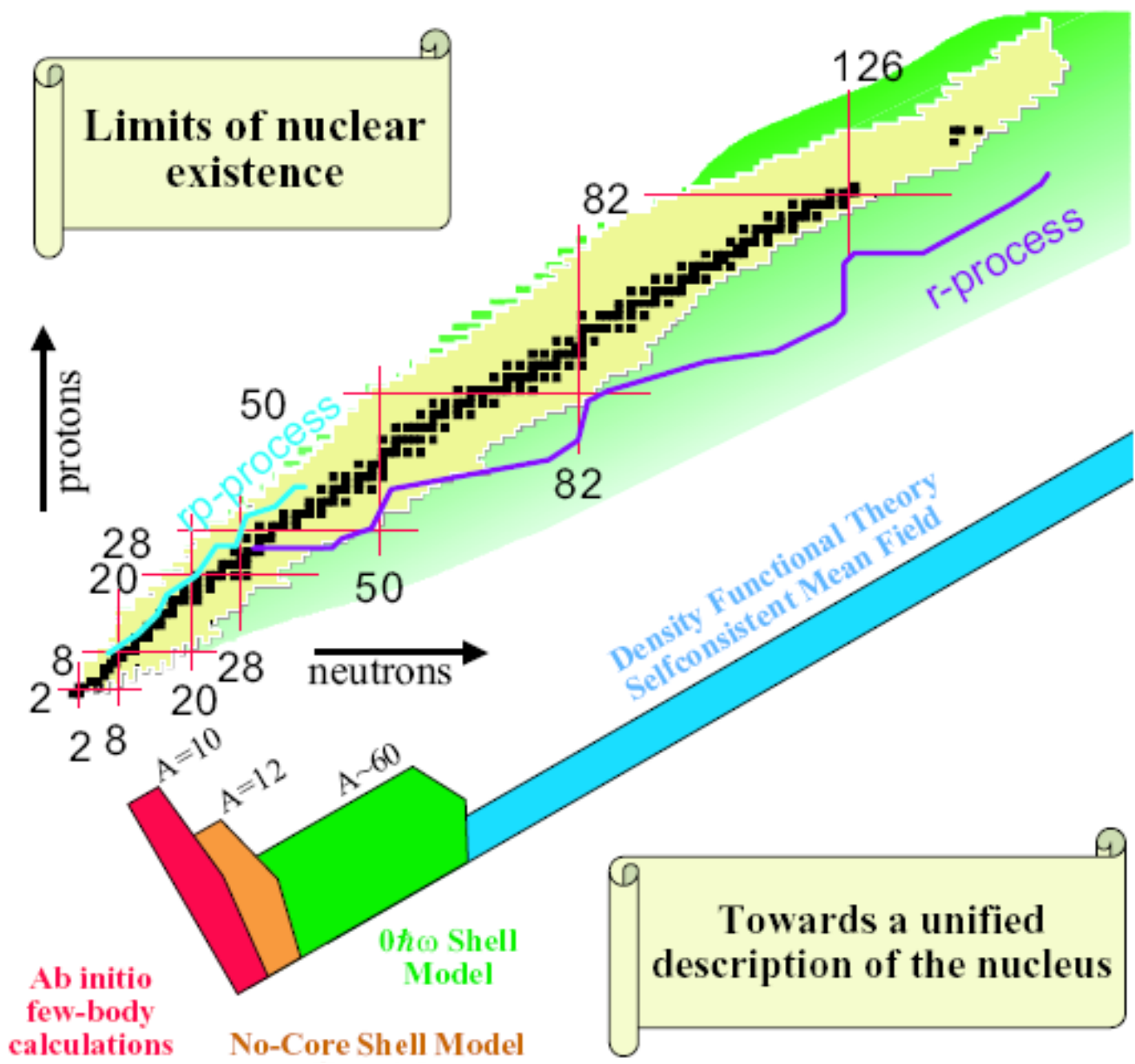


The No Core Shell Model: Its Formulation, Application and Extensions

Bruce R. Barrett
University of Arizona, Tucson



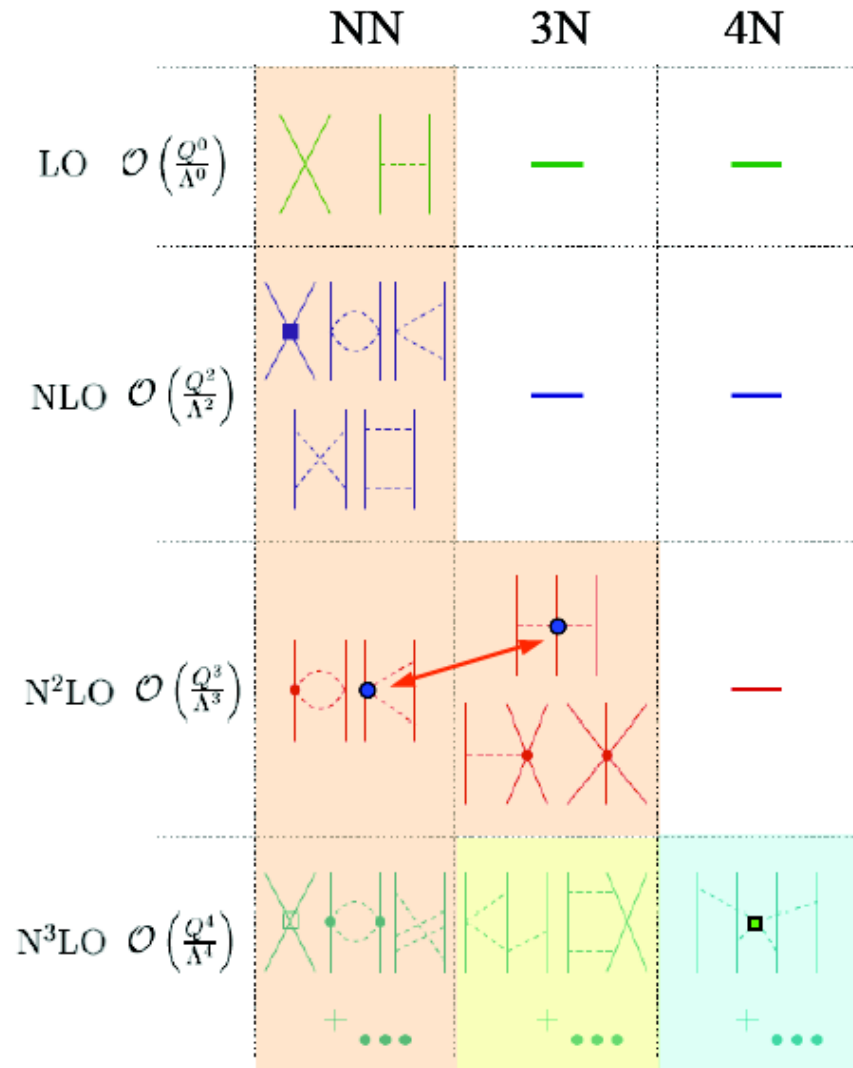


MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons
2. Calculate nuclear properties using nuclear many-body theory

Chiral effective field theory (EFT) for nuclear forces

Separation of scales: low momenta $\frac{1}{\lambda} = Q \ll \Lambda_b$ breakdown scale Λ_b



explains pheno hierarchy:

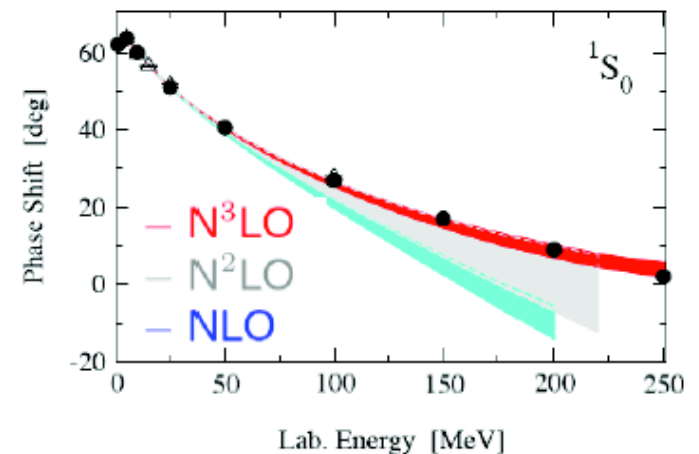
NN > 3N > 4N > ...

NN-3N, πN , $\pi\pi$, electro-weak, ...

consistency

3N, 4N: 2 new couplings to N³LO!

theoretical error estimates



I. Forces among nucleons

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

	$N^3\text{LO}$	Exp
${}^3\text{H}$	7.85 MeV	8.48 MeV
${}^4\text{He}$	25.35(5) MeV	28.30 MeV
${}^6\text{Li}$	28.5(5) MeV	31.99 MeV

