

***Ab Initio* Study of  $^{40}\text{Ca}$  with an Importance-Truncated No-Core Shell Model**

R. Roth\*

*Institut für Kernphysik, TU Darmstadt, Schlossgartenstr. 9, 64289 Darmstadt, Germany*

P. Navrátil†

*Lawrence Livermore National Laboratory, P.O. Box 808, L-414, Livermore, California 94551, USA*

(Received 27 May 2007; published 29 August 2007)

We propose an importance truncation scheme for no-core shell model or configuration interaction approaches, which enables converged calculations for nuclei well beyond the  $p$  shell. It is based on an *a priori* measure for the importance of individual basis states constructed by means of many-body perturbation theory. Only the physically relevant states of the no-core model space are considered, which leads to a dramatic reduction of the basis dimension. We analyze the validity and efficiency of this truncation scheme using different realistic nucleon-nucleon interactions and compare to conventional no-core shell model calculations for  $^4\text{He}$  and  $^{16}\text{O}$ . Then, we present first converged calculations for the ground state of  $^{40}\text{Ca}$  within no-core model spaces including up to  $16\hbar\Omega$  excitations using realistic low-momentum interactions. The scheme is universal and can be easily applied to other quantum many-body problems.

DOI: [10.1103/PhysRevLett.99.092501](https://doi.org/10.1103/PhysRevLett.99.092501)

PACS numbers: 21.60.Cs, 21.30.Fe, 27.40.+z

The theoretical description of nuclei as strongly interacting quantum many-body systems bears two fundamental challenges: (i) The interaction between the constituents is a complicated, residual force resulting from the strong interaction of quantum chromodynamics (QCD). (ii) The nuclear many-body problem, which is dominated by correlations, has to be solved reliably for systems containing from 2 to a few hundred nucleons. There has been substantial progress on both aspects over recent years. In addition to traditional realistic nucleon-nucleon interactions, like the Argonne V18 [1] and the CD Bonn potential [2], which reproduce the experimental nucleon-nucleon scattering data with high precision, interactions derived in the framework of chiral effective field theory became available [3,4]. The latter provide a systematic and consistent picture of two- and three-nucleon interactions based on the symmetries of QCD. Given these interactions the solution of the nuclear many-body problem remains a formidable task. For light nuclei, *ab initio* methods like the no-core shell model [5,6] or the Green's Function Monte Carlo method [7,8] provide tools to solve the many-body problem numerically. Recently, the former has been used to study the properties of mid- $p$  shell nuclei based on chiral two- plus three-nucleon interactions for the first time [9].

Methods like the full no-core shell model (NCSM) or configuration interaction (CI) approaches become computationally intractable for heavier nuclei. Currently, converged NCSM calculations are limited to the  $p$  shell. For heavier nuclei one relies on severe approximations, such as perturbative expansions on top of a Hartree-Fock solution [10], or completely phenomenological approaches. Only few approaches, e.g., the coupled-cluster method [11,12], are able to connect the domain of strict *ab initio* methods

with the domain of approximate models for heavier systems.

In order to extend the scope of NCSM or CI calculations to heavier nuclei we propose an extension using *a priori* information on the importance of individual basis states obtained from many-body perturbation theory. We use this importance measure to truncate the NCSM model space to the physically relevant basis states and thus reduce its dimension substantially. The current limitation of full NCSM calculations results from the sheer dimension of the matrix eigenvalue problem. Typically the many-body basis, which is represented by Slater determinants  $|\Phi_\nu\rangle$  of harmonic-oscillator single-particle states, is truncated at a maximum number  $N_{\text{max}}$  of harmonic-oscillator excitation quanta thus defining the so-called  $N_{\text{max}}\hbar\Omega$  model space. Its ( $m$ -scheme) dimension grows exponentially with the number of nucleons  $A$  and the truncation level  $N_{\text{max}}$ . For  $^{16}\text{O}$  this limits the presently tractable model space to  $N_{\text{max}} = 8$  [13], corresponding to an effective  $m$ -scheme dimension of  $6 \times 10^8$ . For  $^{40}\text{Ca}$  the dimension of the  $8\hbar\Omega$  model space is  $2 \times 10^{12}$ —well beyond the capabilities of current shell model codes. Many of these basis states are irrelevant for the description of any particular eigenstate, e.g., the ground state. Therefore, if one were able to identify the important basis states beforehand, one could reduce the dimension of the matrix eigenvalue problem without losing predictive power. This, as we propose in this Letter, can be done using many-body perturbation theory. This type of problem is not restricted to nuclear physics but common to many areas of quantum many-body theory. For the description of strongly correlated lattice systems, e.g., in the context of ultracold atomic gases in optical lattices [14], or other atomic or condensed matter systems, one encounters the same limitations of exact diagonalization approaches.

