Extrapolation to Infinite Basis Space in No-Core Monte Carlo Shell Model

T. Abe[a], P. Maris[b], T. Otsuka[a,c,d], N. Shimizu[c], Y. Utsuno[e] and J. P. Vary[b]

[a] *Department of Physics, the University of Tokyo, Hongo, Tokyo 113-0033, Japan*
[b] *Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
[c] *Center for Nuclear Study, the University of Tokyo, Hongo, Tokyo 113-0033, Japan*
[d] *National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824, USA*
[e] *Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan*

Abstract

We report a preliminary study of extrapolations to infinite basis space of ground-state energies in the no-core Monte Carlo shell model. Ground-state energies of ^{4}He, ^{8}Be, ^{12}C and ^{16}O are calculated in the basis spaces up to $N_{\text{shell}} = 7$ with the JISP16 two-nucleon interaction. Then we extrapolate these energy eigenvalues obtained in the finite basis spaces to infinity. For the extrapolation to the infinite basis space, we employ two schemes: One of them is the traditional exponential extrapolation scheme. The other is the extrapolation scheme based on the infrared and ultraviolet regulators. From a preliminary investigation, both extrapolation schemes give consistent extrapolated energy eigenvalues in the N_{shell} truncation, however, estimations of the uncertainty are needed. We also compare the MCSM results to the NCFC results obtained from the different basis space truncation, N_{max}. We find reasonable agreement between the MCSM and NCSM results.

Keywords: *No-core shell model; Monte Carlo shell model; infrared and ultraviolet regulators*

1 Introduction

The No-core Shell Model (NCSM) is one of powerful *ab initio* methods to investigate low-energy nuclear structure and reactions in light nuclei [1]. However, the computational cost is expensive and explodes factorially as the number of nucleons increases and/or the basis spaces are enlarged, because the NCSM retains all nucleon degrees of freedom explicitly. At present, the maximum size of the Hamiltonian matrix attainable for the direct diagonalization by the Lanczos technique is around 10^{10-11} in the M-scheme basis space. To avoid the large dimensionality of the Hamiltonian matrix to be diagonalized, several variants of the NCSM have emerged recently. One of these approaches is the Importance-Truncated NCSM [2] where the model spaces are extended by using an importance measure evaluated with perturbation theory. Another approach is the Symmetry-Adapted NCSM [3] where the model spaces are truncated according to selected symmetry groups. The No-core Shell Model with

Proceedings of the International Conference 'Nuclear Theory in the Supercomputing Era — 2014' (NTSE-2014), Khabarovsk, Russia, June 23–27, 2014. Eds. A. M. Shirokov and A. I. Mazur. Pacific National University, Khabarovsk, Russia, 2016, p. 166.

http://www.ntse-2014.khb.ru/Proc/Abe.pdf.

a Core [4] obtains microscopically the core, one- and two-body terms of the conventional shell-model framework, and the Hamiltonian matrix is diagonalized in the smaller basis space. Similar to these attempts, the No-core Monte Carlo Shell Model (MCSM) [5, 6] is one of the promising candidates to go beyond the Full Configuration Interaction (FCI) method which involves a different truncation of the basis space, $N_{\rm shell}$, than the one commonly used in the NCSM, $N_{\rm max}$. A proof of principle study of the MCSM without an assumed inert core has been demonstrated on the Be isotopes [5]. By exploiting the recent development in the MCSM algorithm [7], the no-core calculations with the MCSM algorithm can be performed efficiently on massively parallel supercomputers. From the benchmark calculations, the observables such as the energy, root-mean-square radius, electromagnetic dipole and quadrupole moments, give good agreement between the MCSM and FCI results in applications to p-shell nuclei [6].

Recently, extrapolation methods to the infinite basis space in the harmonic oscillator basis have been developed [8, 9]. In these proceedings, we extend the MCSM calculations in larger basis spaces and extrapolate the ground-state (g. s.) energies of ^{4}He, ^{8}Be, ^{12}C and ^{16}O to the infinite basis space. For the extrapolations, we apply a traditional extrapolation scheme and the recently proposed infrared and ultraviolet cutoff extrapolations in a harmonic oscillator basis.

2 Monte Carlo shell model

The MCSM has been developed mainly for conventional shell-model calculations with an assumed inert core [10]. The shell-model calculations with an assumed inert core by the MCSM have succeeded in obtaining approximate solutions where the direct diagonalization is difficult due to large dimensionalities. Recently, the algorithm and code itself have been significantly revised and rewritten so as to accommodate massively parallel computing environments [7]. We are able now to apply the MCSM method successfully to the no-core calculations [5, 6].

