Prospects for the No Core Shell Model

Bruce R. Barrett University of Arizona, Tucson



Arizona's First University.

INT Program 11-2d

August 17, 2011

OUTLINE

I. Brief Overview of the No Core Shell Model (NCSM)

II. Applications of the NCSM

III. Approaches for Extending the NCSM to Heavier Mass Nuclei

IV. Summary and Outlook

MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear manybody theory

No Core Shell Model

"Ab Initio" approach to microscopic nuclear structure calculations, in which <u>all A</u> nucleons are treated as being active.

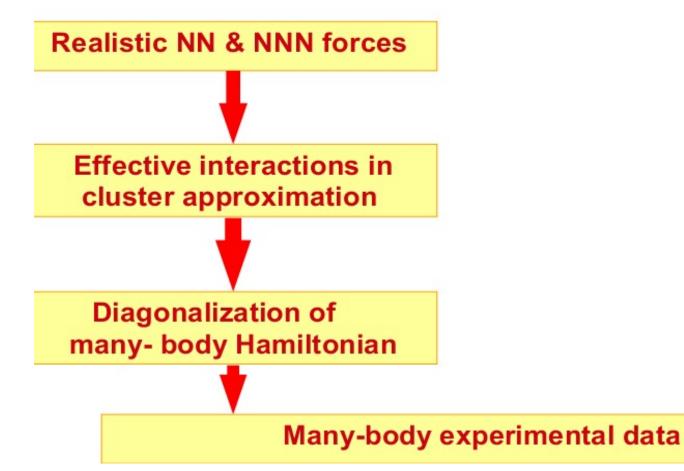
Want to solve the A-body Schrödinger equation

$$H_{A}\Psi^{A} = E_{A}\Psi^{A}$$

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

From few-body to many-body





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 <u>no</u> phenomenological s.p. energies!

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

No-Core Shell-Model Approach

Next, add CM harmonic-oscillator Hamiltonian

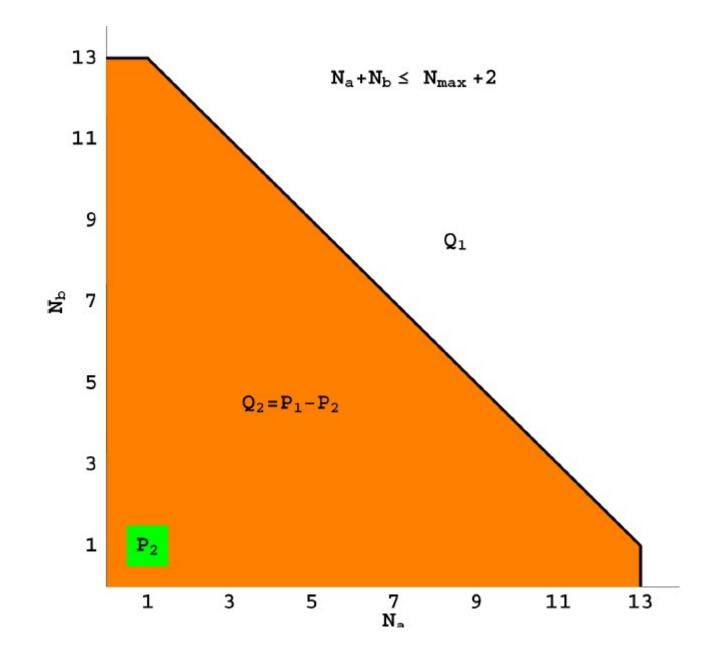
$$H_{CM}^{HO} = \frac{\vec{P}^{2}}{2Am} + \frac{1}{2}Am\Omega^{2}\vec{R}^{2}; \quad \vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_{i}, \quad \vec{P} = Am\dot{\vec{R}}$$

To H_A, yielding

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

V_{ii}

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

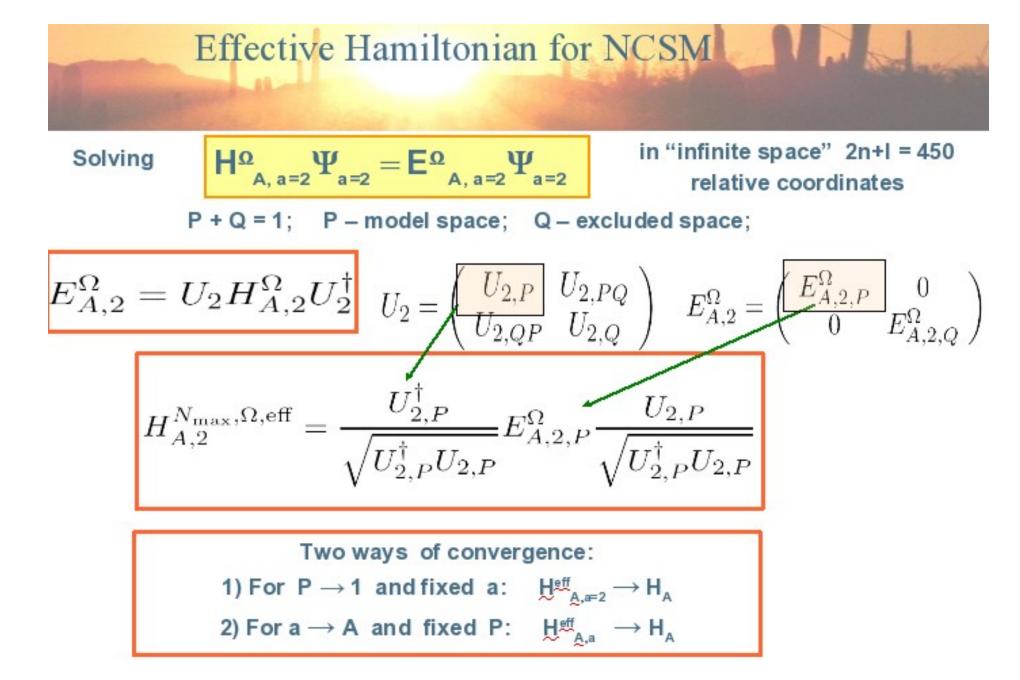


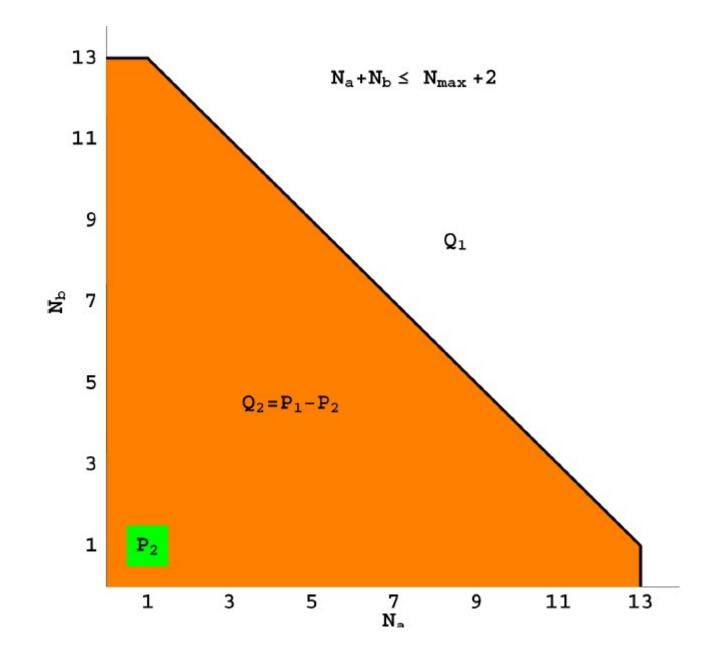
$$egin{aligned} & H\Psi_lpha & = E_lpha\Psi_lpha & W here & H = \sum_{i=1}^A t_i + \sum_{i\leq j}^A v_{ij}. \ & \mathcal{H}\Phi_eta & = E_eta \Phi_eta & \ & \Phi_eta & = P\Psi_eta & \end{aligned}$$