We start out with a translationally invariant Hamiltonian  $H_{\text{int}}$  composed of the intrinsic kinetic energy  $T_{\text{int}} = T - T_{\text{cm}}$  and a two-nucleon interaction  $V_{\text{NN}}$ . In the first part of this Letter, we use the phase-shift equivalent correlated interaction  $V_{\text{UCOM}}$  discussed in Refs. [10,15]. For three- and four-nucleon systems it provides binding energies in good agreement with experiment without the inclusion of an explicit three-nucleon force. In the second part, we use the  $V_{\text{low}k}$  low-momentum interaction [16] to discuss the ground-state structure of  $^{16}\text{O}$  and  $^{40}\text{Ca}$ . Note that no transformation to an effective model-space interaction (Lee-Suzuki transformation) is employed in any of the calculations presented here. Thus, they correspond to CI diagonalizations using the harmonic-oscillator basis in an  $N_{\text{max}}\hbar\Omega$  model space.

The general concept of the importance truncation is as follows: We start with a reference state  $|\Psi_{\text{ref}}\rangle$ , which in the simplest case is a single harmonic-oscillator Slater determinant. Here, we limit ourselves to the ground state, but the scheme can easily be extended to excited states or more than one reference state. Starting from  $|\Psi_{\text{ref}}\rangle$  we can build a many-body space by generating all possible  $n$ -particle- $n$ -hole ( $nph$ ) excitations up to the excitation energy  $N_{\text{max}}\hbar\Omega$ . By increasing  $n$  ( $\leq A$ ), we eventually recover the translationally invariant  $N_{\text{max}}\hbar\Omega$  model space of the NCSM. We now estimate the contribution of a given basis state  $|\Phi_\nu\rangle$  to the exact eigenstate after the diagonalization via many-body perturbation theory. In first-order, the amplitude of the state  $|\Phi_\nu\rangle$  is given by

$$\kappa_\nu = -\frac{\langle\Phi_\nu|H'|\Psi_{\text{ref}}\rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}, \quad (1)$$

where  $H'$  is the Hamiltonian of the perturbation and  $\epsilon_\nu, \epsilon_{\text{ref}}$  are the unperturbed energies of the two configurations. The unperturbed Hamiltonian is just the one-body harmonic-oscillator Hamiltonian,  $H_0 = H_{\text{HO}}$ , with the Slater determinants  $|\Phi_\nu\rangle$  as eigenstates,  $H_{\text{HO}}|\Phi_\nu\rangle = \epsilon_\nu|\Phi_\nu\rangle$ . The perturbation is given by  $H' = H_{\text{int}} - H_{\text{HO}}$ .

If we restrict ourselves to two-body interactions, then  $H'$  contains only one- and two-body terms such that  $\kappa_\nu$  vanishes for  $3p3h$  and higher-order configurations when starting with a  $0p0h$  reference state. In principle, higher orders of perturbation theory are required to generate states beyond the  $2p2h$  level directly. Since this becomes computationally inefficient, we resort to an iterative scheme. In a first iteration we generate  $1p1h$  and  $2p2h$  states starting from a Slater determinant as reference state, retain those with an importance weight  $|\kappa_\nu| \geq \kappa_{\text{min}}$ , and solve the eigenvalue problem in this space. In the next iteration, the dominant components of the ground state  $|\Psi_0\rangle = \sum_\nu C_\nu |\Phi_\nu\rangle$  obtained from the diagonalization in the previous step are used as a reference state, i.e.,  $|\Psi_{\text{ref}}\rangle = \sum_{|\kappa_\nu| \geq C_{\text{ref}}} C_\nu |\Phi_\nu\rangle$ , with  $C_{\text{ref}} \approx 0.005$ . Since this state already contains up to  $2p2h$  admixtures, one obtains non-vanishing importance weights (1) for states up to the  $4p4h$  level. After applying the importance truncation