In the MCSM, a many-body basis state $|\Psi^{J^\pi M}\rangle$ is approximated as a linear combination of non-orthogonal angular-momentum, J, and parity, π, projected deformed Slater determinants with good total angular momentum projection, M,

$$|\Psi^{J^\pi M}\rangle = \sum_{n=1}^{N_b} f_n \sum_{K=-J}^{J} g_{nK}\, P^J_{MK}\, P^\pi |\phi_n\rangle, \tag{1}$$

where P^J_{MK} is the projection operator for the total angular momentum, J, with its z-projection in the laboratory (body-fixed) frame, M (K). P^π is the projection operator for the parity. N_b is the number of Slater determinants. A deformed Slater determinant is described by $|\phi\rangle = \prod_{i=1}^{A} a_i^\dagger|-\rangle$ with the vacuum $|-\rangle$ and the creation operator $a_i^\dagger = \sum_{\alpha=1}^{N_{\rm sp}} c_\alpha^\dagger\, D_{\alpha i}$. $N_{\rm sp}$ is specified by the cutoff of the single particle basis space, $N_{\rm shell}$.

One then stochastically samples the coefficient $D_{\alpha i}$ in all possible many-body basis states around the mean field solutions through auxiliary fields and/or automatically evaluates it by the conjugate gradient method. The coefficients, f_n and g_{nK}, are determined by the diagonalization of the Hamiltonian matrix. With increasing the number of basis states, N_b, the energy eigenvalue converges from above to the exact solution and gives the variational upper bound. In recent MCSM calculations, the energy eigenvalue obtained by the above way is extrapolated by using the energy variance so as to get better estimate of true eigenvalue in the chosen basis space. Recent development and the technical details of the MCSM algorithm can be found in Ref. [7]. The next step is to further extrapolate the MCSM results to those in the infinite basis space to get an *ab initio* solution and to compare them with another solution by the NCFC method [11], which extrapolates from the different truncation of basis space, $N_{\max}$.

3 Extrapolations to infinite basis space

Extrapolation methods to the infinite basis space in the harmonic oscillator basis have been developed in recent years [8, 9]. In this section, we briefly summarize the extrapolation methods applied to the MCSM.

The extrapolation of the results in the harmonic oscillator basis has a long history. Until recently, the exponential fit of the energy with fixed $\hbar\omega$,

$$E(N) = E(N = \infty) + a \exp(-bN), \tag{2}$$

has been traditionally adopted. Here, N describes the size of basis space, and $E(N = \infty)$, a and b are the fit parameters. The NCFC method combines the NCSM with an elaborated scheme based on the traditional extrapolation scheme, which gives an *ab initio* solution by extrapolating the results in the $N = N_{\max}$ truncated basis space to infinity [11].

Recently proposed extrapolation scheme utilizes the infrared (IR) and ultraviolet (UV) cutoff scales [8, 9]. It is just a transformation from a two-parameter problem in $(N, \hbar\omega)$ to (λ, Λ), but the scaling properties can be different. In the harmonic oscillator basis, the IR cutoff scale is defined as $\lambda_{sc} = \sqrt{(m\hbar\omega)/(N + 3/2)}$, which corresponds to the inverse of the root-mean-square radius in the highest harmonic oscillator level in the basis space N, while the UV cutoff scale is defined as $\Lambda = \sqrt{m(N + 3/2)\hbar\omega}$, which is associated with the highest harmonic oscillator level in the basis space N. Note that there is another definition of the IR scale by $\lambda = \sqrt{m\hbar\omega}$, which is characterized by the minimum allowed energy difference between the harmonic oscillator levels. Here, we use λ_{sc}, not λ, as the IR cutoff due to its scaling property. Also note that there is another definition of the UV regulator ($\Lambda' = \sqrt{2}\Lambda$), but the extrapolated energy is not affected by the difference of the definitions. In this study, we use Λ as the UV regulator. The IR-cutoff extrapolation is performed by using UV-saturated results with

$$E(\lambda) = E(\lambda = 0) + a \exp(-b/\lambda), \tag{3}$$

where $E(\lambda = 0)$, a and b are the fit parameters. Note that the IR extrapolation formula, Eq. (3) was derived for a single-particle system and is widely applied to bound states of many-body systems [9]. Although the UV extrapolation formula has yet to be derived, the IR- and UV-cutoff combined extrapolation is applied, for example, in Ref. [12]. The IR- and UV-cutoff extrapolation is given by using the following formula,

$$E(\lambda, \Lambda) = E(\lambda = 0, \Lambda = \infty) + a \exp(-b/\lambda) + c \exp(-\Lambda^2/d^2), \tag{4}$$

where $E(\lambda = 0, \Lambda = \infty)$, a, b, c and d are the fit parameters.