P is a projection operator from S into S

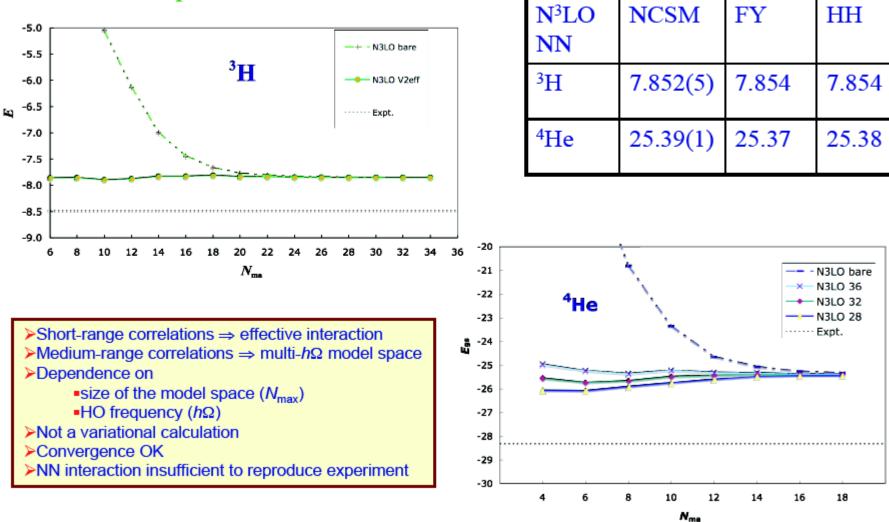
$$< \tilde{\Phi}_{\gamma} | \Phi_{\beta} > = \delta_{\gamma\beta}$$

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

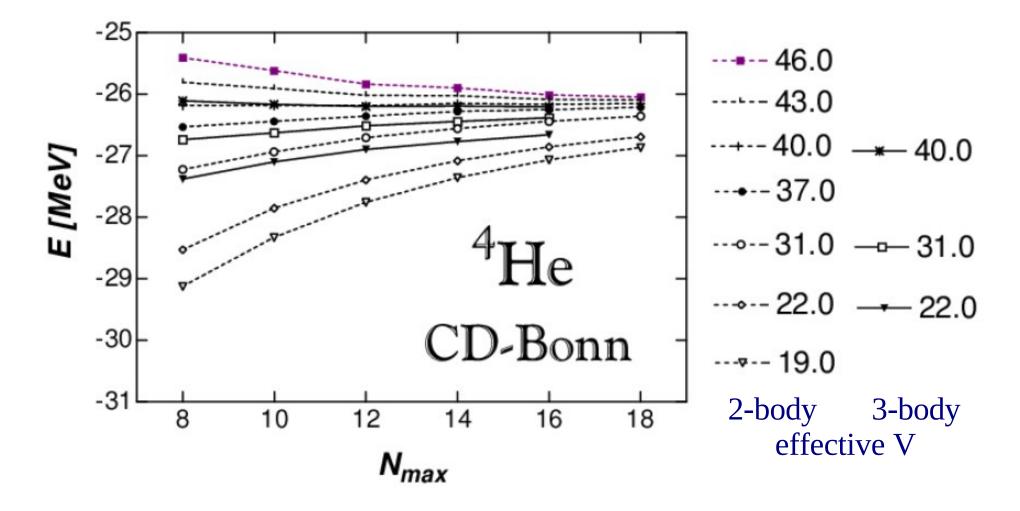


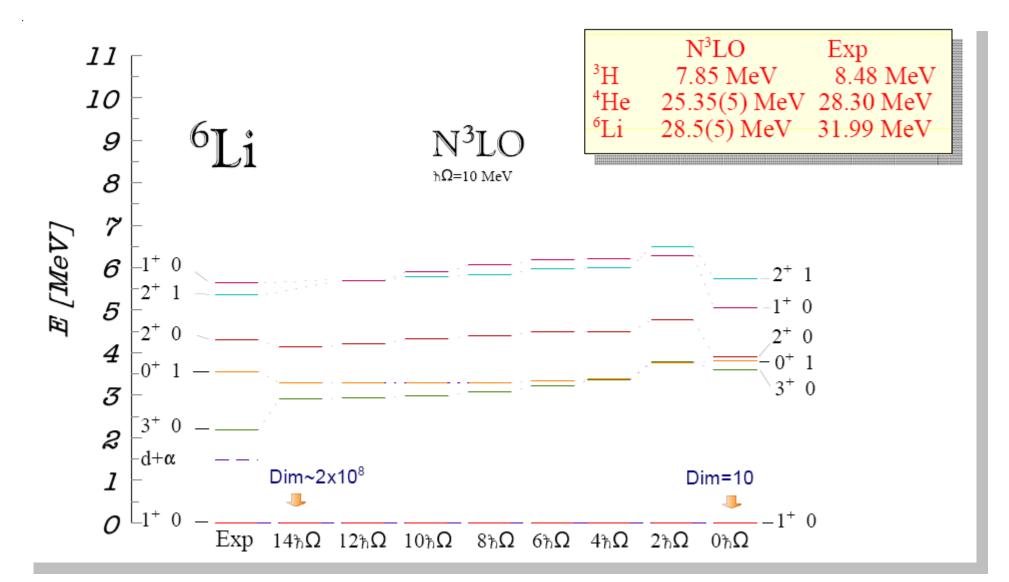


- NCSM convergence test
 - Comparison to other methods



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





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

II. Applications of the NCSM

H. Kamada, *et al.*, Phys. Rev. C <u>64</u>, 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.

BE _{th}≈ 25.91 MeV



H. Kamada, *et al.*, Phys. Rev. C <u>64</u>, 044011 (2001)

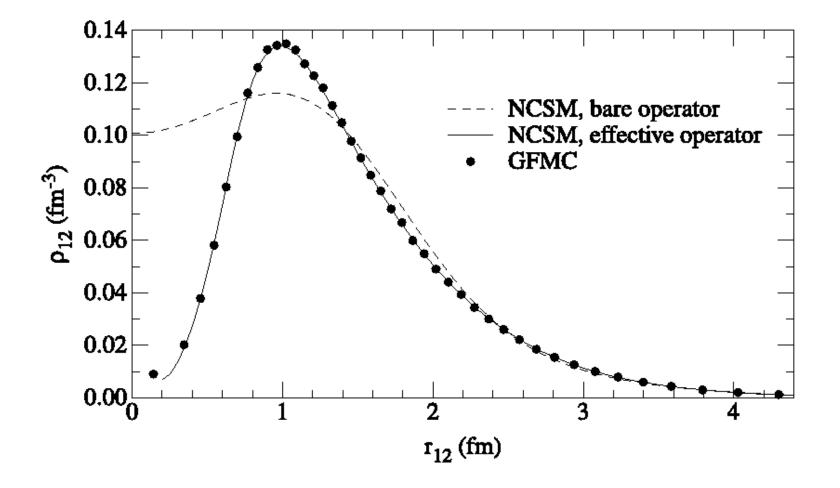


Figure 2. NCSM and GFMC NN pair density in ⁴He.