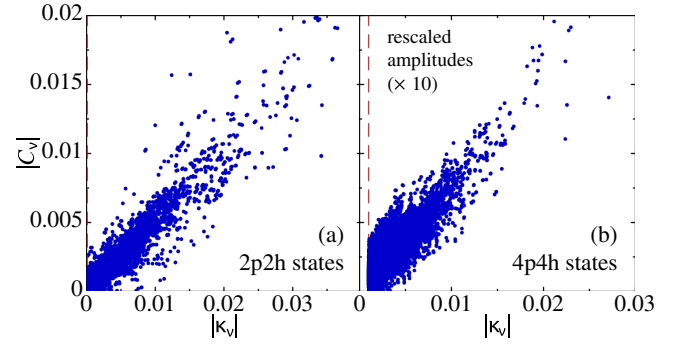


FIG. 1 (color online). Correlation between the *a priori* importance weight  $\kappa_\nu$  and the *a posteriori* amplitudes  $C_\nu$  resulting from the explicit diagonalization. Shown are the  $2p2h$  (a) and  $4p4h$  contributions (b) for a  $6\hbar\Omega$  calculation for  $^{16}\text{O}$  with  $V_{\text{UCOM}}$  at  $\hbar\Omega = 20$  MeV. The dashed vertical line marks a typical truncation parameter  $\kappa_{\text{min}}$ .

$|\kappa_\nu| \geq \kappa_{\text{min}}$  the eigenvalue problem is solved in the extended space. This cycle can be repeated until the full  $N_{\text{max}}\hbar\Omega$  model space is generated in the limit  $\kappa_{\text{min}} = 0$ . For the first applications presented here, we restrict ourselves to the  $4p4h$  level, extensions will be discussed elsewhere.

The correlation plots presented in Fig. 1 demonstrate that this prescription provides a reliable *a priori* estimate for the size of the *a posteriori* amplitudes  $C_\nu$  of the individual basis states after solving the eigenvalue problem. There is a clear correlation between the coefficients  $C_\nu$  and the importance measure  $\kappa_\nu$ . Therefore, the additional truncation of the many-body space to configurations with  $|\kappa_\nu| \geq \kappa_{\text{min}}$  provides an efficient means to remove irrelevant configurations from the outset. Eventually, the eigenvalue problem within the truncated space is solved without further approximation. Hence, formal properties such as the variational principle and the Hylleraas-Undheim theorem remain intact—in contrast to other approaches like the coupled-cluster method [11,12].

The dependence of the ground-state energy on the truncation parameter  $\kappa_{\text{min}}$  is illustrated in Fig. 2 for  $^{16}\text{O}$  and

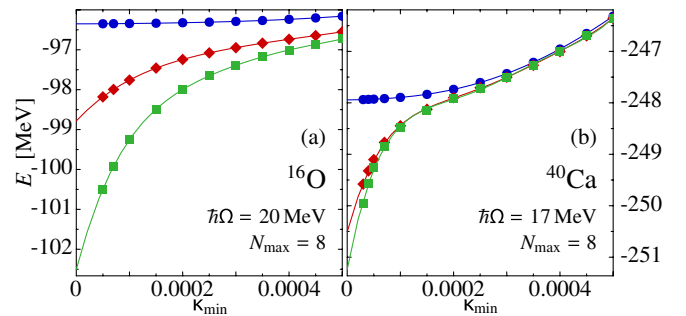


FIG. 2 (color online). Dependence of the ground-state energy of  $^{16}\text{O}$  (a) and  $^{40}\text{Ca}$  (b) on the truncation parameter  $\kappa_{\text{min}}$  obtained with  $V_{\text{UCOM}}$ . The three data sets correspond to model spaces with up to  $2p2h$  (●),  $3p3h$  (◆), and  $4p4h$  states (■), respectively. The lines show a 5th order polynomial interpolation.

$^{40}\text{Ca}$ . The different data sets correspond to calculations with spaces comprising up to  $2p2h$ ,  $3p3h$ , and  $4p4h$  states, respectively. We always observe a very regular behavior, which allows for a robust extrapolation of the energies towards  $\kappa_{\min} = 0$ , corresponding to the complete model space. All results presented here employ a 5th order polynomial extrapolation based on a sequence of calculations for the truncation parameters  $\kappa_{\min}$  indicated in Fig. 2.

