Ab initio Shell Model: With and Without a Core

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Arizona's First University.

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# MICROSCOPIC NUCLEAR-STRUCTURE **THEORY**

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many body theory



A. SchwenkWeinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Meissner, Nogga, Machleidt,

I. Forces among nucleons

1. QCD ---> EFT ---> CPT --> Self-consistent nucleon interactions

2. Need NN and NNN and perhaps NNNN interactions



P. Navratil and E. Caurier, Phys. Rev. C 69, 014311 (2004)

### H. Kamada, *et al.*, *Phys. Rev. C* 64, 044001 (2001)

PHYSICAL REVIEW C, VOLUME 64, 044001

#### Benchmark test calculation of a four-nucleon bound state

In the past, several efficient methods have been developed to solve the Schrödinger equation for fournucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic AV8' NN interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.





# Standard Shell Model

- Maria Goeppert-Mayer J. Hans D. Jensen (1949)
- Nobel Prize for Physics 1963



#### PHENOMENOLOGICAL EFFECTIVE

#### **INTERACTIONS**

1. Usually constructed for a single major shell

- 2. Take experimental single-particle energies
- 3. Determine two-body matrix elements

# $\langle (j_1j_2)TT|V| (j_3j_4)TT \rangle$

by a least-squares fit to some subset of the experimental data





# *Some current shell-model references*

1. E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, and A. P. Zuker, "The Shell Model as a Unified View of Nuclear Structure," *Reviews of Modern Physics* **77**, 427 (2005)

2. B. A. Brown, "The Nuclear Shell Model towards the Drip Lines," *Progress in Particle and Nuclear Physics* **47**, 517 (2001)

3. I. Talmi, "Fifty Years of the Shell Model-The Quest for the Effective Interaction," *Advances in Nuclear Physics*, Vol. **27**, ed. J. W. Negele and E. Vogt (Plenum, NY, 2003)

4. B. R. B., "Effective Operators in Shell-Model Calculations," 10<sup>th</sup> Indian Summer School of Nuclear Physics:Theory of Many-Fermion Systems, *Czechoslovak Journal of Physics* **49**, 1 (1999)



Lecture Notes in Physics, vol. 40.

**Abstract not Available** 

## **The Smithsonian/NASA Astrophysics Data System**





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the University of Arizona, Tucson, June 2-6,1975. Editor: B. R. Barrett,

# **No Core Shell Model**

"Ab Initio" approach to microscopic nuclear structure calculations, in which all  $\underline{A}$  nucleons are treated as being active.

Want to solve the A-body Schrödinger equation

$$
H_A \Psi^A = E_A \Psi^A
$$

R.P. Navrátil, J.P. Vary, B.R.B., PRC 62, 054311 (2000) P. Navratil, et al., J. Phys. G: Nucl. Part. Phys. 36, 083101 (2009)

# *No-Core Shell-Model Approach*

• Start with the purely intrinsic Hamiltonian

$$
H_A = T_{rel} + \mathcal{V} = \frac{1}{A} \sum_{i < j = 1}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i < j = 1}^{A} V_{NN} \left( + \sum_{i < j < k}^{A} V_{ijk}^{3b} \right)
$$

**Note**: There are **no** phenomenological s.p. energies!

Can use any NN potentials Coordinate space: Momentum space: Argonne V8', AV18 Nijmegen I, II CD Bonn, EFT Idaho

# *No-Core Shell-Model Approach*

• Next, add CM harmonic-oscillator Hamiltonian

$$
H_{CM}^{HO} = \frac{\vec{P}^2}{2Am} + \frac{1}{2}Am\Omega^2 \vec{R}^2; \quad \vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i, \quad \vec{P} = Am\vec{R}
$$

# To H<sub>A</sub>, yielding

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

Defines a basis (*i.e.* HO) for evaluating *V ij*

# $H \Psi = E \Psi$

We cannot, in general, solve the full problem in the

complete Hilbert space, so we must truncate to a finite

model space

We must use effective interactions and  $\implies$ operators!