By using the above formulae, Eqs. (2), (3) and (4), we attempt to extrapolate the MCSM results of the g. s. energies in the $N = N_{\mathrm{shell}}$ truncation to the infinite basis space.

4 Results

We have calculated the ground-state energies of ^{4}He, ^{8}Be, ^{12}C and ^{16}O in the basis spaces up to $N_{\mathrm{shell}} = 7$. In this study, we have taken $N_b = 100$ and extrapolated the energies obtained in each basis space by the energy variance. The energy-variance extrapolation is needed to obtain better estimate of true eigenvalue derived from

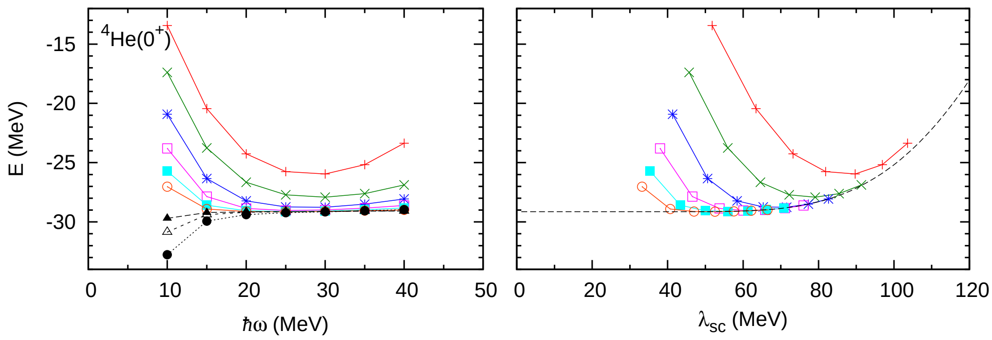

Figure 1: Extrapolations of ^{4}He g. s. energy. The JISP16 two-nucleon interaction is employed and Coulomb interaction is turned off. The color (symbol) difference corresponds to different size of basis space. The red (plus), green (cross), blue (asterisk), pink (open square), aqua (solid square), orange (open circle) symbols with solid lines are the MCSM results in $N_{\rm shell}$ = 2, 3, 4, 5, 6 and 7, respectively. The traditional exponential extrapolation by Eq. (2) is shown in the left panel. The black solid circles with dotted line, black open triangles with short-dashed line, and black solid triangles with long-dashed line denote the extrapolated results to infinite basis space from the MCSM results in $N_{\rm shell}$ = 2−7, 3−7, and 4−7, respectively. The IR-cutoff extrapolation by Eq. (3) is shown in the right panel as the black dotted curve.

the calculated eigenvalue and its variance in the N_b = 100 truncation of each finite MCSM basis space defined by $N_{\rm shell}$. In the MCSM calculations, the JISP16 two-nucleon interaction [13] is employed, and the Coulomb force is turned off. For simplicity, the effect of spurious center-of-motion is neglected. MCSM calculations have been performed on K computer, RIKEN AICS and FX10 at the University of Tokyo. The MCSM results of the energies have been extrapolated to the infinite basis space by using the extrapolation schemes discussed in the previous section. For the extrapolations to the infinite basis space, we take $N_{\rm shell}$ as N in Eqs. (2), (3) and (4).