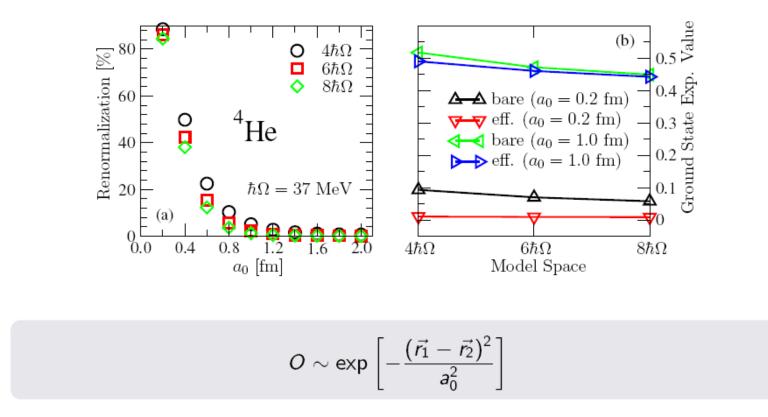
Nucleus	Observable	Model Space	Bare operator	Effective operator
² H	Q_0	$4\hbar\Omega$	0.179	0.270
⁶ Li	$B(E2,1^+0 \rightarrow 3^+0)$	$2\hbar\Omega$	2.647	2.784
⁶ Li	$B(E2,1^+0\rightarrow 3^+0)$	$10\hbar\Omega$	10.221	2
⁶ Li	$B(E2,2^+0\rightarrow 1^+0)$	$2\hbar\Omega$	2.183	2.269
⁶ Li	$B(E2,2^+0\rightarrow 1^+0)$	$10\hbar\Omega$	4.502	-
¹⁰ C	$B(E2,2^+_10\rightarrow 0^+0)$	$4\hbar\Omega$	3.05	3.08
¹² C	$B(E2, 2^+_1 0 \to 0^+ 0)$	$4\hbar\Omega$	4.03	4.05
⁴ He	$\langle g.s. T_{rel} g.s. \rangle$	$8\hbar\Omega$	71.48	154.51

Stetcu, Barrett, Navratil, Vary, Phys. Rev. C 71, 044325 (2005)

- small model space: expect larger renormalization
- large variation with the model space
- three-body forces: might be important, but not the issue
- *a* → *A* for fixed model space;
- $P \to \infty$ for fixed cluster.



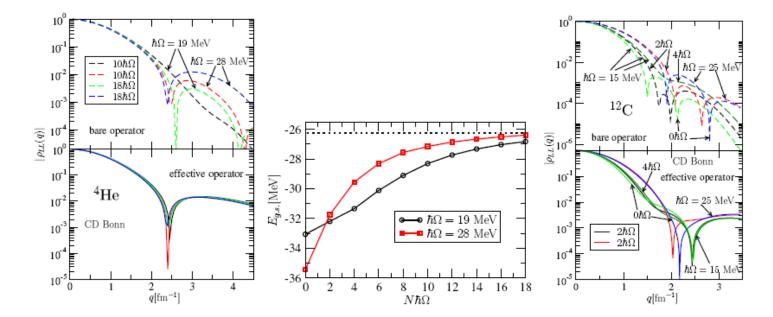
Range dependence



Stetcu, Barrett, Navratil, Vary, Phys. Rev. C 71, 044325 (2005)

Longitudinal-longitudinal distribution function

$$\rho_{LL}(q) = \frac{1}{4Z} \sum_{j \neq i} (1 + \tau_z(i)) (1 + \tau_z(j)) \langle g.s. | j_0(q | \vec{r_i} - \vec{r_j} |) | g.s. \rangle$$



Stetcu, Barrett, Navratil, Vary, nucl-th/0601076

Model space independence at high momentum transfer: good renormalization at the two-body cluster level

PHYSICAL REVIEW C 79, 044606 (2009)

Ab initio many-body calculations of nucleon-nucleus scattering

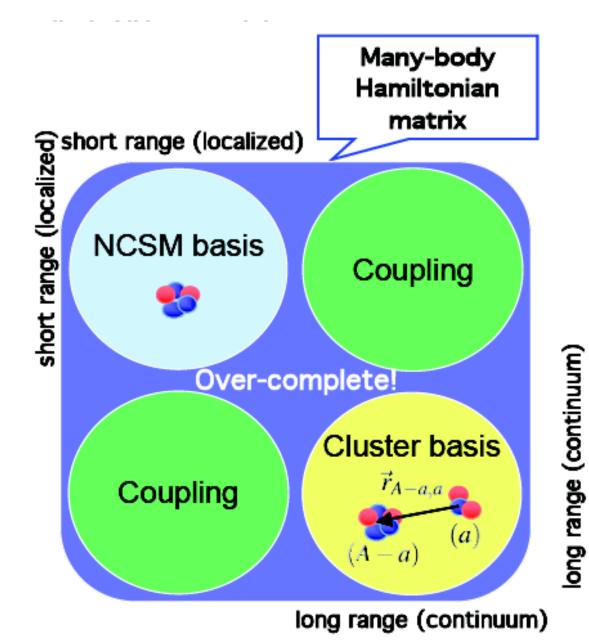
Sofia Quaglioni and Petr Navrátil

Lawrence Livermore National Laboratory, P. O. Box 808, L-414, Livermore, California 94551, USA (Received 7 January 2009; published 16 April 2009)

We develop a new *ab initio* many-body approach capable of describing simultaneously both bound and scattering states in light nuclei, by combining the resonating-group method with the use of realistic interactions, and a microscopic and consistent description of the nucleon clusters. This approach preserves translational symmetry and the Pauli principle. We outline technical details and present phase-shift results for neutron scattering on ³H, ⁴He, and ¹⁰Be and proton scattering on ^{3,4}He, using realistic nucleon-nucleon (*NN*) potentials. Our A = 4 scattering results are compared to earlier *ab initio* calculations. We find that the CD-Bonn *NN* potential in particular provides an excellent description of nucleon-⁴He *S*-wave phase shifts. In contrast, the experimental nucleon-⁴He *P*-wave phase shifts are not well reproduced by any *NN* potential we use. We demonstrate that a proper treatment of the coupling to the *n*-¹⁰Be continuum is successful in explaining the parity-inverted ground state in ¹¹Be.

DOI: 10.1103/PhysRevC.79.044606

PACS number(s): 21.60.De, 25.10.+s, 27.10.+h, 27.20.+n



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

PHYSICAL REVIEW C 81, 021301(R) (2010)

Ab initio nuclear structure simulations: The speculative ¹⁴F nucleus

P. Maris,¹ A. M. Shirokov,^{1,2,*} and J. P. Vary¹

¹Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011-3160, USA ²Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow RU-119991, Russia (Received 13 November 2009; published 4 February 2010)

We present results from *ab initio* no-core full configuration simulations of the exotic proton-rich nucleus ¹⁴F, whose first experimental observation is expected soon. Calculations with the JISP16 *NN* interaction are performed up to the $N_{max} = 8$ basis space. The binding energy is evaluated using an extrapolation technique. This technique is generalized to excitation energies, verified in calculations of ⁶Li, and applied to ¹⁴F and ¹⁴B, the ¹⁴F mirror, for which some data are available.

DOI: 10.1103/PhysRevC.81.021301

PACS number(s): 21.60.De, 21.10.Dr, 27.20.+n

Origin of the Anomalous Long Lifetime of ¹⁴C

P. Maris,¹ J. P. Vary,¹ P. Navrátil,^{2,3} W. E. Ormand,^{3,4} H. Nam,⁵ and D. J. Dean⁵

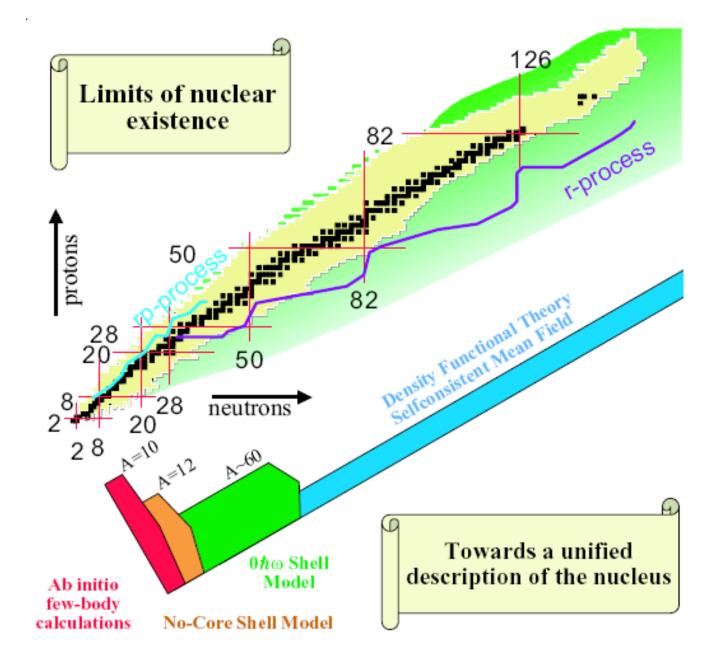
 ¹Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011-3160, USA ²TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia, V6T 2A3, Canada
 ³Lawrence Livermore National Laboratory, L-414, P.O. Box 808, Livermore, California 94551, USA
 ⁴Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA ⁵Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831, USA (Received 27 January 2011; published 20 May 2011)

