



LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Effective Interactions from No Core Shell Model

E. Dikmen, A. F. Lisetskiy, B. R. Barrett, P.
Navratil, J. P. Vary

February 3, 2009

Nuclear Physics and Astrophysics: From Stable Beams to
Exotic Nuclei
Cappadocia, Turkey
June 25, 2008 through June 30, 2008

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

Effective Interactions from No Core Shell Model

E. Dikmen*, A. F. Lisetskiy†, B. R. Barrett†, P. Navratil** and J. P. Vary‡

*Department of Physics, Suleyman Demirel University, Isparta, Turkey

†Department of Physics, University of Arizona, Tucson, AZ 85721, USA

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

‡Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

Abstract. We construct the many-body effective Hamiltonian for pf-shell by carrying out $2\hbar\Omega$ NCSM calculations at the 2-body cluster level. We demonstrate how the effective Hamiltonian derived from realistic nucleon-nucleon (NN) potentials for the $2\hbar\Omega$ NCSM space should be modified to properly account for the many-body correlations produced by truncating to the major pf-shell. We obtain two-body effective interactions for the pf-shell by using direct projection and use them to reproduce the results of large scale NCSM for other light Ca isotopes.

Keywords: NCSM, ab-initio, effective interactions

PACS: 21.10.Hw, 23.20.En, 23.20.Lv, 23.20.-g, 27.40.+z

In recent years remarkable progress in *ab-initio* microscopic nuclear structure studies has been made in calculating nuclear properties, e.g., low-lying spectra, transition strengths etc., of the nuclei with $A < 14$ [1]. Large basis no-core shell model (NCSM) calculations has been successful to reproduce the low-lying spectra in light nuclei [2]. When we apply the NCSM calculations to nuclei in the $A > 12$ mass region, the model spaces required to obtain converged results are too huge to be handled by existing computers. The problem remains of how to reproduce the many-body correlations present in the large space in a tractable, smaller model space.

In this study we demonstrate how the effective Hamiltonian derived from realistic NN potentials for the $2\hbar\Omega$ NCSM space should be modified to properly account for the many-body correlations produced by truncating to the pf-shell, in the spirit of Ref. [3]. We obtain two-body effective interactions for the pf-shell by using direct projection and use them to reproduce the results of large scale NCSM for other light Ca isotopes.

The NCSM calculations start with the intrinsic Hamiltonian of the A -nucleon system,

$$H = \sum_{i=1}^A \frac{\vec{p}_i^2}{2m} + \sum_{i<j=1}^A V_{ij}^{NN}, \quad (1)$$

where m is the nucleon mass and V_{ij}^{NN} , the bare NN interaction. We can modify H by adding the center-of-mass harmonic oscillator (HO) potential to allow us to work with convenient basis states. The new A - and Ω -dependent Hamiltonian can be written as

$$H_{A,n=A}^{\Omega} = \sum_{i=1}^{n=A} \left[\frac{\vec{p}_i^2}{2m} + \frac{1}{2} m \Omega^2 \vec{r}_i^2 \right] + \sum_{i<j=1}^{n=A} \left[V_{ij}^{NN} - \frac{m \Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]. \quad (2)$$

The exact solution of the Eq.(1) requires an A -body effective interaction for the A -nucleon system, and such a solution is not currently possible. However, if we make

a two-body cluster approximation ($n = 2$) for the effective interaction, this allows us to solve the eigenvalue problem, even in the almost “infinite” space, e.g. $N_{max} = 450$, where N_{max} is the maximal number of excited HO quanta. Note that the A -body correlations for the considered A -nucleon system enter into the bare Hamiltonian $H_{A,n=2}^{\Omega}$ through the last term in Eq.(2), as well as the indirect dependence on Ω due the truncation of the model space. The solution of the two-body cluster Hamiltonian $H_{A,n=2}^{\Omega}$ in the almost “full” space gives us the eigenvalues $E_{A,2;k}$ and corresponding eigenvectors $|k\rangle$.