Fig. 1 shows the extrapolations of the ^{4}He g. s. energy to the infinite basis space. In the figure, each color (symbol) corresponds to a different value of $N_{\rm shell}$. The red (plus), green (cross), blue (asterisk), pink (open square), aqua (solid square), orange (open circle) symbols with solid lines are the MCSM results in $N_{\rm shell}$ = 2, 3, 4, 5, 6 and 7, respectively. The traditional extrapolation is demonstrated in the left panel, while the IR-cutoff extrapolation in the right panel. In the left panel, the black symbols connected with dotted lines are the extrapolated results obtained by the traditional extrapolation scheme, Eq. (2). The black solid circles with dotted line, black open triangles with short-dashed line, and black solid triangles with long-dashed line denote the extrapolated results to infinite basis space from the MCSM results in $N_{\rm shell}$ = 2−7, 3−7, and 4−7, respectively. Traditional exponential fits to the MCSM results with $\hbar\omega$ = 15−35 MeV in $N_{\rm shell}$ = 3−7 give the ^{4}He g. s. energy ranging from −29.389 to −29.077 MeV. In the right panel, the dotted curve is the fit function of Eq. (3) determined by the MCSM results, which demonstrates the IR-cutoff extrapolation. The IR-cutoff extrapolation gives −29.142 MeV where λ_{sc} = 0. These extrapolated results give a good agreement with the NCFC result of −29.164(2) MeV, which is obtained by the traditional exponential extrapolation to infinite basis space from a different truncation of the basis space governed by $N_{\rm max}$.

Fig. 2 shows the extrapolations of the ^{8}Be g. s. energy to the infinite basis space. The notation conventions in Fig. 2 are the same as in Fig. 1. As shown in the left panel of Fig. 2, the traditional exponential fits to the MCSM results with $\hbar\omega$ = 25−35 MeV in $N_{\rm shell}$ = 3−7 give the ^{8}Be g. s. energy ranging from −59.289 to −57.396 MeV. From the right panel of Fig. 2, the IR-cutoff extrapolation gives −58.676 MeV. These

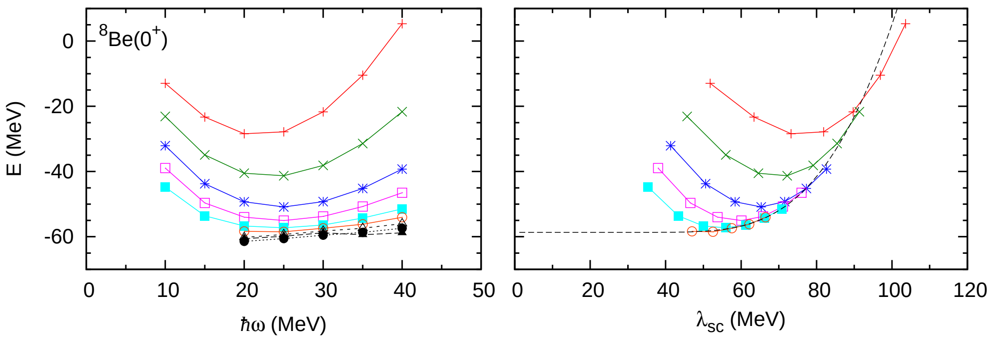

Figure 2: Extrapolations of ^{8}Be g. s. energy. Same caption as in Fig. 1, but for ^{8}Be.

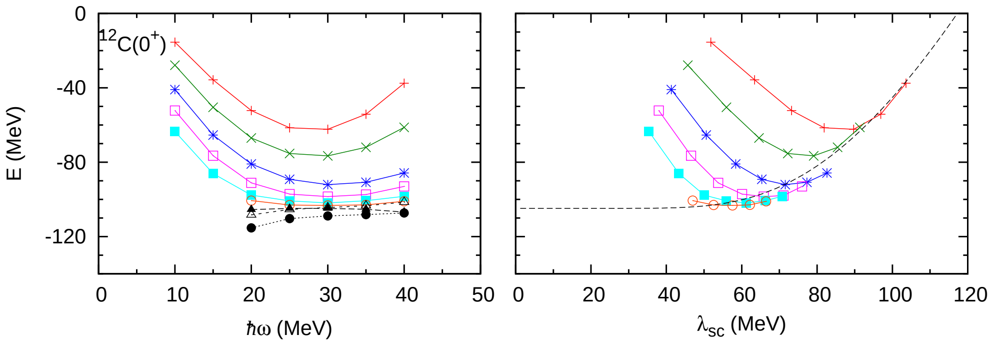

Figure 3: Extrapolations of ^{12}C g. s. energy. Same caption as in Fig. 1, but for ^{12}C.