A first indication of the efficiency of the importance truncation scheme is given in Fig. 3. Shown are the ground-state energies of  $^4\text{He}$  and  $^{16}\text{O}$  as function of  $N_{\max}$  computed for the  $V_{\text{UCOM}}$  interaction using the importance truncation (after extrapolation to  $\kappa_{\min} = 0$ ) in comparison to the full NCSM calculation performed with the ANTOINE code [17]. For  $^4\text{He}$  the truncated calculation including up to  $4p4h$  configurations generates the full  $N_{\max} \hbar\Omega$  model space in the limit  $\kappa_{\min} = 0$ . The excellent agreement between full and truncated calculation in this case proves the reliability of the importance truncation scheme. Nonetheless, the dimension of the eigenvalue problem is drastically reduced by the importance truncation: For  $N_{\max} = 20$  the dimension of the full NCSM model space is beyond  $2 \times 10^7$ , whereas the dimension of the truncated basis is of the order  $10^5$ .

For  $^{16}\text{O}$  a similar picture emerges, the importance-truncated calculations up to the  $4p4h$  level are in very good agreement with the full NCSM. For the  $8\hbar\Omega$  model space the full calculation yields a slightly lower ground-

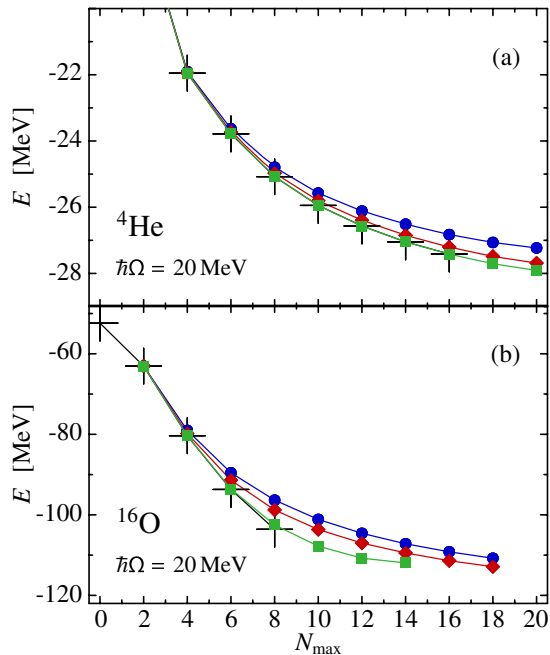


FIG. 3 (color online). Convergence of the ground-state energy for  $^4\text{He}$  (a) and  $^{16}\text{O}$  (b) versus  $N_{\max}$  obtained using  $V_{\text{UCOM}}$ . Shown are three data sets corresponding to model spaces with up to  $2p2h$  (●),  $3p3h$  (◆), and  $4p4h$  states (■), respectively. Black crosses (+) indicate the results of full NCSM calculations. Lines to guide the eye.

state energy, which is due to states beyond the  $4p4h$  level. The relevance of  $4p4h$  correlations is a specific property of  $^{16}\text{O}$  ( $\alpha$ -clustering) and is revealed through the comparably strong effect of those states on the ground-state energy.

The  $N_{\max}$  dependence of the ground-state energy of  $^{40}\text{Ca}$  for two different oscillator frequencies is presented in Fig. 4. In comparison to  $^{16}\text{O}$ , the impact of  $4p4h$  configurations is negligible and it is expected that higher-order configurations will not affect the ground-state energy. For the oscillator frequency  $\hbar\Omega = 17$  MeV even the inclusion of  $3p3h$  states does not lead to a significant effect. An exponential extrapolation of the  $3p3h$  energies for  $\hbar\Omega = 17$  MeV to infinite model-space size gives  $E_{\infty} \approx -316$  MeV, which can be compared to the experimental binding energy of  $-342.05$  MeV. Keeping in mind that our calculation—because of the restriction to the  $3p3h$  level—provides an upper bound, this result is very encouraging. It shows that the phase-shift equivalent two-nucleon interaction  $V_{\text{UCOM}}$  is able to provide a realistic description of binding energies also for heavier nuclei without the inclusion of an additional three-body interaction.