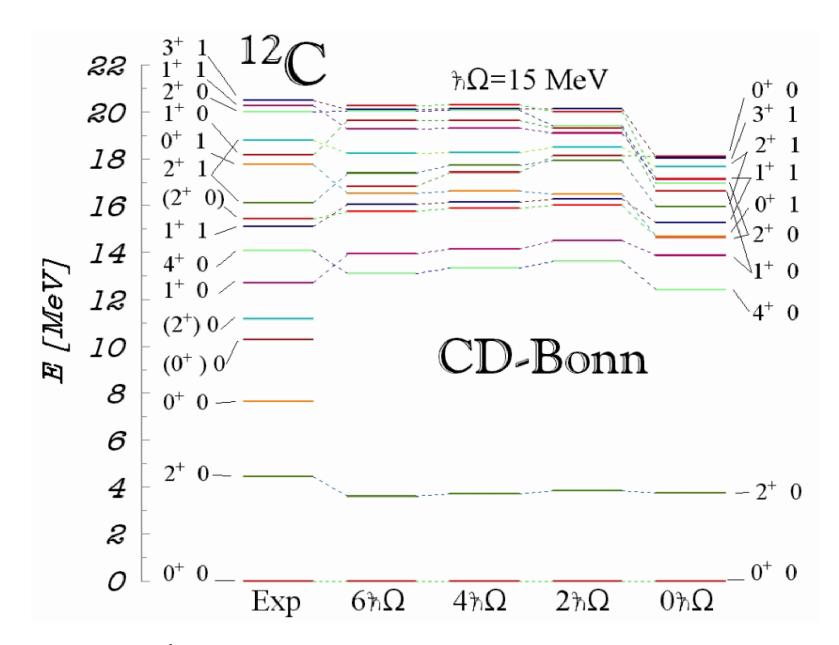
We report the microscopic origins of the anomalously suppressed beta decay of ¹⁴C to ¹⁴N using the *ab initio* no-core shell model with the Hamiltonian from the chiral effective field theory including three-nucleon force terms. The three-nucleon force induces unexpectedly large cancellations within the *p* shell between contributions to beta decay, which reduce the traditionally large contributions from the nucleon-nucleon interactions by an order of magnitude, leading to the long lifetime of ¹⁴C.

DOI: 10.1103/PhysRevLett.106.202502

PACS numbers: 21.10.Tg, 21.60.De, 23.40.-s, 27.20.+n

III. Extending the NCSM to Heavier Mass Nuclei





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

Beyond the No Core Shell Model 1. The ab initio Shell Model with a Core

- 2. Importance Truncation
- 3. The NCSM in an Effective Field Theory (EFT) Framework
- 4. MC-NCSM (U of Tokyo/Iowa State U)
- 5. Other approaches

1. The *ab initio* Shell Model with a Core

PHYSICAL REVIEW C 78, 044302 (2008)

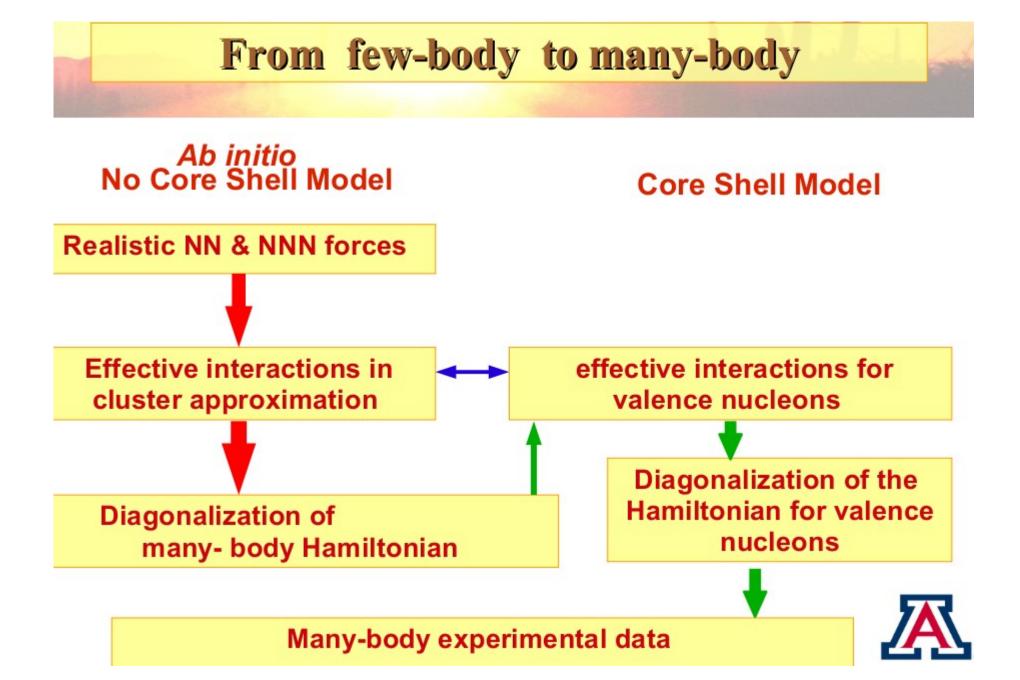
Ab-initio shell model with a core

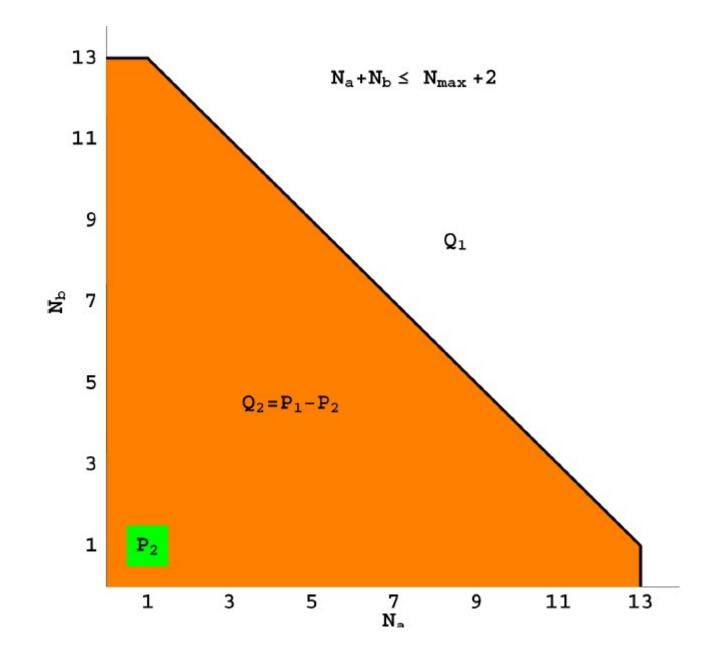
A. F. Lisetskiy,^{1,*} B. R. Barrett,¹ M. K. G. Kruse,¹ P. Navratil,² I. Stetcu,³ and J. P. Vary⁴ ¹Department of Physics, University of Arizona, Tucson, Arizona 85721, USA ²Lawrence Livermore National Laboratory, Livermore, California 94551, USA ³Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA ⁴Department 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.