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

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

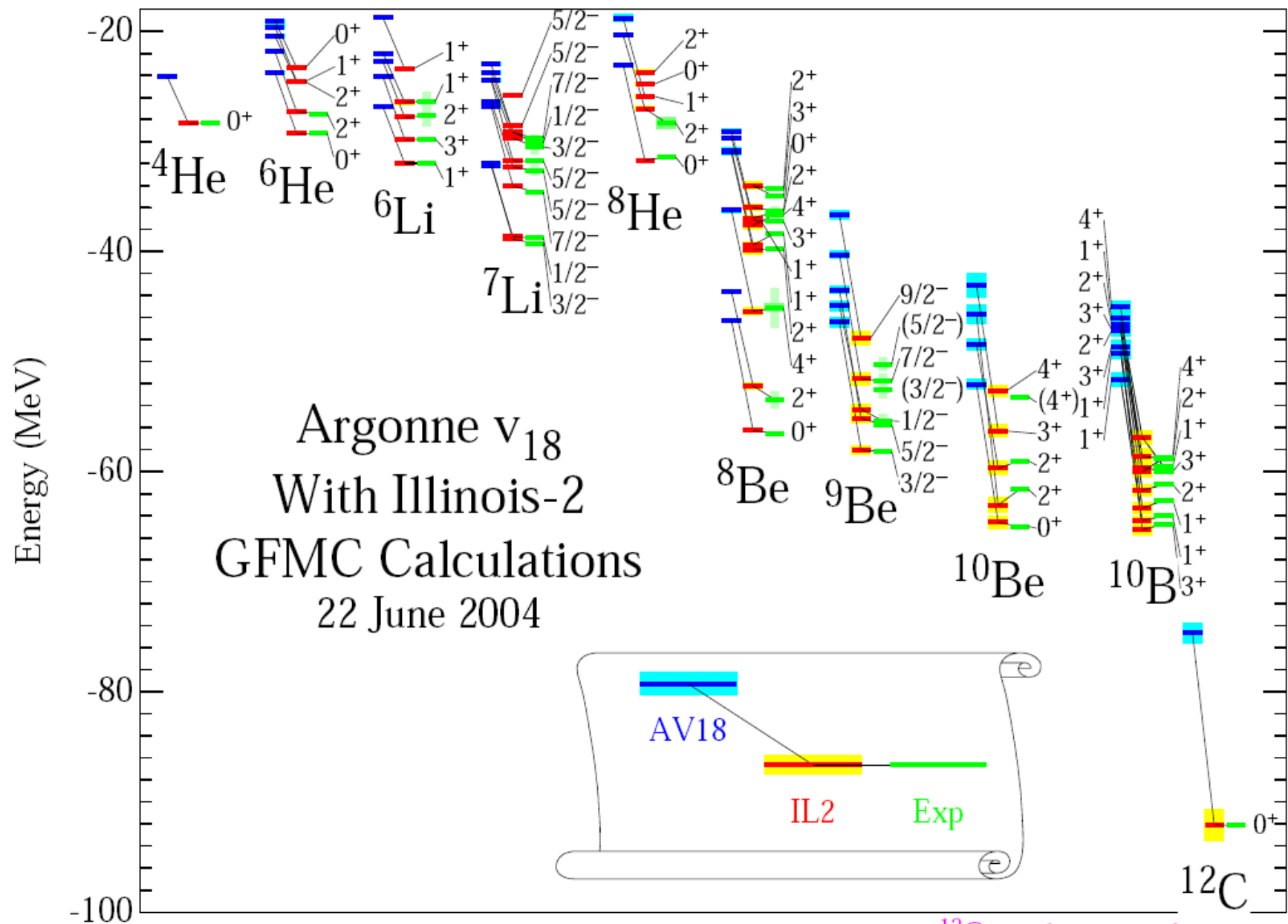
PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon 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.

$$BE_{\text{th}} \approx 25.91 \text{ MeV}$$

$$BE_{\text{exp}} \approx 28.296 \text{ MeV}$$



^{12}C results are preliminary.

No Core Shell Model

“*Ab Initio*” approach to microscopic nuclear structure calculations, in which all 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: 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

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

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

\Rightarrow We must use effective interactions and operators!

Effective Interaction

- Must truncate to a **finite** model space

$$V_{ij} \dashrightarrow V_{ij}^{\text{effective}}$$

- In general, V_{ij}^{eff} is an A -body interaction

- We want to make an a -body cluster approximation

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

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

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

$$\Phi_\beta = P\Psi_\beta$$

P is a projection operator from S into \mathcal{S}

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

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

Effective Hamiltonian for NCSM

Solving

$$\mathbf{H}_{A,a=2}^{\Omega} \Psi_{a=2} = \mathbf{E}_{A,a=2}^{\Omega} \Psi_{a=2}$$

in "infinite space" $2n+1 = 450$
relative coordinates

$P + Q = 1$; P – model space; Q – excluded space;