# *Effective Interaction*

• Must truncate to a finite model space



- In general,  $V_{ii}^{\text{eff}}$  is an A-body interaction *ij*
- We want to make an *a*-body cluster approximation

$$
\mathcal{H} = \mathcal{H}^{(I)} + \mathcal{H}^{(A)} \underset{a < A}{\geq} \mathcal{H}^{(I)} + \mathcal{H}^{(a)}
$$

$$
H\Psi_{\alpha} = E_{\alpha}\Psi_{\alpha} \quad \text{where} \quad H = \sum_{i=1}^{A} t_i + \sum_{i \leq j}^{A} v_{ij}.
$$

$$
\mathcal{H}\Phi_{\beta} = E_{\beta}\Phi_{\beta}
$$

$$
\Phi_{\beta} = P\Psi_{\beta}
$$

 $P$  is a projection operator from  $S$  into  $S$ 

$$
\langle \tilde{\Phi}_{\gamma} | \Phi_{\beta} \rangle = \delta_{\gamma \beta}
$$

$$
\mathcal{H} = \sum_{\beta \in \mathcal{S}} |\Phi_{\beta} \rangle E_{\beta} < \tilde{\Phi}_{\beta}
$$





- **NCSM** convergence test
	- Comparison to other methods



P. Navratil, INT Seminar, November 13, 2007, online





P. Navrátil, J. P. Vary and B. R. B., Phys. Rev. C 62, 054311 (2000)

C. FORSSÉN, P. NAVRÁTIL, W. E. ORMAND, AND E. CAURIER





P. Navrátil and W. E. Ormand, Phys. Rev. C **68**, 034305 (2003)



P. Navratil

H. Kamada, *et al.*, *Phys. Rev. C* 64, 044011 (2001)



Figure 2. NCSM and GFMC NN pair density in <sup>4</sup>He.



*Towards a unified description of the nucleus*

# **The goal of nuclear structure theory:**

exact treatment of nuclei based on NN, NNN,... interactions

 $\Rightarrow$  need to build a bridge between:

0 $\hbar\Omega$  Shell Model calculations: 16 < A < 120 *ab initio few-body & light nuclei calculations: A*  $\leq 24$  $\Rightarrow$   $\rightarrow$ 

Density Functional Theory calculations:  $A \geq 100$ .<br>i/

#### PHYSICAL REVIEW C 78, 044302 (2008)

#### *Ab-initio* shell model with a core

A. F. Lisetskiy, <sup>1,\*</sup> B. R. Barrett, <sup>1</sup> M. K. G. Kruse, <sup>1</sup> P. Navratil, <sup>2</sup> I. Stetcu, <sup>3</sup> and J. P. Vary<sup>4</sup> <sup>1</sup>Department of Physics, University of Arizona, Tucson, Arizona 85721, USA <sup>2</sup>Lawrence Livermore National Laboratory, Livermore, California 94551, USA <sup>3</sup>Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA <sup>4</sup>Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA (Received 20 June 2008; published 10 October 2008)

We construct effective two- and three-body Hamiltonians for the p-shell by performing  $12\hbar\Omega$  ab initio no-core shell model (NCSM) calculations for  $A = 6$  and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the  $0\hbar\Omega$  space. We then separate these effective Hamiltonians into inert core, one- and two-body contributions (also three-body for  $A = 7$ ) and analyze the systematic behavior of these different parts as a function of the mass number A and size of the NCSM basis space. The role of effective three- and higher-body interactions for  $A > 6$ is investigated and discussed.