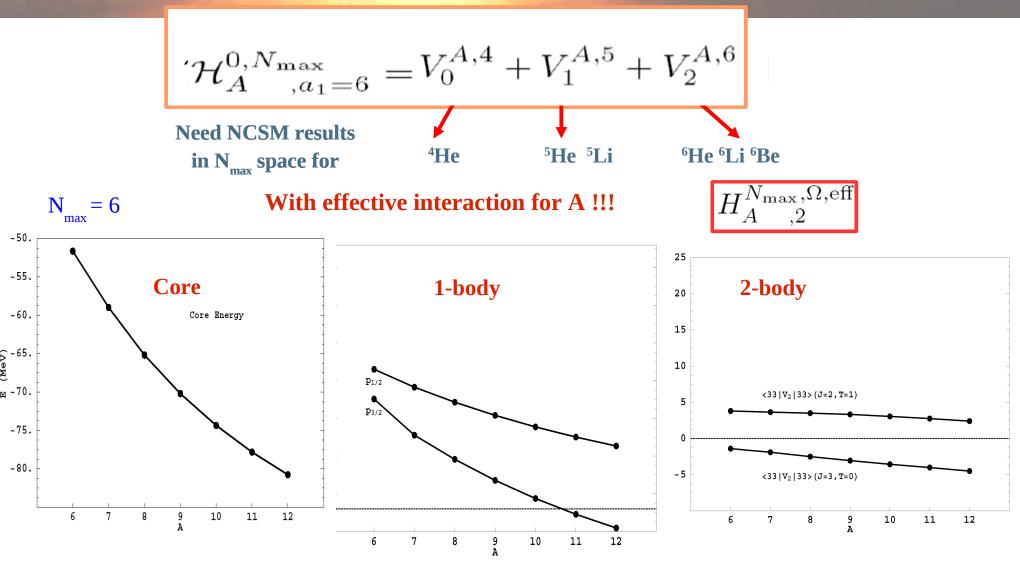
DOI: 10.1103/PhysRevC.78.044302

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

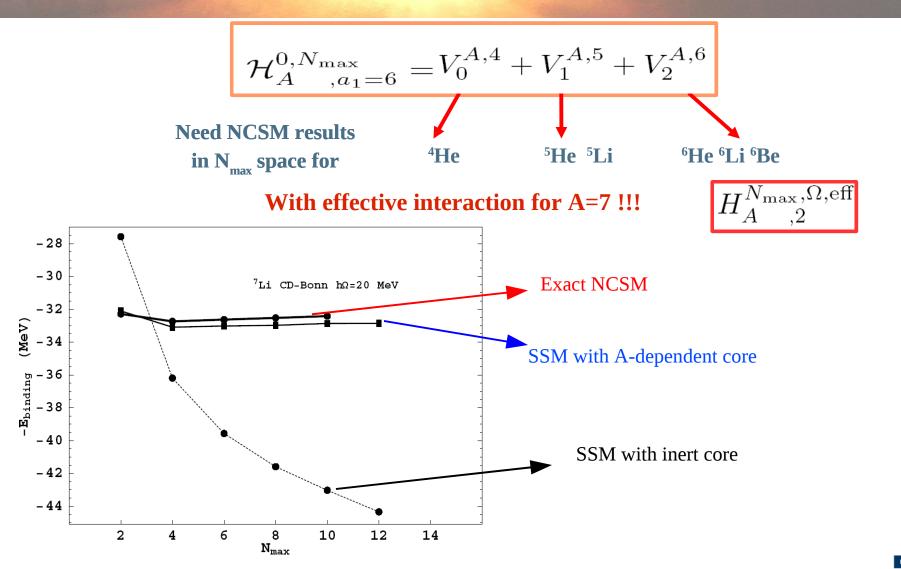




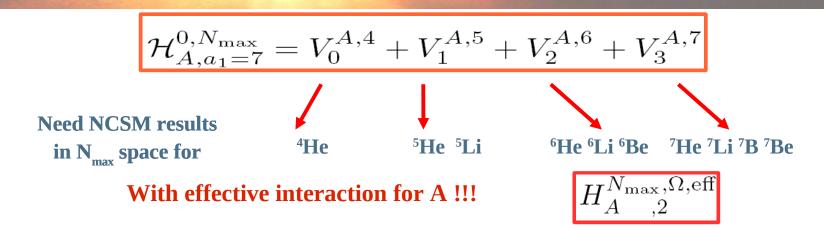
2-body Valence Cluster approximation for A=6



2-body Valence Cluster approximation for A=7



3-body Valence Cluster approximation for A>6



Construct 3-body interaction in terms of 3-body matrix elements: Yes

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



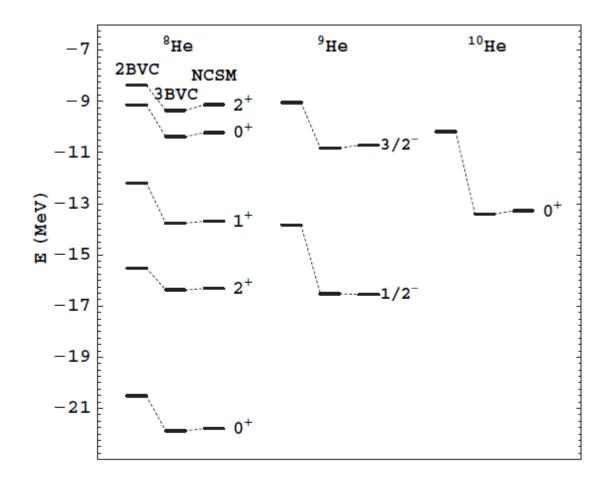


FIG. 9. Comparison of spectra for ⁸He, ⁹He, and ¹⁰He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\text{max}} = 6$ and $\hbar\Omega = 20$ MeV using the CD-Bonn interaction.

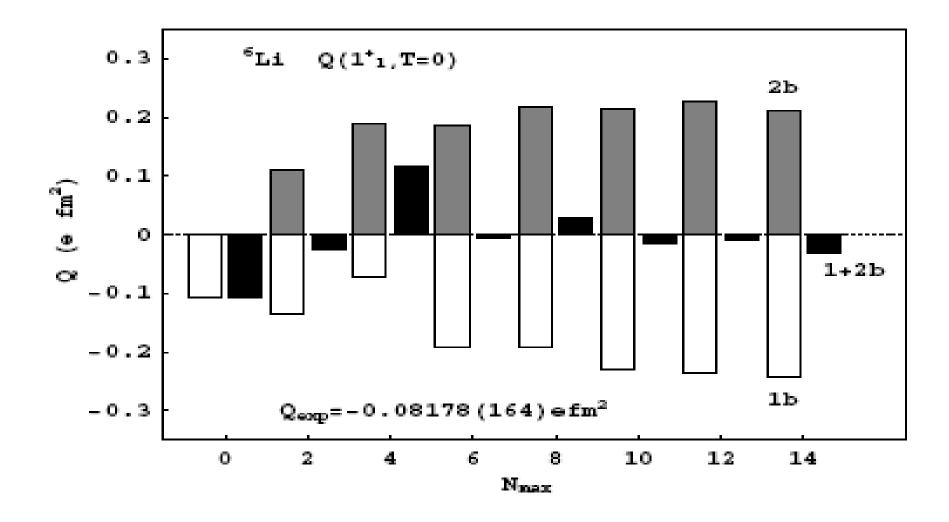
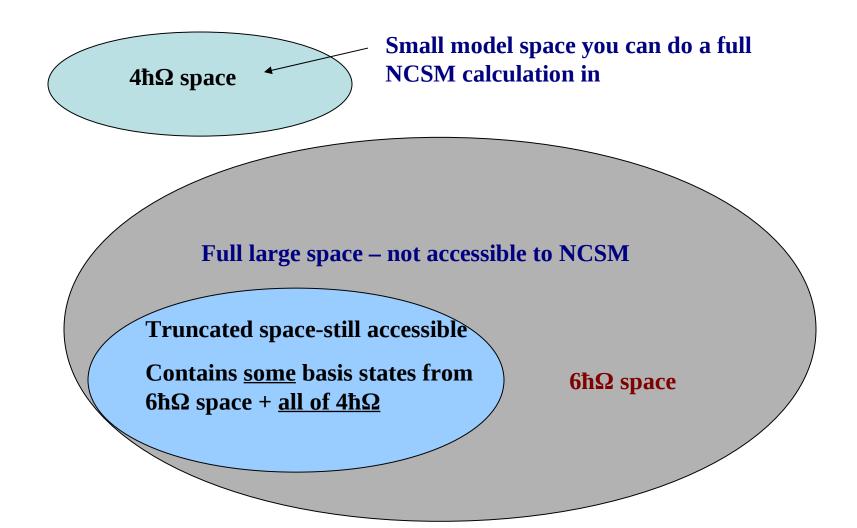


FIG. 6: The quadrupole moment of the ground state for ⁶Li $(1^+(T = 0))$ is shown in terms of one- and two-body contributions as a function of increasing model space size.