$$E_{A,2}^{\Omega} = U_2 H_{A,2}^{\Omega} U_2^{\dagger}$$

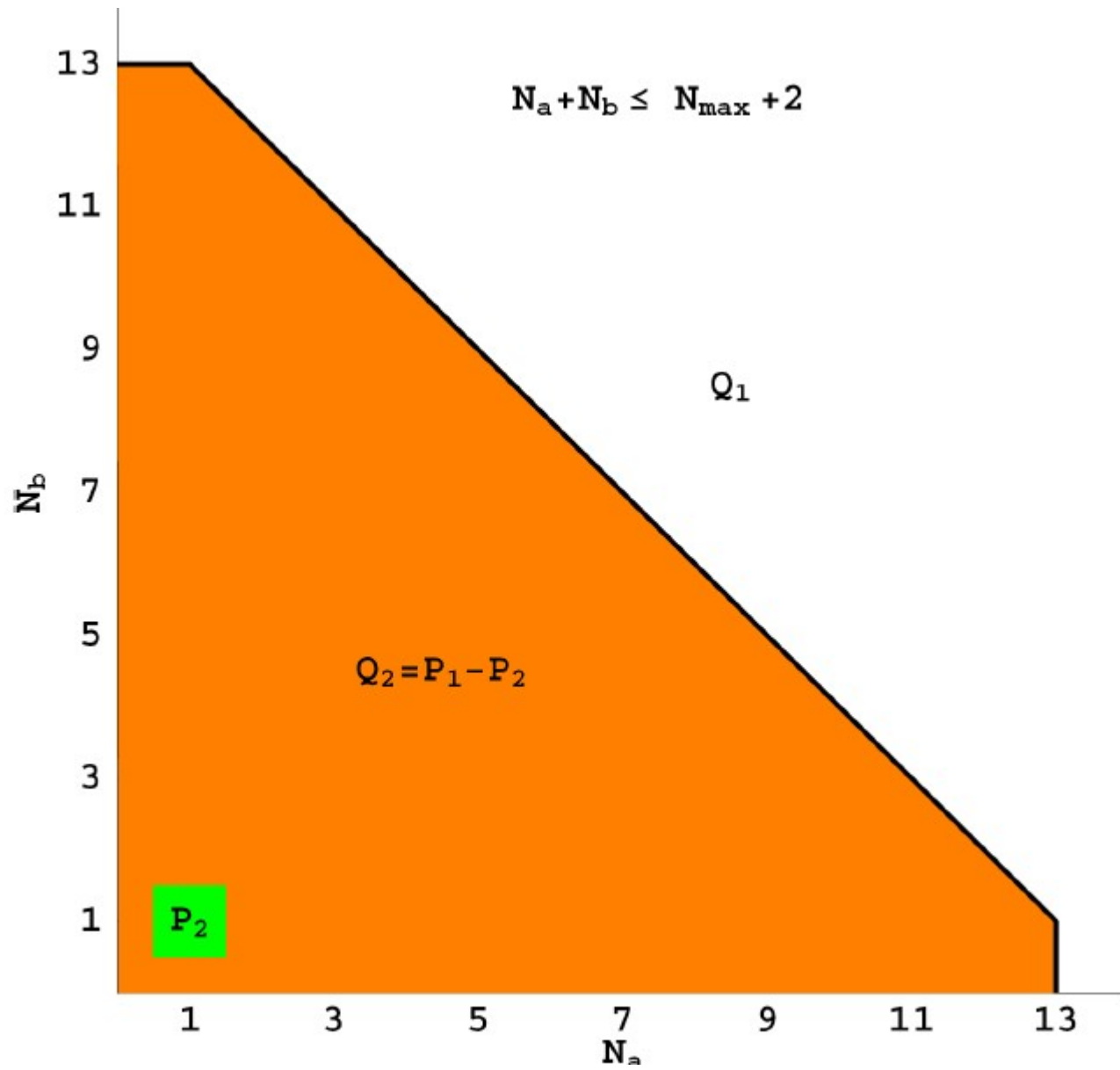
$$U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \quad E_{A,2}^{\Omega} = \begin{pmatrix} E_{A,2,P}^{\Omega} & 0 \\ 0 & E_{A,2,Q}^{\Omega} \end{pmatrix}$$

$$H_{A,2}^{N_{\max}, \Omega, \text{eff}} = \frac{U_{2,P}^{\dagger}}{\sqrt{U_{2,P}^{\dagger} U_{2,P}}} E_{A,2,P}^{\Omega} \frac{U_{2,P}}{\sqrt{U_{2,P}^{\dagger} U_{2,P}}}$$

Two ways of convergence:

1) For $P \rightarrow 1$ and fixed a : $\tilde{H}_{A,a=2}^{\text{eff}} \rightarrow H_A$

2) For $a \rightarrow A$ and fixed P : $\tilde{H}_{A,a}^{\text{eff}} \rightarrow H_A$