In this intermediate mass regime the importance truncation works very efficiently: The dimension of the importance-truncated space used for  $^{40}\text{Ca}$  around  $N_{\max} = 16$  is of the order of  $10^7$ , which is smaller than the full NCSM space at  $N_{\max} = 4$ . In order to warrant that contributions of spurious center-of-mass excitations to the energy are negligible, we monitor the expectation value of the operator  $H_{\text{HO}}^{\text{cm}} - \frac{3}{2}\hbar\Omega$ . We obtain typical values of 100 keV and below proving that the importance truncation does not generate spurious center-of-mass excitations, which are otherwise absent in a complete  $N_{\max} \hbar\Omega$  model space.

Following these benchmark calculations with  $V_{\text{UCOM}}$ , we apply the importance truncation for a systematic study of the ground states of  $^{16}\text{O}$  and  $^{40}\text{Ca}$  with the  $V_{\text{lowk}}$  low-momentum interaction derived from the Argonne V18 potential with a cutoff momentum  $\Lambda = 2.1 \text{ fm}^{-1}$  [18].

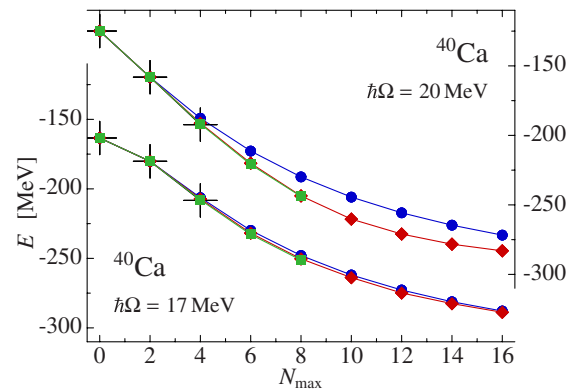


FIG. 4 (color online). Convergence of the ground-state energy of  $^{40}\text{Ca}$  as function of model-space size  $N_{\max}$  for  $\hbar\Omega = 17$  MeV (lower curves, left-hand axis) and  $20$  MeV (upper curves, right-hand axis) using the  $V_{\text{UCOM}}$  interaction. Symbols as described in Fig. 3.

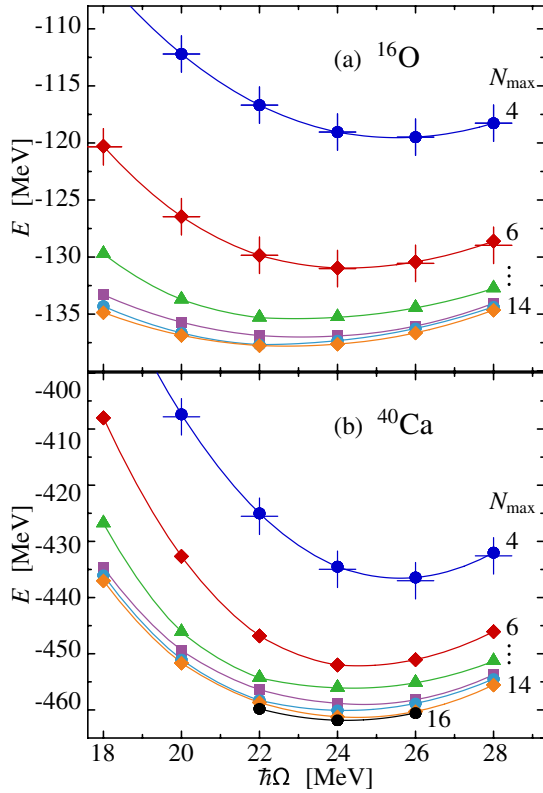


FIG. 5 (color online). Ground-state energy of  $^{16}\text{O}$  (a) and  $^{40}\text{Ca}$  (b) as function of the harmonic-oscillator frequency  $\hbar\Omega$  for different model-space sizes up to  $N_{\text{max}} = 16$  obtained with the  $V_{\text{lowk}}$  interaction. For  $^{16}\text{O}$  up to  $4p4h$  configurations are included, for  $^{40}\text{Ca}$  up to  $3p3h$ . Crosses indicate the results of full NCSM calculations.

The  $V_{\text{lowk}}$  interaction shows an even faster convergence than  $V_{\text{UCOM}}$  and therefore provides a useful reference for a quantitative comparison of different many-body approaches, although it significantly overestimates the binding energies and underestimates the radii in comparison to experiment.