We utilize a unitary transformation to construct effective Hamiltonian $H_{A,2}^{\Omega,eff}$ in the truncated model space. The diagonalization of the bare Hamiltonian $H_{A,n=2}^{\Omega}$ means that we know the unitary transformation U , such that $H_{A,2;diag}^{\Omega} = UH_{A,2}^{\Omega}U^{\dagger}$ where $H_{A,2;diag}^{\Omega}$ is the diagonal matrix containing the eigenvalues $E_{A,2;k}$. By introducing the model P -space, one builds the matrix $H_{A,2;diag}^{\Omega;p} = PH_{A,2;diag}^{\Omega}P$. The effective Hamiltonian $H_{A,2}^{\Omega,eff}$ can be calculated using the following formula:

$$H_{A,2}^{\Omega,eff} = \frac{U_{pp}^{\dagger}}{\sqrt{U_{pp}^{\dagger}U_{pp}}} H_{A,2;diag}^{\Omega;p} \frac{U_{pp}}{\sqrt{U_{pp}^{\dagger}U_{pp}}}, \quad (3)$$

where the matrix U_{pp} is the $d_p \times d_p$ square matrix corresponding to the P -space.

After a unitary transformation of the bare Hamiltonian $H_{A,2}^{\Omega}$ to the $2\hbar\Omega$ model space in the case of ^{42}Sc , we obtain the 42-body Hamiltonian by using the coefficients of fractional parentage from 2-body to 42-body system. The corresponding 42-body effective Hamiltonian of ^{42}Sc in the $2\hbar\Omega$ space can be expressed in terms of the 2-body effective Hamiltonian of ^{42}Sc in the same space. If we replace the eigenvalues and eigenvectors of $H_{42,42}^{N_{max},\Omega,eff}$ in a subspace of the $2\hbar\Omega$ space, called P_2 , with those of $H_{42,2}^{\Omega;p}$ in Eq. (3), we can perform a secondary unitary transformation of $H_{42,42}^{N_{max},\Omega,eff}$ from the $2\hbar\Omega$ model space to the smaller subspace P_2 , e.g., the pf -space. The new effective Hamiltonian would be in the $0\hbar\Omega$ or pf - model space and reproduces exactly the lowest d_{P_2} eigenvalues of the Hamiltonian $H_{42,42}^{N_{max},\Omega,eff}$.

$$H_{42,42}^{0,\Omega,eff} = \frac{U_{pp}^{42,\dagger}}{\sqrt{U_{pp}^{42,\dagger}U_{pp}^{42}}} H_{42,42;pp}^{2,\Omega} \frac{U_{pp}^{42}}{\sqrt{U_{pp}^{42,\dagger}U_{pp}^{42}}} \quad (4)$$

The 42-body effective Hamiltonian $H_{42,42}^{0,\Omega,eff}$ can be represented in terms of 1-body, 2-body, 3-body, and so on effective Hamiltonians:

$$H_{eff} = H_{eff}(1) + H_{eff}(2) + H_{eff}(3) + H_{eff}(4) + \dots \quad (5)$$

The obtained 42-body effective Hamiltonian $H_{42,42}^{0,\Omega,eff}$ is for ^{42}Sc . This means that it has only 1-body and 2-body terms. If we repeat the entire procedure for ^{41}Sc , we obtain only 1-body terms of the effective Hamiltonian in pf -space. Then we subtract the 1-body terms from the effective Hamiltonian of ^{42}Sc , and we obtain the pure effective 2-body matrix elements in the pf -space. By using the single particle energies from ^{41}Sc and the