From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

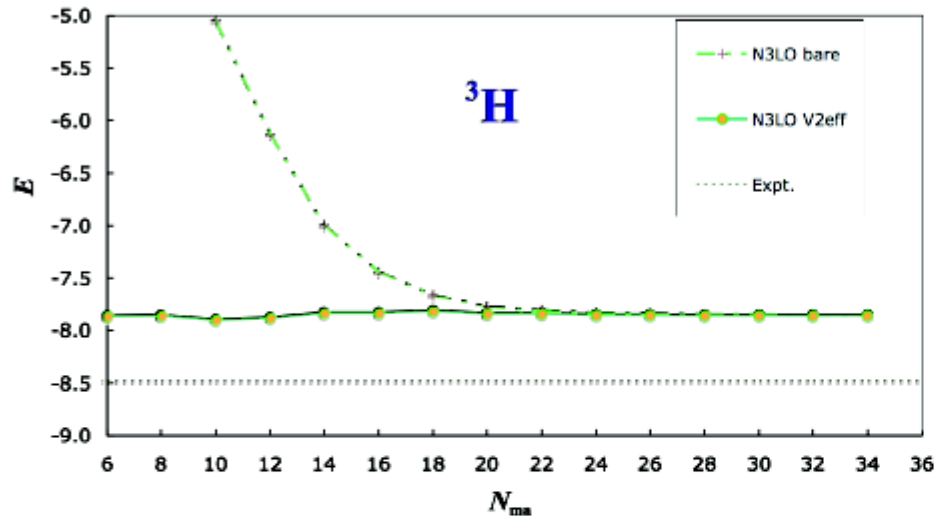
Effective interactions in
cluster approximation