DOI: 10.1103/PhysRevC.78.044302

PACS number(s):  $21.10$ . Hw,  $21.60$ . Cs,  $23.20$ . Lv,  $27.20 + n$ 









P. Navrátil and E. Caurier, Phys. Rev. C **69**, 014311 (2004)

## NCSM results for <sup>6</sup>Li with CD-Bonn NN potential

**Dimensions p-space: 10; Nmax =12: 48 887 665; Nmax = 14: 211 286 096** 





$$
H\Psi_{\alpha} = E_{\alpha}\Psi_{\alpha} \quad \text{where} \quad H = \sum_{i=1}^{A} t_i + \sum_{i \leq j}^{A} v_{ij}.
$$

$$
\mathcal{H}\Phi_{\beta} = E_{\beta}\Phi_{\beta}
$$

$$
\Phi_{\beta} = P\Psi_{\beta}
$$

 $P$  is a projection operator from  $S$  into  $S$ 

$$
\langle \tilde{\Phi}_{\gamma} | \Phi_{\beta} \rangle = \delta_{\gamma \beta}
$$

$$
\mathcal{H} = \sum_{\beta \in \mathcal{S}} |\Phi_{\beta} \rangle E_{\beta} < \tilde{\Phi}_{\beta}
$$



## **Effective Hamiltonian for SSM**

Two ways of convergence: 1) For P  $\rightarrow$  1 and fixed a:  $H^{\text{eff}}_{\text{A},a=2}$   $\rightarrow$  H<sub>A</sub>: previous slide 2) For  $a_1 \rightarrow A$  and fixed  $P_1$ :  $Heff_{Aa1} \rightarrow H_A$ 

 $P_1 + Q_1 = P$ ;  $P_1$  - small model space;  $Q_1$  - excluded space;

$$
\mathcal{H}_{A,a_1}^{N_{1,\max},N_{\max}} = \frac{U_{a_1,P_1}^{A,\dagger}}{\sqrt{U_{a_1,P_1}^{A,\dagger}U_{a_1,P_1}^A}}E_{A,a_1,P_1}^{N_{\max},\Omega}\frac{U_{a_1,P_1}^A}{\sqrt{U_{a_1,P_1}^{A,\dagger}U_{a_1,P_1}^A}}
$$

**Valence Cluster Expansion**  $N_{1,max} = 0$  space (p-space);  $a_1 = A_c + a_v$ ;  $a_1$  - order of cluster;  $A_c$  - number of nucleons in core;  $a_v$  - order of valence cluster;

$$
\mathcal{H}_{A,a_1}^{0,N_{\max}}=\sum_k^{a_{\mathrm{v}}}V_k^{A,A_c+k}
$$

Two-body VCE for <sup>6</sup>Li  
\n
$$
\mathcal{H}_{A=6,a_1=6}^{0,N_{\text{max}}} = V_0^{6,4} + V_1^{6,5} + V_2^{6,6}
$$
\nNeed NCSM results  
\nin N<sub>max</sub> space for  
\nWith effective interaction for A=6 III:  $H_{A=6,2}^{N_{\text{max}},\Omega,\text{eff}}$   
\nCore Energy  
\n
$$
V_0^{6,4} = -51.644 \text{ MeV}
$$
\n
$$
V_1^{6,5} = \mathcal{H}_{6,5}^{0,N_{\text{max}}} - V_0^{6,4} \quad \langle ab; JT | V_1^{6,5} | cd; JT \rangle = (\epsilon_a + \epsilon_b) \delta_{a,c} \delta_{b,d}
$$
\nSingle Particle  
\nEnergies  
\n
$$
V_2^{6,6} = \mathcal{H}_{6,6}^{0,N_{\text{max}}} - \mathcal{H}_{6,5}^{0,N_{\text{max}}}
$$
\n
$$
V_2^{6,6} = \mathcal{H}_{6,6}^{0,N_{\text{max}}} - \mathcal{H}_{6,5}^{0,N_{\text{max}}}
$$
\n
$$
\langle p_{3/2}p_{3/2} | V_2^{6,6} | p_{3/2}p_{3/2} \rangle_{J=3,7=0} = -1.825 \text{ MeV}
$$
\nTBMEs