2. Importance Truncation

The idea of Importance Truncation



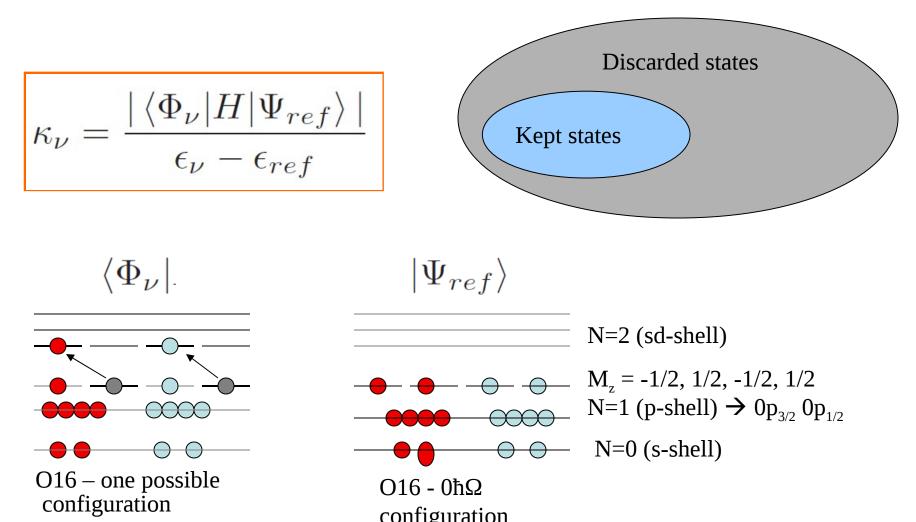
Formalism of Importance truncation.

 First order multi-configurational perturbation theory gives...

$$\begin{split} |\Psi^{(1)}\rangle &= -\sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle \Phi_{\nu} | W | \Psi_{\text{ref}} \rangle}{\epsilon_{\nu} - \epsilon_{\text{ref}}} | \Phi_{\nu} \rangle \\ &= -\sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle \Phi_{\nu} | H | \Psi_{\text{ref}} \rangle}{\epsilon_{\nu} - \epsilon_{\text{ref}}} | \Phi_{\nu} \rangle. \end{split}$$

$$W=H-H_0$$

Importance truncation schematically

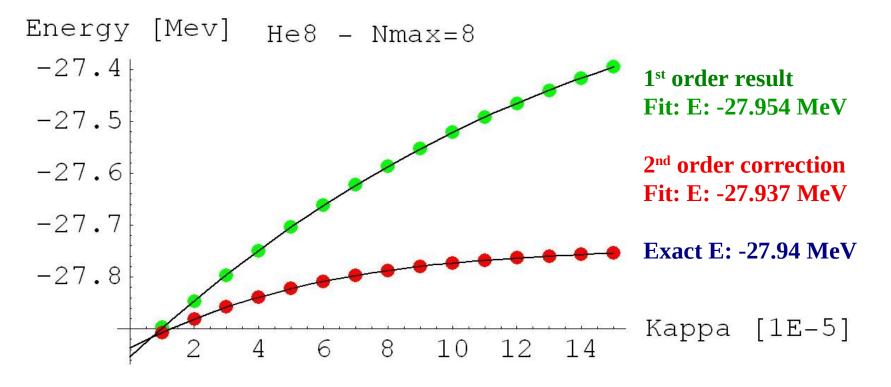


Corrections to the energy

• 2nd order perturbation theory gives you an estimate of the correction to the energy from the discarded state. The first order result is equal to zero.

$$\Delta_{\text{excl}}(\kappa_{\min}) = -\sum_{\substack{\nu \notin \mathcal{M}(\kappa_{\min})}} \frac{|\langle \Phi_{\nu} | H | \Psi_{\text{ref}} \rangle|^2}{\epsilon_{\nu} - \epsilon_{\text{ref}}}$$

⁸He: IT started at $N_{max} = 6$, final space $N_{max} = 8$



Interaction: ⁸He SRG N3LO

3. The NCSM in an Effective Field Theory (EFT) Framework



Available online at www.sciencedirect.com



Physics Letters B 653 (2007) 358-362

PHYSICS LETTERS B

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

I. Stetcu a,b,*, B.R. Barrett a, U. van Kolcka

^a Department of Physics, University of Arizona, Tucson, AZ 85721, USA
^b Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Received 5 March 2007; received in revised form 8 July 2007; accepted 31 July 2007

Available online 9 August 2007

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 ²H, ³H and ⁴Hebe exactly reproduced. The first (0⁺; 0) excited state of ⁴He and the ground state of ⁶Li are then obtained by means of NCSM calculations in several spaces and frequencies. After we remove the harmonic-oscillator frequency dependence, we predict for ⁴He an energy level for the first (0⁺; 0) excited state in remarkable agreement with the experimental value. The corresponding ⁶Li binding energy is about 70% of the experimental value, consistent with the expansion parameter of the EFT.

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PACS: 21.30.-x; 21.60.Cs; 24.10.Cn; 45.50.Jf

J. Phys. G: Nucl. Part. Phys. 37 (2010) 064033 (11pp)

doi:10.1088/0954-3899/37/6/064033

Effective interactions for light nuclei: an effective (field theory) approach

I Stetcu¹, J Rotureau², B R Barrett^{2,3} and U van Kolck²

¹ Department of Physics, University of Washington, Seattle, WA 98195, USA
 ² Department of Physics, University of Arizona, Tucson, AZ 85721, USA

E-mail: bbarrett@physics.arizona.edu

Received 12 December 2009 Published 26 April 2010 Online at stacks.iop.org/JPhysG/37/064033

Abstract

One of the central open problems in nuclear physics is the construction of effective interactions suitable for many-body calculations. We discuss a recently developed approach to this problem, where one starts with an effective field theory containing only fermion fields and formulated directly in a no-core shell-model space. We present applications to light nuclei and to systems of a few atoms in a harmonic-oscillator trap. Future applications and extensions, as well as challenges, are also considered.

Why EFT + NCSM?

EFT:

- 1. Captures the relevant degrees of freedom/symmetries
- 2. Builds in the correct long-range behavior
- 3. Has a systematic way for including the short-range behavior/order by order
- 4. Many-body and two-body interactions treated in the same framework
- 5. Explains naturally the hierarchy of the (many-body) forces

NCSM:

- 1. Flexible many-body method/easy to implement
- 2. Equivalent SD and Jacobi formulations
- 3. Can handle both NN and NNN interactions
- 4. In principle applies to any nucleus/extensions to heavier nuclei

Effective Field Theory (1/3)

i) Separation of scale :

 $M_{_{QCD}} \sim 1 \text{ GeV} (\text{mass of nucleon})$ $M_{_{nucl}} \sim 100 \text{ MeV} (typical momentum in a nucleus})$ $M_{_{struct}} \sim 10 \text{ MeV} (binding energy of a nucleon in a nucleus})$

-> details of physics at short distance (high energy) are irrelevant for low energy physics.