Diagonalization of
many-body Hamiltonian

Many-body experimental data

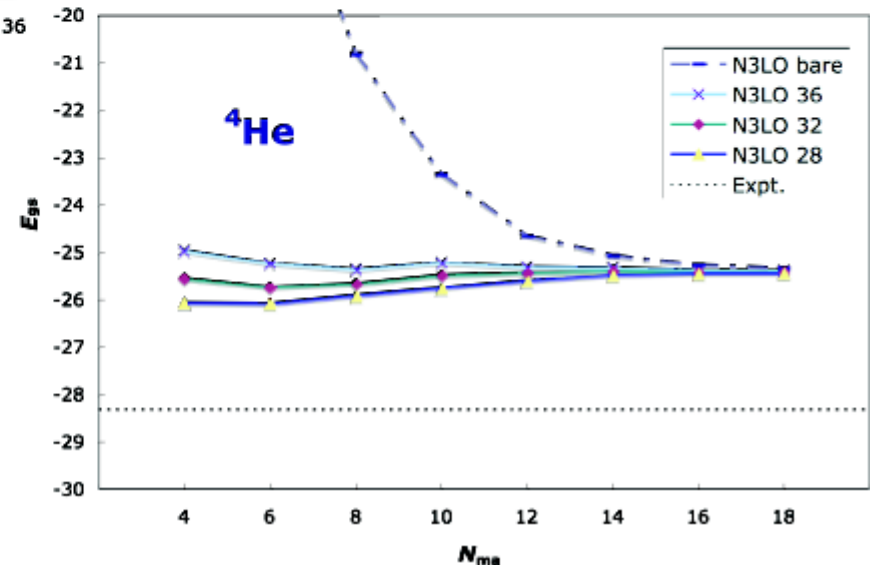
- NCSM convergence test