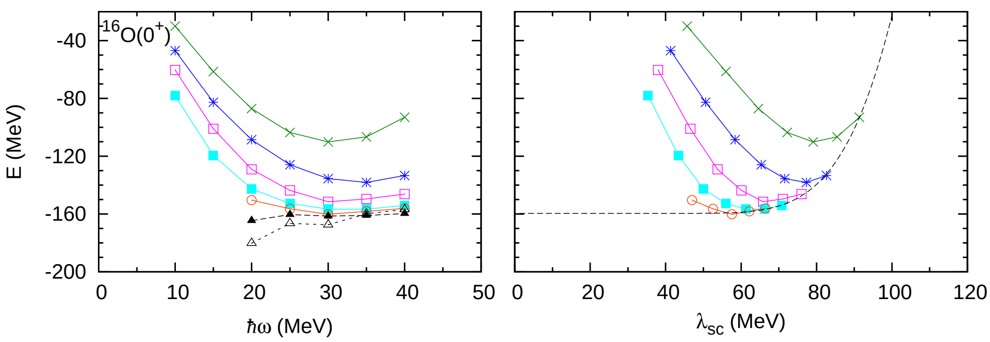

Figure 4: Extrapolations of ^{16}O g. s. energy. Same caption as in Fig. 1, but for ^{16}O, besides the absence of the $N_{\rm shell} = 2$ results and the traditional extrapolation to the infinite basis space from the MCSM results in $N_{\rm shell} = 2$–7.

extrapolated results are in a good agreement with the NCFC result of $-59.1(1)$ MeV.

Fig. 3 shows the extrapolations of the ^{12}C g. s. energy to the infinite basis space. The notation conventions in Fig. 3 are the same as in Fig. 1. From the left panel of Fig. 3, the traditional exponential fits to the MCSM results with $\hbar\omega = 25 - 35$ MeV in $N_{\rm shell} = 3 - 7$ give the ^{12}C g. s. energy ranging from -105.392 to -103.393 MeV. From the right panel of Fig. 3, the IR-cutoff extrapolation gives -104.812 MeV. Note that the NCFC result is not yet available.

Fig. 4 shows the extrapolations of the ^{16}O g. s. energy to the infinite basis space. The notation conventions in Fig. 4 are the same as in Fig. 1, except for the absence of the $N_{\rm shell} = 2$ results and for the traditional extrapolation to the infinite basis space

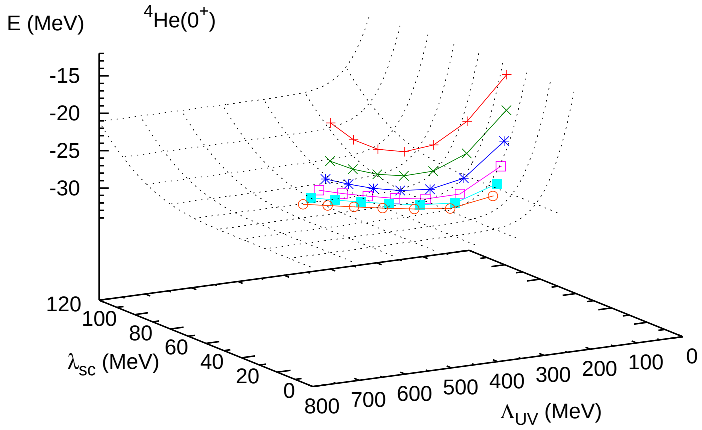

Figure 5: IR- and UV-cutoff extrapolations of ^{4}He g. s. energy. The color (symbol) difference corresponds to different size of basis spaces, see Fig. 1 for details. The black mesh shows the IR- and UV-cutoff extrapolations by Eq. (4).

from the MCSM results in $N_{\rm shell} = 2{-}7$. From the left panel of Fig. 4, the traditional exponential fits to the MCSM results with $\hbar\omega = 25{-}35$ MeV in $N_{\rm shell} = 4{-}7$ give the ^{16}O g. s. energy ranging from -161.435 to -160.378 MeV. From the right panel of Fig. 4, the IR-cutoff extrapolation gives -159.592 MeV. Note that the NCFC result, as in the case of ^{12}C, is not yet available.

Fig. 5 shows the IR- and UV-extrapolation of the ^{4}He g. s. energy to the infinite basis space. In the figure, each color (symbol) corresponds to a different value of N_{shell} as in Fig. 1. The dotted mesh is obtained by the fit with Eq. (4) to the MCSM results, which demonstrate the IR- and UV-cutoff extrapolation. The IR- and UV-cutoff extrapolation gives -29.139 MeV where $\lambda_{sc} = 0$ and $\Lambda = \infty$. Although the IR- and UV-cutoff extrapolated result is in a good agreement with those of the traditional and IR-cutoff extrapolations shown in Fig. 1 and also with the NCFC, further investigation on the extrapolation uncertainties is necessary to confirm these extrapolated results. The IR- and UV-cutoff extrapolations for ^{8}Be, ^{12}C and ^{16}O are under way.