-> in EFT low energy degrees of freedom are explicitly included (high momenta are integrated out).

ii) The Lagrangian / potential consistent with symmetries is expanded as a Taylor Series:

$$V(\vec{p}',\vec{p}) = \sum_{i,j} C_{i,j}(\vec{p})^i (\vec{p}')^j$$

Effective Field Theory (2/3)

iii) Regularization and renormalization :

-> cut-off Λ (separation between low and high energy physics)

$$V(\vec{p}',\vec{p}) \Longrightarrow \sum_{i,j} C_{i,j}(\Lambda)(\vec{p})^i (\vec{p}')^j$$

-> no dependence on cut-off for observables (for a high enough cut-off), dependence absorbed by coupling constants (fitted with observables).

Effective Field Theory (3/3)

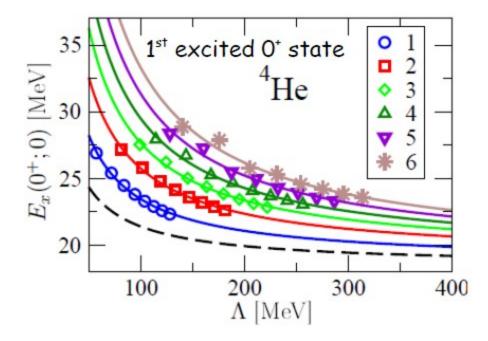
iv) Find the power counting ("truncation of the Taylor series"):

-> hierarchy between the different contributions

-> results improvable order by order (Leading Order, Next-to-Leading-Order, Next-to-Next-to-Leading-Order.....)

Pionless EFT for nuclei within the NCSM: Without pions--> Breakdown momentum roughly 100 MeV/c

$$\begin{split} H &= \frac{1}{2m_N A} \sum_{[i < j]} (\vec{p}_i - \vec{p}_j)^2 + C_0^1 \sum_{[i < j]^1} \delta(\vec{r}_i - \vec{r}_j) \\ &+ C_0^0 \sum_{[i < j]^0} \delta(\vec{r}_i - \vec{r}_j) + D_0 \sum_{[i < j < k]} \delta(\vec{r}_i - \vec{r}_j) \delta(\vec{r}_j - \vec{r}_k), \end{split}$$
et. al., 2007



Stetcu

-> calculation at **Leading order** : two N-N contact interactions in the ${}^{3}S_{1,} {}^{1}S_{0}$ channel and a threebody contact interaction in the 3nucleon $S_{1/2}$ channel

-> coupling constants fitted to the binding energy of the deuteron, triton and ⁴He.

Difficulties:

fixing the couplings to few-body states is cumbersome HO: bound states only no immediate connection to the scattering observables

Question : How to construct an EFT within a bound many-body model space beyond Leading-Order ? Answer : by trapping nuclei in a harmonic potential

T. Busch, et al., Found. Phys. 28, 549 (1998)

$$\frac{\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega}\right)}{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega}\right)} = -\frac{bk}{2}\cot\delta$$

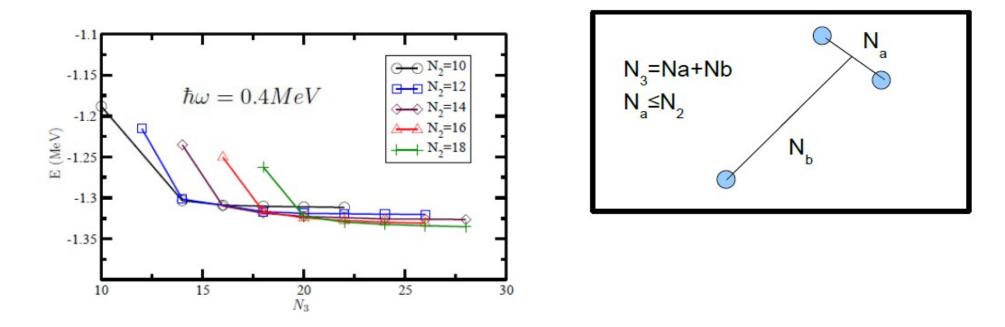
energy in the trap (bound state physics) phase shift (scattering physics)
$$k\cot\delta = -\frac{1}{a_2} + \frac{1}{2}r_2k^2 + \dots,$$

Effective Range Expansion

J. Rotureau, ORNL, March 2011

3 nucleons at Leading-Order $% J^{\pi}=\frac{3}{2}^{+}$ in the trap coupled to $J^{\pi}=\frac{3}{2}^{+}$

for a fixed two-body cutoff (N_2) , the size of the model space (N_3) is increased until convergence



-> convergence of energy as the two-body cutoff N₂ increases -> as expected no need for a three body force at Leading Order. J. Rotureau, ORNL, March 2011

SUMMARY

The NCSM is an *ab initio* method for calculating nuclear structure.

It has been applied to nuclei throughout the Op-shell, where it has been able:

- a.) to predict new results, e.g., the spectrum of 14-F,
- b.) to explain previously non-understood observations, e.g., the lifetime of 14-C by including three nucleon forces,
- c.) to describe the binding energies, low-lying spectra and other observables for 0p-shell nuclei,
- d.) to serve as input for *ab initio* nuclear reaction calculations, *etc*.

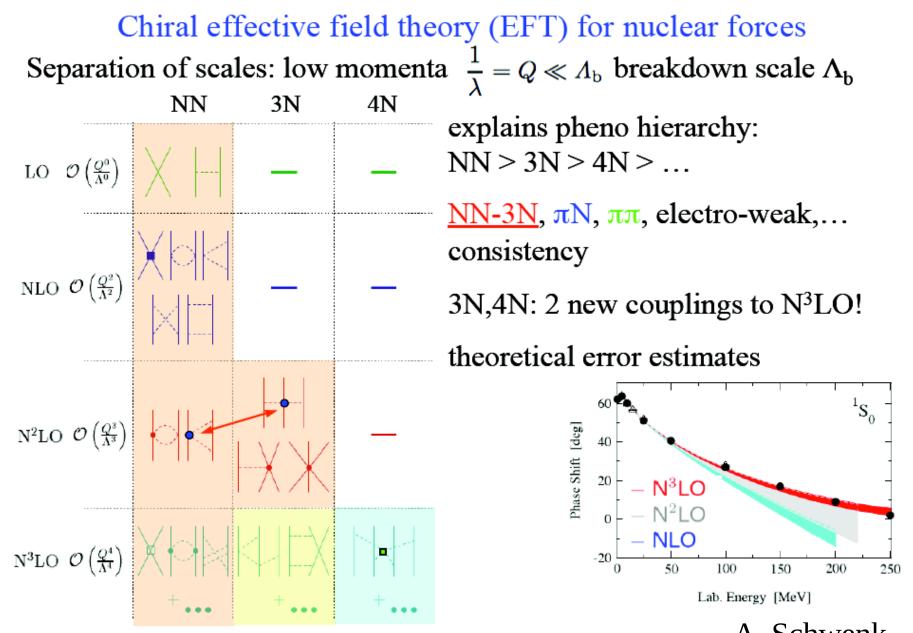
But there are challenges and much else still to do.

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. Further extensions of these microscopic advances for nuclear structure to nuclear reactions.