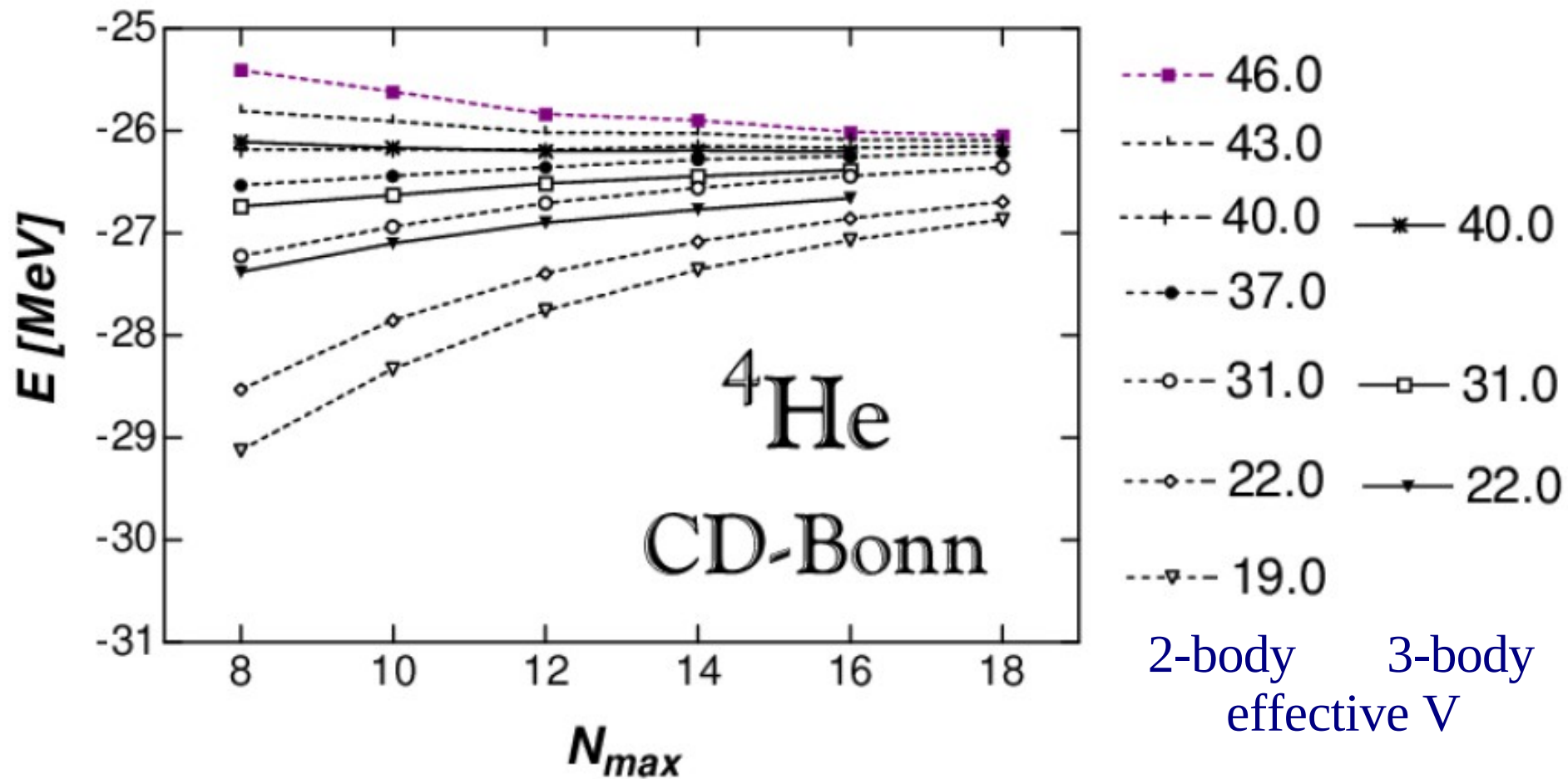
- Comparison to other methods

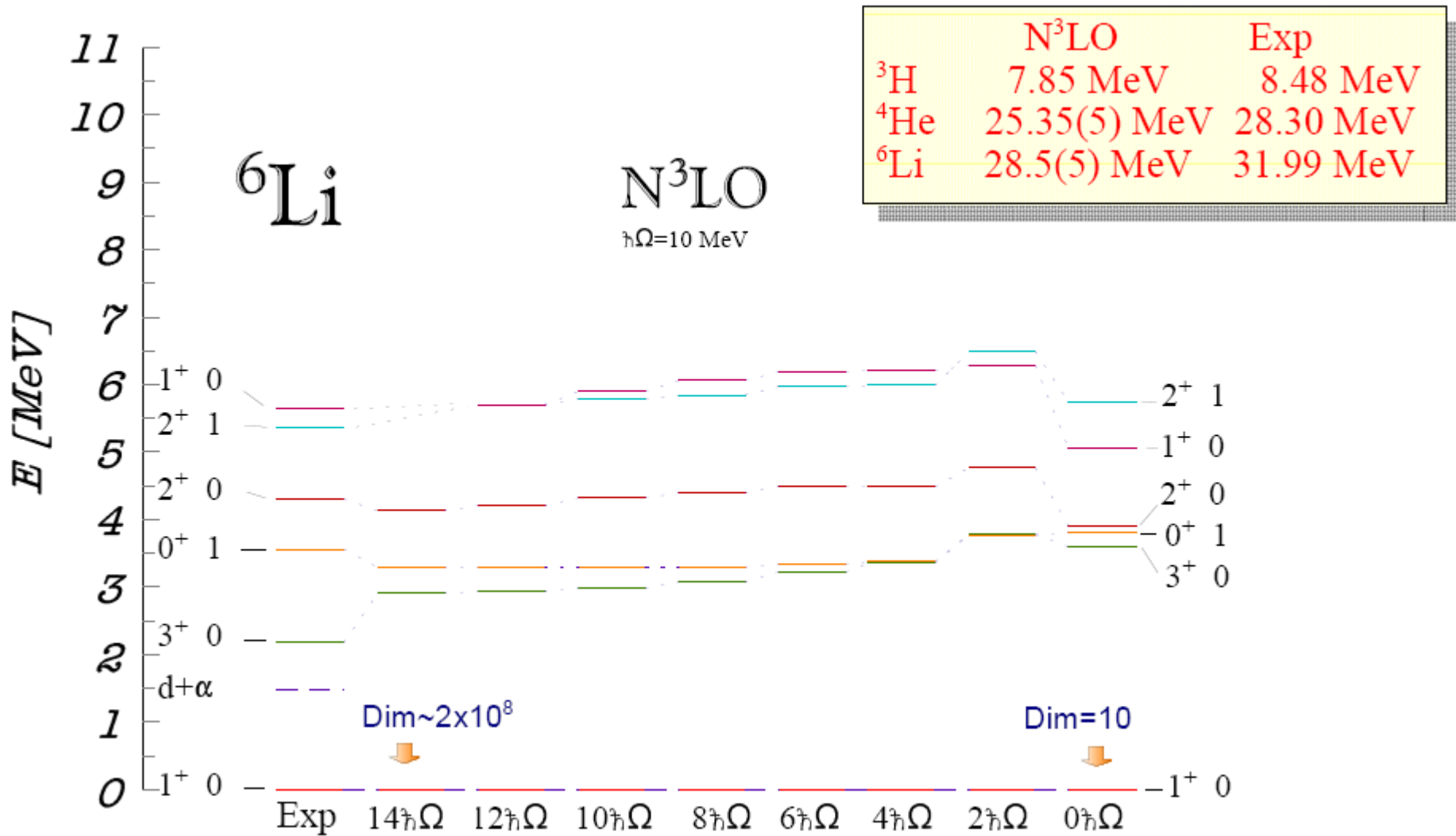