Finally, we summarize the extrapolated results in Table 1. These MCSM results are preliminary. We have to obtain better MCSM results in each basis space by increasing N_b so as to quantify the uncertainties both of the energy-variance extrapolation in the finite basis space and of the extrapolations to the infinite basis space.

5 Summary

We have shown preliminary results of extrapolations to the infinite basis space for ground-state energies in no-core Monte Carlo shell model. The g. s. energies of ^{4}He,

Table 1: Comparison of the extrapolated g. s. energies of ^{4}He, ^{8}Be, ^{12}C and ^{16}O. The entries of Traditional, IR, IR and UV, and NCFC are the extrapolated MCSM results by Eqs. (2), (3), and (4), and the NCFC result, respectively. Energies are in MeV.

	Traditional	IR	IR and UV	NCFC
^{4}He 0^+ g. s. energy	$-29.389 \div -29.007$	-29.142	-29.139	$-29.164(2)$
^{8}Be 0^+ g. s. energy	$-59.289 \div -57.396$	-58.676		$-59.1(1)$
^{12}C 0^+ g. s. energy	$-105.392 \div -103.393$	-104.812		
^{16}O 0^+ g. s. energy	$-161.435 \div -160.378$	-159.592		

^{8}Be, ^{12}C and ^{16}O were calculated in the basis spaces up to $N_{\rm shell} = 7$ with the JISP16 two-nucleon interaction and without the Coulomb interaction. Then we extrapolate these energy eigenvalues obtained in the finite basis spaces to the infinite basis limit by the traditional exponential scheme and the schemes with the IR and UV cutoffs. From this preliminary investigation, both extrapolation schemes give consistent extrapolated energy eigenvalues in the $N_{\rm shell}$ truncation, however, estimations of the uncertainty are needed. We also compare the MCSM results for the ^{4}He and ^{8}Be g. s. energies to the NCFC results obtained from the different $N_{\rm max}$ basis space truncations. The agreement between them seems to be reasonable.

Acknowledgments

This work was supported in part by the SPIRE Field 5 from MEXT, Japan (hp130024 and hp140210). We also acknowledge Grants-in-Aid for Young Scientists (Nos. 20740127 and 21740204), for Scientific Research (Nos. 20244022 and 23244049), and for Scientific Research in Innovative Areas (No. 20105003) from JSPS, and the CNS-RIKEN joint project for large-scale nuclear structure calculations. This work was also supported in part by the US DOE Grants No. DESC0008485 (SciDAC-3/NUCLEI) and DE-FG02-87ER40371, by the US NSF Grant No. PHY-0904782, and through JUSTIPEN under grant No. DE-FG02-06ER41407. A part of the MCSM calculations was performed on K computer at RIKEN AICS and FX10 at the University of Tokyo. Computational resources for the FCI and NCFC calculations were provided by the National Energy Research Scientific Computing Center (NERSC) supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and by the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

References

[1] P. Navrátil, J. P. Vary and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000); Phys. Rev. C **62**, 054311 (2000); S. Quaglioni and P. Navrátil, Phys. Rev. Lett. **101**, 092501 (2008); Phys. Rev. C **79**, 044606 (2009); for a recent review, see, e. g., B. R. Barrett, P. Navrátil and J. P. Vary, Progr. Part. Nucl. Phys. **69**, 131 (2013).

[2] R. Roth and P. Navrátil, Phys. Rev. Lett. **99**, 092501 (2007); R. Roth, Phys. Rev. C **79**, 064324 (2009); R. Roth, J. Langhammer, A. Calci, S. Binder and P. Navrátil, Phys. Rev. Lett. **107**, 072501 (2011); R. Roth, S. Binder, K. Vobig, A. Calci, J. Langhammer and P. Navrátil, *ibid.* **109**, 052501 (2012).