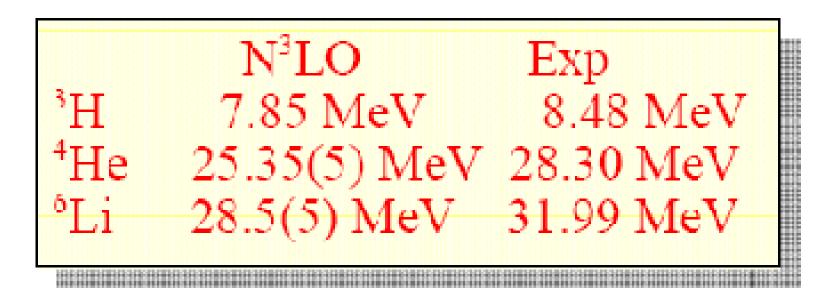
COLLABORATORS

M. C. Birse, University of Manchester, UK Sybil de Clark, University of Arizona Michael Kruse, University of Arizona Alexander Lisetskiy, Mintec Inc., Tucson Petr Navratil, TRIUMF, Vancouver, B.C. Canada Erich Ormand, Lawrence Livermore National Laboratory Sofia Quaglioni, Lawrence Livermore National Laboratory Jimmy Rotureau, University of Arizona Ionel Stetcu, University of Washington Ubirajara van Kolck, University of Arizona James P. Vary, Iowa State University



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

- I. Forces among nucleons
- 1. QCD --> EFT --> CPT --> self-consistent nucleon interactions
- 2. Need NN and NNN and perhaps also NNNN interactions



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

$$\begin{split} H_{int} &= \frac{1}{A} \sum_{i>j=1}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i>j=1}^{A} V_{ij} + \sum_{i>j>k=1}^{A} V_{ijk} + \dots \\ H &= H_{int} + \frac{\vec{P}_{CM}^2}{2mA} + \frac{1}{2} m A \omega^2 \vec{R}_{CM}^2 \\ &= \sum_{i=1}^{A} \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 r_i^2 \right) + \sum_{i
NCSM: unitary transformation h_{rel} Renormalization for trap $\Omega = \omega \sqrt{\frac{A-2}{A}}$$$

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EFT FOR TWO PARTICLES IN A TRAP

Original motivation: to understand gross features of nuclear systems from a QCD perspective

At the heart of an effective theory: a truncation of the Hilbert space / all interactions allowed by symmetries are generated / power counting

$$\frac{\Gamma(3/4 - \varepsilon/2)}{\Gamma(1/4 - \varepsilon/2)} = \frac{b}{2a_2}$$

$$\frac{\Gamma(3/4 - \varepsilon/2)}{\Gamma(1/4 - \varepsilon/2)} = -\frac{b}{2} \left(-\frac{1}{a_2} + \frac{r_2}{b^2} \varepsilon + \dots \right)$$

In finite model spaces:

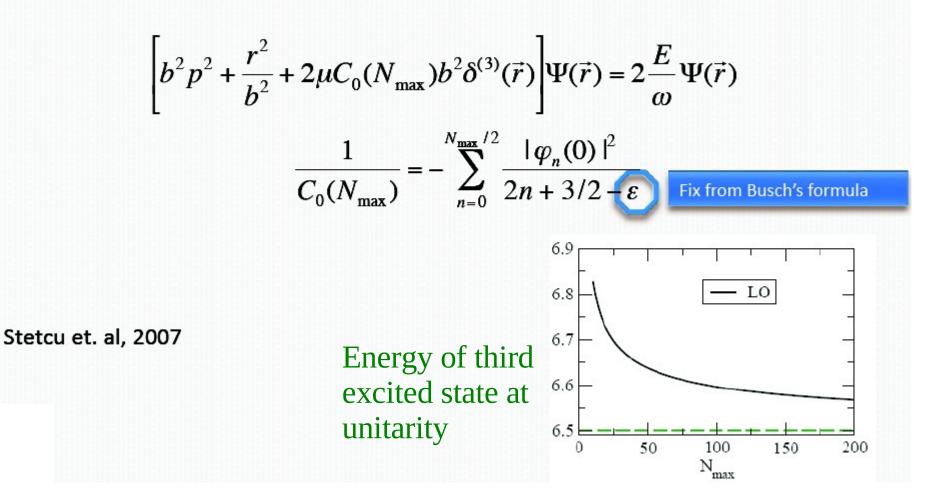
$$egin{aligned} V_{LO}(ec{p},ec{p}') &= C_0 \ V_{N\,LO}(ec{p},ec{p}') &= C_2(p^2+p'^2) \ V_{N^2LO}(ec{p},ec{p}') &= C_4(p^2+p'^2)^2 \end{aligned}$$

 $C_0, C_2, C_4,...$ Constants to be determined in each model space so that select observables are preserved

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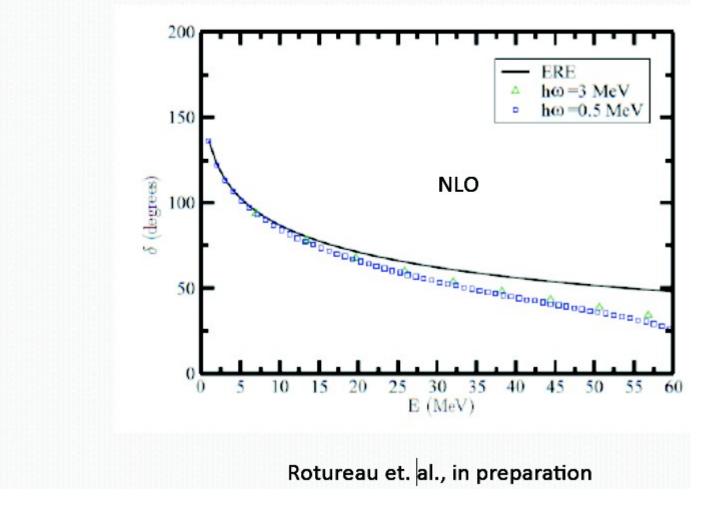
LO RENORMALIZATION

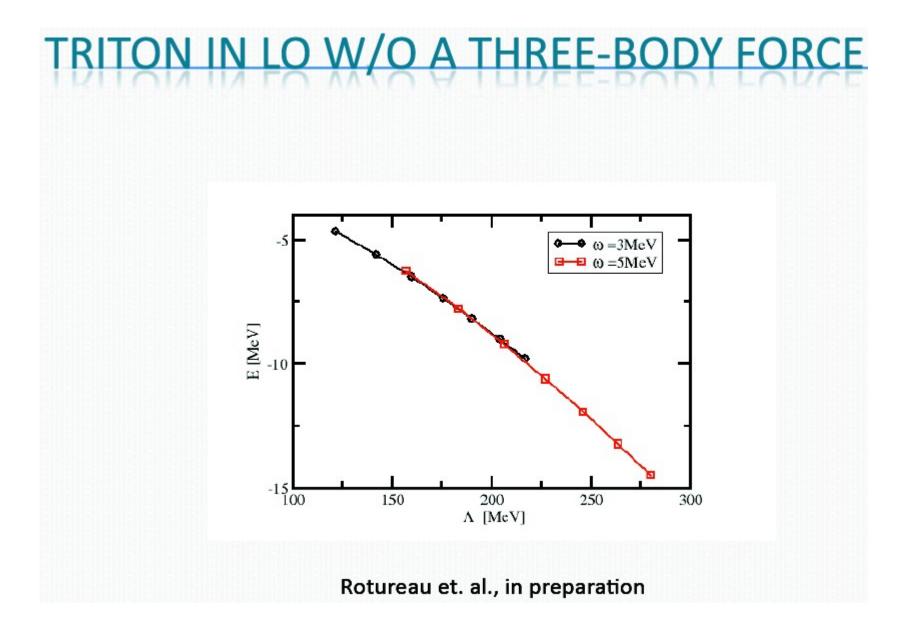
$$\Psi(\vec{r}) = \sum_{n=0}^{N_{\text{max}}/2} A_n \varphi_n(\vec{r})$$



TRAPPED NUCLEONS

Triplet S NN phase shift





III. New Methods/Transformative Ideas (???)

- 1. "soft" NN interactions plus weak NNN interactions
- 2. Coupled Cluster calculations with NNN interactions
- 3. Universal Nuclear Energy Density Functional
- 4. Building more correlations into smaller model space:a) Fermionic Molecular Dynamics Approach (T. Neff, et al.)b) Extensions of the NCSM:
 - i) Projected NCSM/SSM
 - ii) Symplectic (3,R) NCSM (J. Draayer, et al.)
 - iii) Importance Truncated NCSM (Navratil and Roth)
 - iv) NCSM + Resonating Group Method (Navratil & Quaglioni)