## 2-body Valence Cluster **approximation for A=6**



2-body Valence Cluster approximation for A=7



2-body Valence Cluster approximation for A=7

$$
\mathcal{H}_{A}^{0,N_{\mathrm{max}}}=V_{0}^{A,4}+V_{1}^{A,5}+V_{2}^{A,6}
$$





3-body Valence Cluster approximation for A>6



 **P<sup>1</sup> + Q1 = P; P<sup>1</sup>** Construct 3-body interaction in terms of 3-body matrix elements: Yes

$$
V_3^{A,7} = \mathcal{H}_{A,7}^{0,N_{\max}} - \mathcal{H}_{A,6}^{0,N_{\max}}.
$$



## 3-body Valence Cluster approximation for A>6





#### Effective operators from exact many-body renormalization

A. F. Lisetskiy, <sup>1,2,\*</sup> M. K. G. Kruse, <sup>1</sup> B. R. Barrett, <sup>1</sup> P. Navratil, <sup>3</sup> I. Stetcu, <sup>4</sup> and J. P. Vary<sup>5</sup> <sup>1</sup>Department of Physics, University of Arizona, Tucson, Arizona 85721, USA <sup>2</sup>National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824-1321, USA <sup>3</sup>Lawrence Livermore National Laboratory, Livermore, California 94551, USA <sup>4</sup>Department of Physics, University of Washington, P. O. Box 351560, Seattle, Washington 98195-1560, USA <sup>5</sup>Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA (Received 15 June 2009; published 28 August 2009)

We construct effective two-body Hamiltonians and E2 operators for the p shell by performing  $16\hbar\Omega$  ab initio no-core shell model (NCSM) calculations for  $A = 5$  and  $A = 6$  nuclei and explicitly projecting the many-body Hamiltonians and E2 operator onto the  $0\hbar\Omega$  space. We then separate the effective E2 operator into one-body and two-body contributions employing the two-body valence cluster approximation. We analyze the convergence of proton and neutron valence one-body contributions with increasing model space size and explore the role of valence two-body contributions. We show that the constructed effective  $E2$  operator can be parametrized in terms of one-body effective charges giving a good estimate of the NCSM result for heavier  $p$ -shell nuclei.

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PACS number(s):  $27.20.+n$ ,  $21.10.Hw$ ,  $21.60.Cs$ ,  $23.20.Lv$ 

$$
E_J = \mathcal{U}_J \mathcal{H}_J \mathcal{U}_J^{\dagger}.
$$
 (4)

This same eigenstate matrix  $\mathcal{U}_J$  can also be used to calculate the matrix elements of other effective operators,  $\mathcal{O}_{A,a_1}^{\text{eff}}(\lambda k; JJ')$ , between basis states with spins J and J' in the  $0\hbar\Omega$  space:

$$
\mathcal{M}_{A,a_1}^{\text{eff}}(\lambda k; JJ') = \mathcal{U}_J \mathcal{O}_{A,a_1}^{\text{eff}}(\lambda k; JJ') \mathcal{U}_{J'}^{\dagger},\tag{5}
$$



FIG. 6: The quadrupole moment of the ground state for <sup>6</sup>Li  $(1^+(T = 0))$  is shown in terms of one- and two-body contributions as a function of increasing model space size.

# **Summary**

3-step technique to construct effective Hamiltonian for SSM with a core :

- #1 2-body UT of bare NN Hamiltonian (2-body cluster approximation)
- #2 NCSM diagonalization in large  $N_{max}$  space for  $A = 4,5,6,7$

 #3 many-body UT of NCSM Hamiltonian (up to 3-body valence cluster approximation) Results:

- 1) strong mass dependence of core  $\&$  one-body parts of  $H<sup>eff</sup>$
- 2) 3-body effective interaction plays crucial role

3) negligible role of 4-body and higher-order interactions for identical nucleons

4) similar approach can be applied for calculating effective operators for other physical quantities



## COLLABORATORS

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# SOME REMAINING CHALLENGES

- 1. Understanding the fundamental interactions among the nucleons in terms of QCD, e.g., NN, NNN, ....
- 2. Determination of the mean field (the monopole effect).
- 3. Microscopic calculations of medium- to heavy-mass nuclei:
	- a.) How to use the advances for light nuclei to develop techniques for heavier nuclei.
	- b.) Building in more correlations among the nucleons in small model spaces, e.g., effective interactions for heavier nuclei.
- 4. Extensions of these microscopic advances for nuclear structure to nuclear reactions.