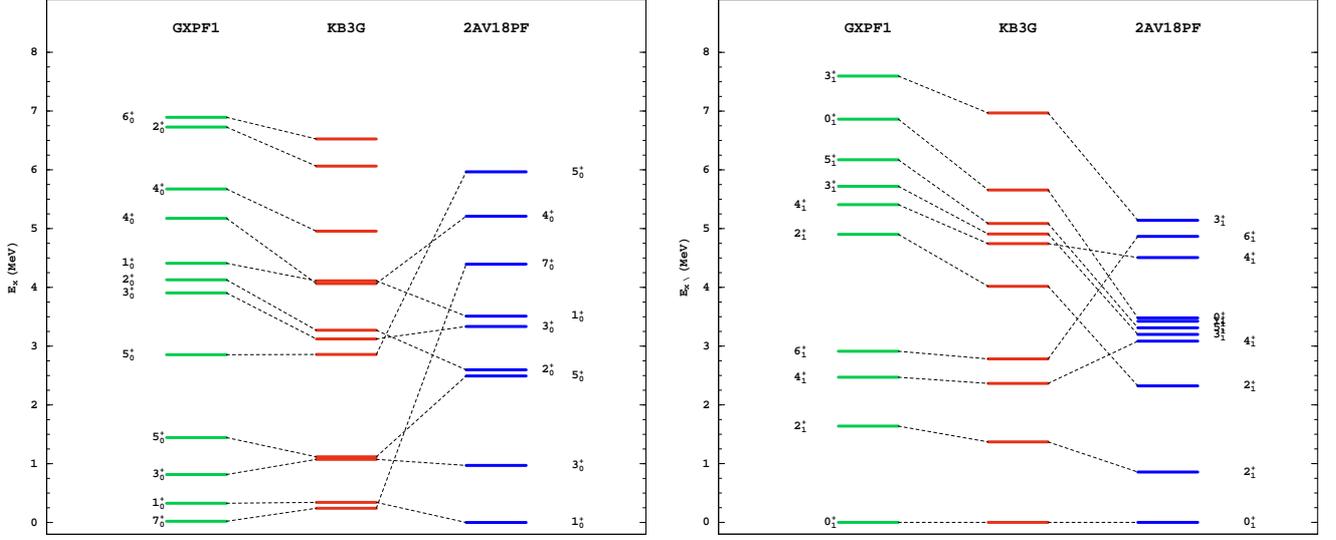


FIGURE 1. The excitation energies of the $J^{\pi}_{T=0}$ and $J^{\pi}_{T=1}$ states for ^{42}Sc calculated in the $2\hbar\Omega$ space with the AV18 potential. The KB3G and GXPF1 spectra are shown for comparison. The value of $\hbar\Omega = 10$ MeV has been used for the AV18 calculations.

pure effective 2-body interactions in the pf -space, we can perform standard shell-model calculations for ^{42}Sc . By construction, the standard shell model calculations for ^{42}Sc are supposed to give exactly the same results as the NCSM calculations for ^{42}Sc in the $2\hbar\Omega$ space. Following the prescription outlined above, we have calculated the effective pf -space Hamiltonian for ^{42}Sc by using the many-body $2\hbar\Omega$ Hamiltonian constructed from the AV18 [4] NN interactions. We have performed the standard shell model (SM) calculation with this effective pf -space interaction, from now on we call it 2AV18PF for ^{42}Sc . For the NCSM with the $2\hbar\Omega$ space effective interactions for ^{42}Sc , from now on we call it 2AV18. Results for both effective interactions for spectra of ^{42}Sc are exactly the same. We have also performed the standard SM calculations by using the well known pf -shell effective interactions KB3G [5] and GXPF1 [6] for comparison. The resulting effective Hamiltonian $H_{42,42}^{0,\Omega,\text{eff}}$ reproduces the excitation energies of the lowest pf -space dominated states of $2\hbar\Omega$ NCSM calculations for ^{42}Sc , as shown in Figs. 1. In Fig. 1 we see that all $T = 0$ states are more or less lower, while 7_0^+ and 5_0^+ states are too high with respect to the results of KB3G and GXPF1 interactions. For $T = 1$ in Fig. 1 only the 4_1^+ and 6_1^+ states are higher, all the others are lower. The effective interaction 2AV18PF gives reasonable spectra for ^{42}Sc compared to the spectra resulting from the KB3G and GXPF1 effective interactions. We plot the standard SM and NCSM results for the two lowest excited states of each spin for ^{44}Ca and ^{46}Ca in Fig. 2. We notice that the standard SM matches almost exactly the $2\hbar\Omega$ NCSM excitation energies, although the dimension of the $2\hbar\Omega$ space for ^{44}Ca is 11 million (m-scheme), while the dimension of the pf -space is only 565. The very small differences for excitation energies may be attributed to not enough Lanczos convergence and three- and four-body pf -space correlations, as well the density dependence, which is not considered by the two-body 2AV18PF interaction.