The convergence of the ground-state energy of  $^{16}\text{O}$  and  $^{40}\text{Ca}$  as function of the oscillator frequency  $\hbar\Omega$  for different model-space sizes up to  $N_{\text{max}} = 16$  is illustrated in Fig. 5. For  $^{16}\text{O}$  configurations up to the  $4p4h$  level have been included, for  $^{40}\text{Ca}$  up to  $3p3h$  configurations are considered. For both nuclei we observe a very rapid convergence of the energies, such that fully converged results are obtained. For  $^{16}\text{O}$  with  $N_{\text{max}} = 14$  and  $\hbar\Omega = 22$  MeV we obtain a ground-state energy of  $-137.7$  MeV, and a root-mean-square radius of 2.03 fm (point nucleons). An exponential extrapolation at  $\hbar\Omega = 22$  MeV yields  $E_{\infty} = -138.0$  MeV. This result can be compared with a recent coupled-cluster calculation (CCSD) using the same interaction, which yields an extrapolated energy of  $-142.8$  MeV [18,19]. This is in good agreement with our result keeping in mind that our calculation provides a variational upper bound, since configurations beyond  $4p4h$  are not included. For  $^{40}\text{Ca}$  with  $N_{\text{max}} = 16$  and  $\hbar\Omega =$

24 MeV we obtain a ground-state energy of  $-461.8$  MeV and a rms radius of 2.27 fm. An exponential extrapolation results in  $E_{\infty} = -462.7$  MeV. In addition to the observables shown here, we have also extracted charge form factors and translationally invariant density profiles from the eigenvectors in the importance-truncated space.

In conclusion, we have presented an importance truncation scheme which reduces the model space of NCSM or CI approaches to the physically relevant states. The relevance of individual basis states is quantified using an *a priori* importance measure derived from many-body perturbation theory. This novel scheme has proven very robust and extends the range of reliable NCSM calculations to regions of the nuclear chart far beyond the  $p$  shell. In this Letter, we have shown the first converged NCSM calculations for the ground state of  $^{40}\text{Ca}$  with two different realistic NN interactions. The scheme is universal and can easily be adapted to other quantum many-body problems treated by diagonalization techniques.

Supported by the Deutsche Forschungsgemeinschaft through SFB 634. This work was partly performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48. This work was supported in part by the Department of Energy under Grant No. DE-FC02-07ER41457.

\*robert.roth@physik.tu-darmstadt.de

†navratil1@llnl.gov

- [1] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
- [2] R. Machleidt, Phys. Rev. C **63**, 024001 (2001).
- [3] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001(R) (2003).
- [4] E. Epelbaum *et al.*, Phys. Rev. C **66**, 064001 (2002).
- [5] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000).
- [6] P. Navrátil and W. E. Ormand, Phys. Rev. Lett. **88**, 152502 (2002).
- [7] S. C. Pieper and R. B. Wiringa, Annu. Rev. Nucl. Part. Sci. **51**, 53 (2001).
- [8] S. C. Pieper, R. B. Wiringa, and J. Carlson, Phys. Rev. C **70**, 054325 (2004).
- [9] P. Navrátil *et al.*, Phys. Rev. Lett. **99**, 042501 (2007).
- [10] R. Roth *et al.*, Phys. Rev. C **73**, 044312 (2006).
- [11] K. Kowalski *et al.*, Phys. Rev. Lett. **92**, 132501 (2004).
- [12] M. Włoch *et al.*, Phys. Rev. Lett. **94**, 212501 (2005).
- [13] E. Caurier *et al.*, Rev. Mod. Phys. **77**, 427 (2005).
- [14] F. Schmitt, M. Hild, and R. Roth, J. Phys. B **40**, 371 (2007).
- [15] R. Roth *et al.*, Phys. Rev. C **72**, 034002 (2005).
- [16] S. K. Bogner, T. T. S. Kuo, and A. Schwenk, Phys. Rep. **386**, 1 (2003).
- [17] E. Caurier and F. Nowacki, Acta Phys. Pol. B **30**, 705 (1999).
- [18] G. Hagen (private communication).
- [19] G. Hagen *et al.*, arXiv:0707.1516.