Lett. **116**, 121101 (2016).
[5] F. T. Avignone, S. R. Elliott, and J. Engel, Rev. Mod. Phys. **80**, 481 (2008).
[6] J. Engel, S. Pittel, and P. Vogel, Int. J. Mod. Phys. E **01**, 1 (1992).
[7] P. Klos, J. Menéndez, D. Gazit, and A. Schwenk, Phys. Rev. D **88**, 083516 (2013).
[8] J. C. Hardy and I. S. Towner, Phys. Rev. C **91**, 025501 (2015).
[9] E. Epelbaum, H.-W. Hammer, and U.-G. Meißner, Rev. Mod. Phys. **81**, 1773 (2009).
[10] R. Machleidt and D. R. Entem, Phys. Rep. **503**, 1 (2011).
[11] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C **75**, 061001 (2007).
[12] J. Carlson, S. Gandolfi, F. Pederiva, S. C. Pieper, R. Schiavilla, K. E. Schmidt, and R. B. Wiringa, Rev. Mod. Phys. **87**, 1067 (2015).
[13] B. R. Barrett, P. Navrátil, and J. P. Vary, Prog. Part. Nucl. Phys. **69**, 131 (2013).
[14] G. Hagen, T. Papenbrock, M. Hjorth-Jensen, and D. J. Dean, Rep. Prog. Phys. **77**, 096302 (2014).
[15] H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rep. **621**, 165 (2016).
[16] W. Dickhoff and C. Barbieri, Prog. Part. Nucl. Phys. **52**, 377 (2004).
[17] R. Roth, Phys. Rev. C **79**, 064324 (2009).
[18] T. Otsuka, T. Suzuki, J. D. Holt, A. Schwenk, and Y. Akaishi, Phys. Rev. Lett. **105**, 032501 (2010).
[19] G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, and T. Papenbrock, Phys. Rev. Lett. **108**, 242501 (2012).
[20] A. Cipollone, C. Barbieri, and P. Navrátil, Phys. Rev. Lett. **111**, 062501 (2013).
[21] H. Hergert, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett. **110**, 242501 (2013).
[22] J. D. Holt, J. Menéndez, and A. Schwenk, Eur. Phys. J. A **49**, 39 (2013).
[23] J. D. Holt, T. Otsuka, A. Schwenk, and T. Suzuki, J. Phys. G **39**, 085111 (2012).
[24] G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, and T. Papenbrock, Phys. Rev. Lett. **109**, 032502 (2012).
[25] F. Wienholtz *et al.*, Nature (London) **498**, 346 (2013).
[26] H. Hergert, S. K. Bogner, T. D. Morris, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. C **90**, 041302 (2014).
[27] V. Somà, A. Cipollone, C. Barbieri, P. Navrátil, and T. Duguet, Phys. Rev. C **89**, 061301 (2014).
[28] G. Hagen, A. Ekström, C. Forssén, G. R. Jansen, W. Nazarewicz, T. Papenbrock, K. A. Wendt, S. Bacca, N. Barnea, B. Carlsson, C. Drischler, K. Hebeler, M. Hjorth-Jensen, M. Miorelli, G. Orlandini, A. Schwenk, and J. Simonis, Nat. Phys. **12**, 186 (2016).
[29] R. F. Garcia Ruiz *et al.*, Nat. Phys. **12**, 594 (2016).
[30] T. T. S. Kuo and G. E. Brown, Nucl. Phys. **85**, 40 (1966).
[31] M. Hjorth-Jensen, T. T. S. Kuo, and E. Osnes, Phys. Rep. **261**, 125 (1995).
[32] J. D. Holt, J. W. Holt, T. T. S. Kuo, G. E. Brown, and S. K. Bogner, Phys. Rev. C **72**, 041304 (2005).
[33] A. F. Lisetskiy, B. R. Barrett, M. K. G. Kruse, P. Navratil, I. Stetcu, and J. P. Vary, Phys. Rev. C **78**, 044302 (2008).
[34] K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. C **85**, 061304 (2012).
[35] S. K. Bogner, H. Hergert, J. D. Holt, A. Schwenk, S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett. **113**, 142501 (2014).
[36] G. R. Jansen, J. Engel, G. Hagen, P. Navratil, and A. Signoracci, Phys. Rev. Lett. **113**, 142502 (2014).
[37] E. Dikmen, A. F. Lisetskiy, B. R. Barrett, P. Maris, A. M. Shirokov, and J. P. Vary, Phys. Rev. C **91**, 064301 (2015).