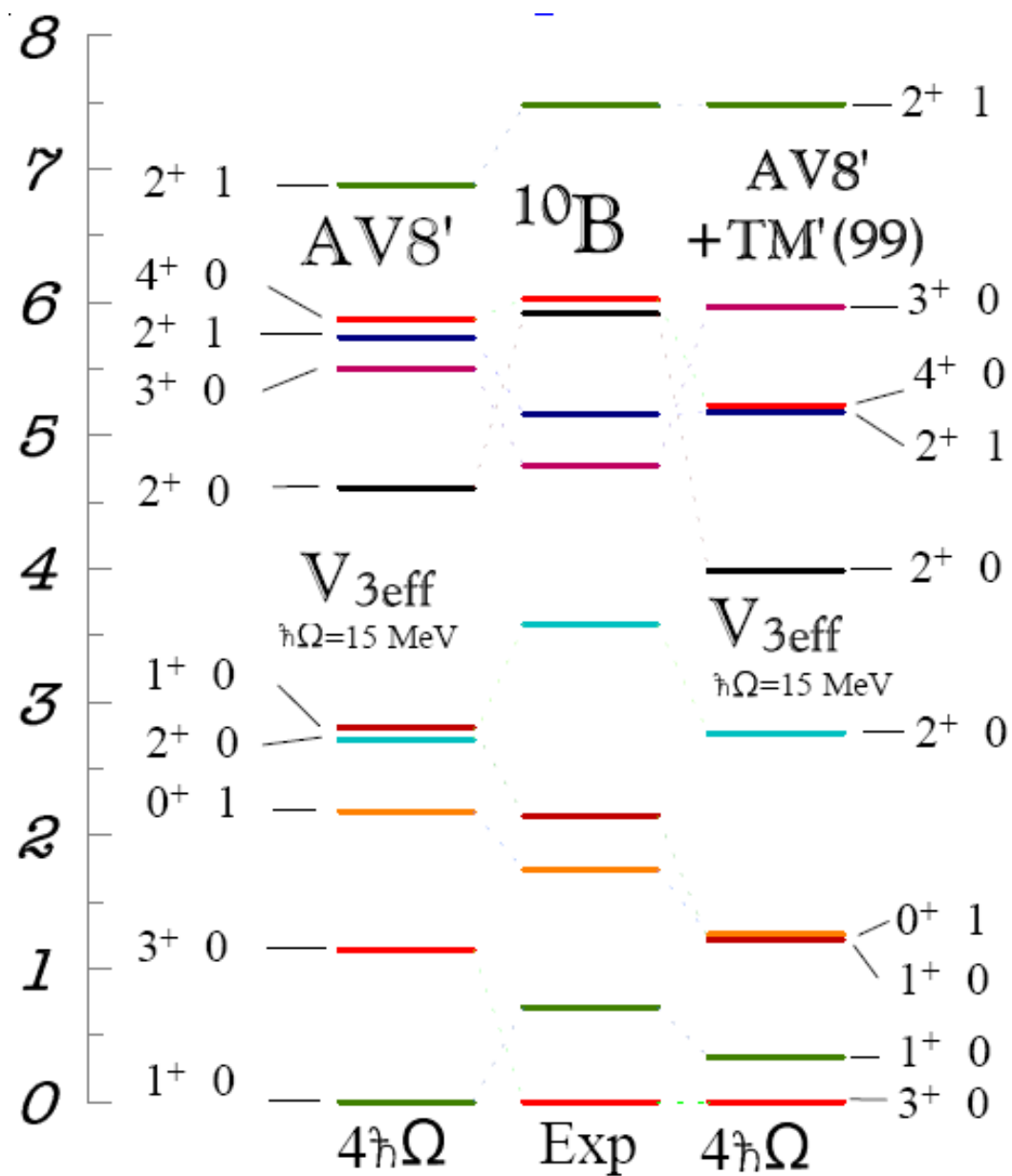
$\text{N}^3\text{LO NN}$	NCSM	FY	HH
^3H	7.852(5)	7.854	7.854
^4He	25.39(1)	25.37	25.38