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#### No-core shell model in an effective-field-theory framework

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Editor: W. Haxton

#### **Abstract**

We present a new approach to the construction of effective interactions suitable for many-body calculations by means of the no-core shell model (NCSM). We consider an effective field theory (EFT) with only nucleon fields directly in the NCSM model spaces. In leading order, we obtain the strengths of the three contact interactions from the condition that in each model space the experimental ground-state energies of  ${}^{2}H$ .  ${}^{3}H$  and  ${}^{4}He$  be exactly reproduced. The first  $(0^+; 0)$  excited state of <sup>4</sup>He and the ground state of <sup>6</sup>Li are then obtained by means of NCSM calculations in several spaces and frequencies. After we remove the harmonic-oscillator frequency dependence, we predict for <sup>4</sup>He an energy level for the first  $(0^+;0)$ excited state in remarkable agreement with the experimental value. The corresponding <sup>6</sup>Li binding energy is about 70% of the experimental value, consistent with the expansion parameter of the EFT.

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S. Quaglioni and P. Navratil, Phys. Rev. Lett. 101, 092501  $(2008)$ 

long range (continuum)

# I. Forces among nucleons

1. QCD ---> EFT ---> CPT --> Self-consistent nucleon interactions

2. Need NN and NNN and perhaps NNNN interactions

## 3. Which approach is best?

- a) Chiral Effective Field Theory
- b) Find NN interaction which minimizes the NNN interaction and then treat the NNN interaction perturbatively.
- c) Contract the NNN interaction into the nuclear medium as 0-, 1-, and 2-body density dependent parts + a small residual NNN force.
- d) Other approaches: V\_low-k, Similarity Renormalization Group (SRG), Unitary Correlation Operator Method (UCOM), INOY,...

#### V.F. WEISSKOPF

how matter came about, and they add a great deal of significance and importance to nuclear physics and to certain experiments in nuclear physics which would have only little importance to the problems we have discussed here. Perhaps in the next conference we should have a session where we discuss these things; it is not enough just to go to Mr. Cameron or Mr. Fowler and ask him what shall we measure, we ought to know why we do it.

The second and last point I would like to raise is this. To round up the conference I come back to the first remark of Peierls, when he opened up the conference and asked the question, why are we interested in nuclear structure. May I add my own little verse to this. I have heard many people say that Nuclear Structure is not a fundamental problem, the real thing is high energy physics; the object of nuclear structure is after all nothing else but solving a Schroedinger equation for A particles. I strongly disagree with this point of view. The discovery and the understanding of phenomena hidden in a many-body problem can be a task of fundamental importance, if the object itself is of central interest. A car shows on the state of the second social

Physics inquires into the nature of things. The nucleus, our nucleus, is an essential part of nature, it is the centre of the atom. It is not just a little phenomenon, it is the most prominent constituent of matter. The understanding of the phenomena occurring in this nucleus is therefore of paramount importance. Hence Nuclear Physics is an essential part of physics. I found out that some theorists, both in the east and in the west, consider the sales only thing worth doing is elementary particle physics. Experimentalists usually don't say so because they work with real matter (and hence they know that the nucleus is an important thing. These theorists, however, worship the theory of elementary particles, a theory which in fact doesn't even exist. They knock their heads daily against a wall of dispersion-relations, Mandelstam representations and the like. Let them do it. After all the proton and the meson are also an important part of nature. In fact we should give them all the moral support they need. They are a brave lot who fight a very difficult fight and some day they will find the theory . But don't let yourself be talked into believing that the nucleus is not interesting. It is so small and it has so few parts and still it shows a tremendous variety of phenomena. Its investigation requires the whole arsenal of presently available. experimental techniques and its understanding makes use of almost all branches of theoretical physics. What a marvellous invention! It is worth devoting a lifetime to it.

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