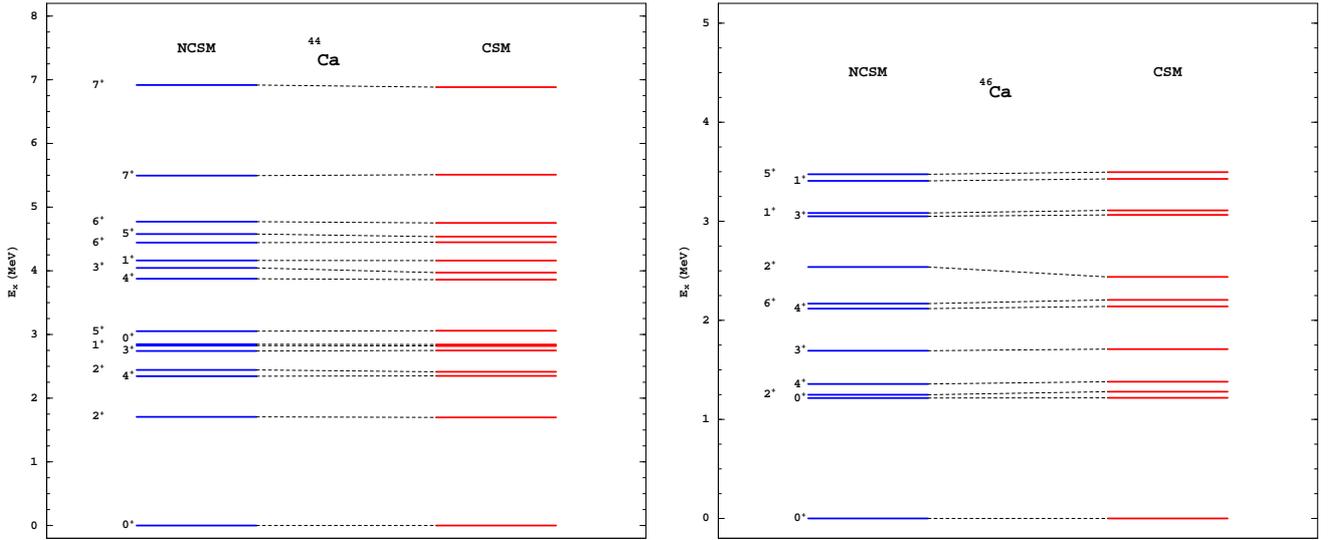


FIGURE 2. The standard SM and NCSM spectrum for ^{44}Ca and ^{46}Ca with 2AV18PF and 2AV18 interactions, respectively.

In conclusion, we have derived pf -shell effective 1-body and 2-body Hamiltonians from 41-body and 42-body $2\hbar\Omega$ Hamiltonians constructed by using AV18 NN potentials. We introduce a two step procedure: first, a unitary transformation of bare Hamiltonian into the $2\hbar\Omega$ model space and the second, a secondary unitary transformation of the diagonalized $2\hbar\Omega$ Hamiltonian into the pf -space. We have performed the NCSM calculations for ^{42}Sc by using the effective interaction 2AV18 obtained at the first step, the standard SM calculations for ^{42}Sc by using the effective interaction 2AV18PF obtained at the second step. Both spectra from the NCSM and the standard SM are exactly the same for ^{42}Sc .

***This work was supported in part by NSF grant PHY-0555396, the Scientific and Technological Council of Turkey, TUBITAK-BIDEB and TUBITAK 105T092, and prepared by LLNL under Contract DE-AC52-07NA27344.

REFERENCES

1. R. Roth and P. Navratil, Phys. Rev. Lett. **99**, 092501 (2007); I.Stetcu, B.R. Barrett, P. Navratil, and J.P. Vary, Phys. Rev. C **73**, 037307 (2006); P. Navratil, W.E. Ormand, C. Forssen, and E. Caurier, Eur. Phys. J. A **25**, Supplement 1, 481 (2005);
2. P. Navratil, J. P. Vary, W. E. Ormand, and B. R. Barrett, Phys. Rev. Lett. **87**, 172502 (2001); P. Navratil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett **84**, 5728 (2000).
3. P. Navratil, M. Thoresen, and B. R. Barrett, Phys. Rev. C **55**, R573 (1997).
4. R. B. Wiringa, V. G. J. Stocks, and R. Schiavilla, Phys. Rev. C. **51**, 38 (1995); S. Pieper and R. B. Wiringa, Annu. Rev. Nucl. Part. Sci. **51**, 53 (2001).
5. A. Poves and A. P. Zuker, Phys. Rep. **70**, 235 (1981); A. Poves, J. Sanchez-Solano, E. Caurier, and F. Nowacki, Nucl. Phys. A **694**, 157 (2001).
6. M. Honma, T. Otsuka, B. A. Brown, and T. Mizusaki, Phys. Rev. C **69**, 034335 (2004).