[3] T. Dytrych, K. D. Sviratcheva, C. Bahri, J. P. Draayer and J. P. Vary, Phys. Rev. Lett. **98**, 162503 (2007); Phys. Rev. C **76**, 014315 (2007); J. Phys. G **35**, 095101 (2008); T. Dytrych, K. D. Launey, J. P. Draayer, P. Maris, J. P. Vary, E. Saule, U. Catalyurek, M. Sosonkina, D. Langr and M. A. Caprio, Phys. Rev. Lett. **111**, 252501 (2013); for reviews, see T. Dytrych, K. D. Sviratcheva, J. P. Draayer, C. Bahri and J. P. Vary, J. Phys. G **35**, 123101 (2008); J. P. Draayer, T. Dytrych, K. D. Launey and D. Langr, Progr. Part. Nucl. Phys. **67**, 516 (2012).

[4] A. F. Lisetskiy, B. R. Barrett, M. K. G. Kruse, P. Navrátil, I. Stetcu and J. P. Vary, Phys. Rev. C **78**, 044302 (2008); A. F. Lisetskiy, M. K. G. Kruse, B. R. Barrett, P. Navrátil, I. Stetcu and J. P. Vary, *ibid.* **80**, 024315 (2009).

[5] L. Liu, T. Otsuka, N. Shimizu, Y. Utsuno and R. Roth, Phys. Rev. C **86**, 014304 (2012).

[6] T. Abe, P. Maris, T. Otsuka, N. Shimizu, Y. Utsuno and J. P. Vary, Phys. Rev. C **86**, 054301 (2012).

[7] N. Shimizu, Y. Utsuno, T. Mizusaki, T. Otsuka, T. Abe and M. Honma, Phys. Rev. C **82**, 061305(R) (2010); N. Shimizu, Y. Utsuno, T. Mizusaki, M. Honma, Y. Tsunoda and T. Otsuka, *ibid.* **85**, 054301 (2012); Y. Utsuno, N. Shimizu, T. Otsuka and T. Abe, Comp. Phys. Comm. **184**, 102 (2013); N. Shimizu, T. Abe, Y. Tsunoda, Y. Utsuno, T. Yoshida, T. Mizusaki, M. Honma and T. Otsuka, Progr. Theor. Exp. Phys. 01A205 (2012).

[8] S. A. Coon, M. I. Avetian, M. K. G. Kruse, U. van Kolck, P. Maris and J. P. Vary, Phys. Rev. C **86**, 054002 (2012); S. A. Coon, arXiv:1303.6358 [nucl-th] (2013); S. A. Coon and M. K. G. Kruse, arXiv:1408.0738 [nucl-th] (2014).

[9] R. J. Furnstahl, G. Hagen and T. Papenbrock, Phys. Rev. C **86**, 031301(R) (2012); S. N. More, A. Eksrom, R. J. Furnstahl, G. Hagen and T. Papenbrock, *ibid.* **87**, 044326 (2013); R. J. Furnstahl, S. N. More and T. Papenbrock, *ibid.* **89**, 044301 (2014); R. J. Furnstahl, G. Hagen, T. Papenbrock and K. A. Wendt, arXiv:1408.0252 [nucl-th] (2014); S. Konig, S. K. Bogner, R. J. Furnstahl, S. N. More and T. Papenbrock, arXiv:1409.5997 [nucl-th] (2014).

[10] M. Honma, T. Mizusaki and T. Otsuka, Phys. Rev. Lett. **75**, 1284 (1995); *ibid.* **77**, 3315 (1996); T. Otsuka, M. Honma and T. Mizusaki, *ibid.* **81**, 1588 (1998); for a review, see T. Otsuka, M. Honma, T. Mizusaki, N. Shimizu and Y. Utsuno, Progr. Part. Nucl. Phys. **47**, 319 (2001).

[11] P. Maris, J. P. Vary and A. M. Shirokov, Phys. Rev. C **79**, 14308 (2009); P. Maris, A. M. Shirokov and J. P. Vary, *ibid.* **81**, 021301 (2010); C. Cockrell, J. P. Vary and P. Maris, *ibid.* **86**, 034325 (2012); P. Maris and J. P. Vary, Int. J. Mod. Phys. E **22**, 1330016 (2013).

[12] E. D. Jurgenson, P. Maris, R. J. Furnstahl, W. E. Ormand and J. P. Vary, Phys. Rev. C **87**, 054312 (2013).

[13] A. M. Shirokov, J. P. Vary, A. I. Mazur and T. A. Weber, Phys. Lett. B **644**, 33 (2007); A. M. Shirokov, J. P. Vary, A. I. Mazur, S. A. Zaytsev and T. A. Weber, *ibid.* **621**, 96 (2005).