[38] S. R. Stroberg, H. Hergert, J. D. Holt, S. K. Bogner, and A. Schwenk, Phys. Rev. C **93**, 051301(R) (2016).
[39] G. R. Jansen, M. D. Schuster, A. Signoracci, G. Hagen, and P. Navrátil, Phys. Rev. C **94**, 011301 (2016).
[40] T. Yanai and G. K.-L. Chan, J. Chem. Phys. **124**, 194106 (2006); **127**, 104107 (2007).
[41] Three-body forces will be induced by the decoupling of the valence space, even if they are not present in the initial Hamiltonian.
[42] C. Caesar, J. Simonis *et al.*, Phys. Rev. C **88**, 034313 (2013).
[43] J. D. Holt, J. Menéndez, J. Simonis, and A. Schwenk, Phys. Rev. C **90**, 024312 (2014).
[44] B. Brown, Prog. Part. Nucl. Phys. **47**, 517 (2001).
[45] E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves, and A. P. Zuker, Rev. Mod. Phys. **77**, 427 (2005).
[46] G. Hagen, T. Papenbrock, D. J. Dean, A. Schwenk, A. Nogga, M. Włoch, and P. Piecuch, Phys. Rev. C **76**, 034302 (2007).
[47] R. Roth, S. Binder, K. Vobig, A. Calci, J. Langhammer, and P. Navrátil, Phys. Rev. Lett. **109**, 052501 (2012).

[48] K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011).
[49] H. Hergert, S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C **87**, 034307 (2013).
[50] H. Hergert, Phys. Scr. **92**, 023002 (2017).
[51] For this Hamiltonian, we find that the effect of the 3*N* force induced by the IM-SRG flow is typically of the same sign and comparable magnitude to that of the free-space SRG evolution.
[52] T. Duguet, P. Bonche, P.-H. Heenen, and J. Meyer, Phys. Rev. C **65**, 014310 (2001).
[53] S. Perez-Martin and L. M. Robledo, Phys. Rev. C **78**, 014304 (2008).
[54] D. J. Thouless, Phys. Rev. **107**, 1162 (1957).
[55] M. Gaudin, Nucl. Phys. **15**, 89 (1960).
[56] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.118.032502, which includes Refs. [57–59], for more details.
[57] T. D. Morris, N. M. Parzuchowski, and S. K. Bogner, Phys. Rev. C **92**, 034331 (2015).
[58] S. R. White, J. Chem. Phys. **117**, 7472 (2002).
[59] W. Kutzelnigg and D. Mukherjee, J. Chem. Phys. **107**, 432 (1997).
[60] L. Kong, M. Nooijen, and D. Mukherjee, J. Chem. Phys. **132**, 234107 (2010).
[61] E. Gebrerufael, A. Calci, and R. Roth, Phys. Rev. C **93**, 031301 (2016).
[62] A. Carbone, A. Rios, and A. Polls, Phys. Rev. C **90**, 054322 (2014).
[63] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001 (2003).
[64] P. Navrátil, Few-Body Syst. **41**, 117 (2007).
[65] R. Roth, A. Calci, J. Langhammer, and S. Binder, Phys. Rev. C **90**, 024325 (2014).
[66] B. A. Brown and W. D. M. Rae, Nucl. Data Sheets **120**, 115 (2014).
[67] S. Binder, J. Langhammer, A. Calci, and R. Roth, Phys. Lett. B **736**, 119 (2014).
[68] A. Cipollone, C. Barbieri, and P. Navrátil, Phys. Rev. C **92**, 014306 (2015).
[69] M. Wang, G. Audi, A. H. Wapstra, F. G. Kondev, M. MacCormick, X. Xu, and B. Pfeiffer, Chin. Phys. C **36**, 1603 (2012).
[70] C. Stumpf, J. Braun, and R. Roth, Phys. Rev. C **93**, 021301 (2016).
[71] S. Binder, P. Piecuch, A. Calci, J. Langhammer, P. Navrátil, and R. Roth, Phys. Rev. C **88**, 054319 (2013).
[72] V. Somà, C. Barbieri, and T. Duguet, Phys. Rev. C **89**, 024323 (2014).
[73] P. Navrátil and W. E. Ormand, Phys. Rev. Lett. **88**, 152502 (2002); E. Caurier, P. Navrátil, W. E. Ormand, and J. P. Vary, Phys. Rev. C **66**, 024314 (2002).
[74] S. C. Pieper, K. Varga, and R. B. Wiringa, Phys. Rev. C **66**, 044310 (2002).
[75] C. Sanderson, Technical Report, Report No. NICTA, 2010.