- Short-range correlations \Rightarrow effective interaction
- Medium-range correlations \Rightarrow multi- $h\Omega$ model space
- Dependence on
 - size of the model space (N_{max})
 - HO frequency ($h\Omega$)
- Not a variational calculation
- Convergence OK
- NN interaction insufficient to reproduce experiment









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

Origin of the anomalous long lifetime of ^{14}C

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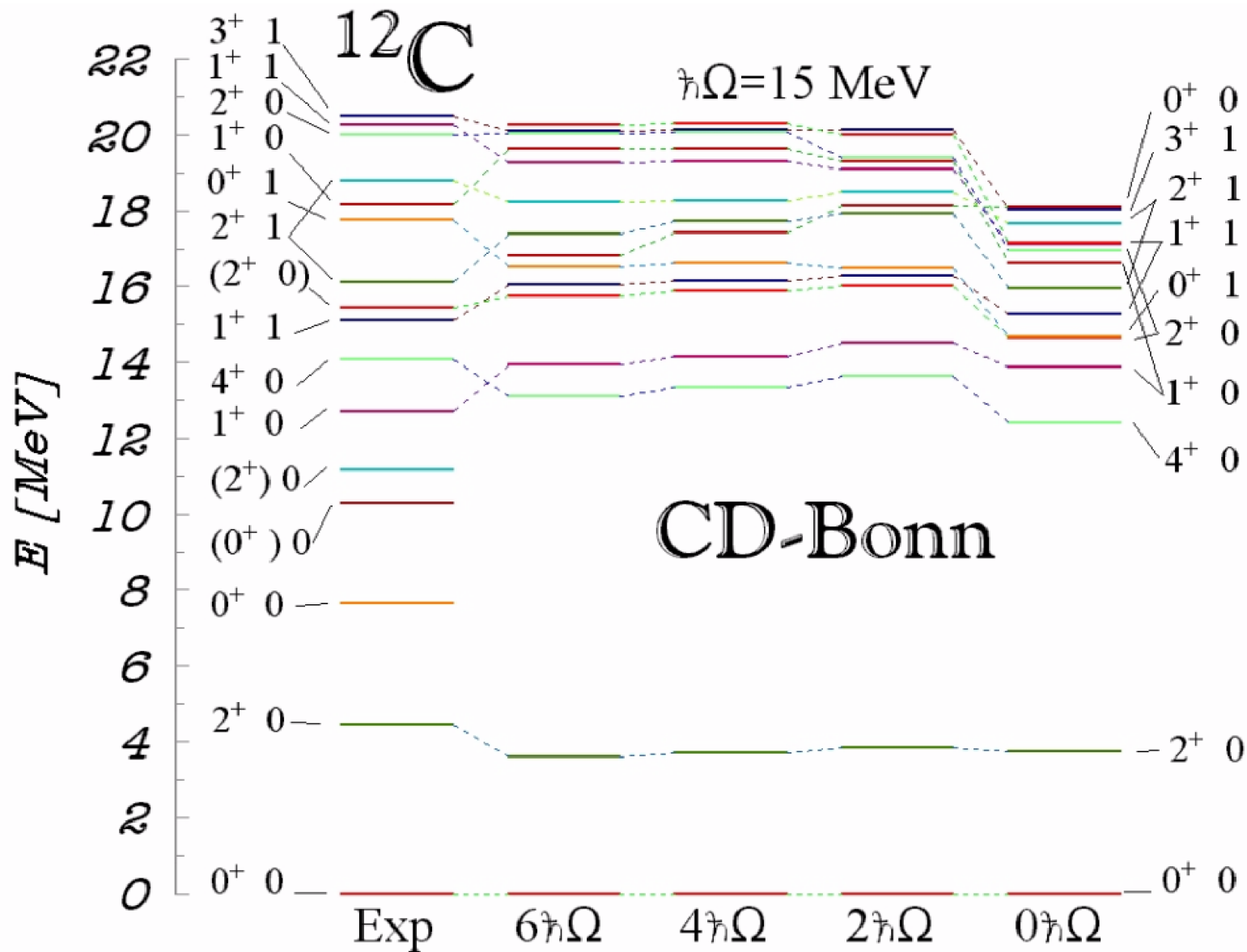
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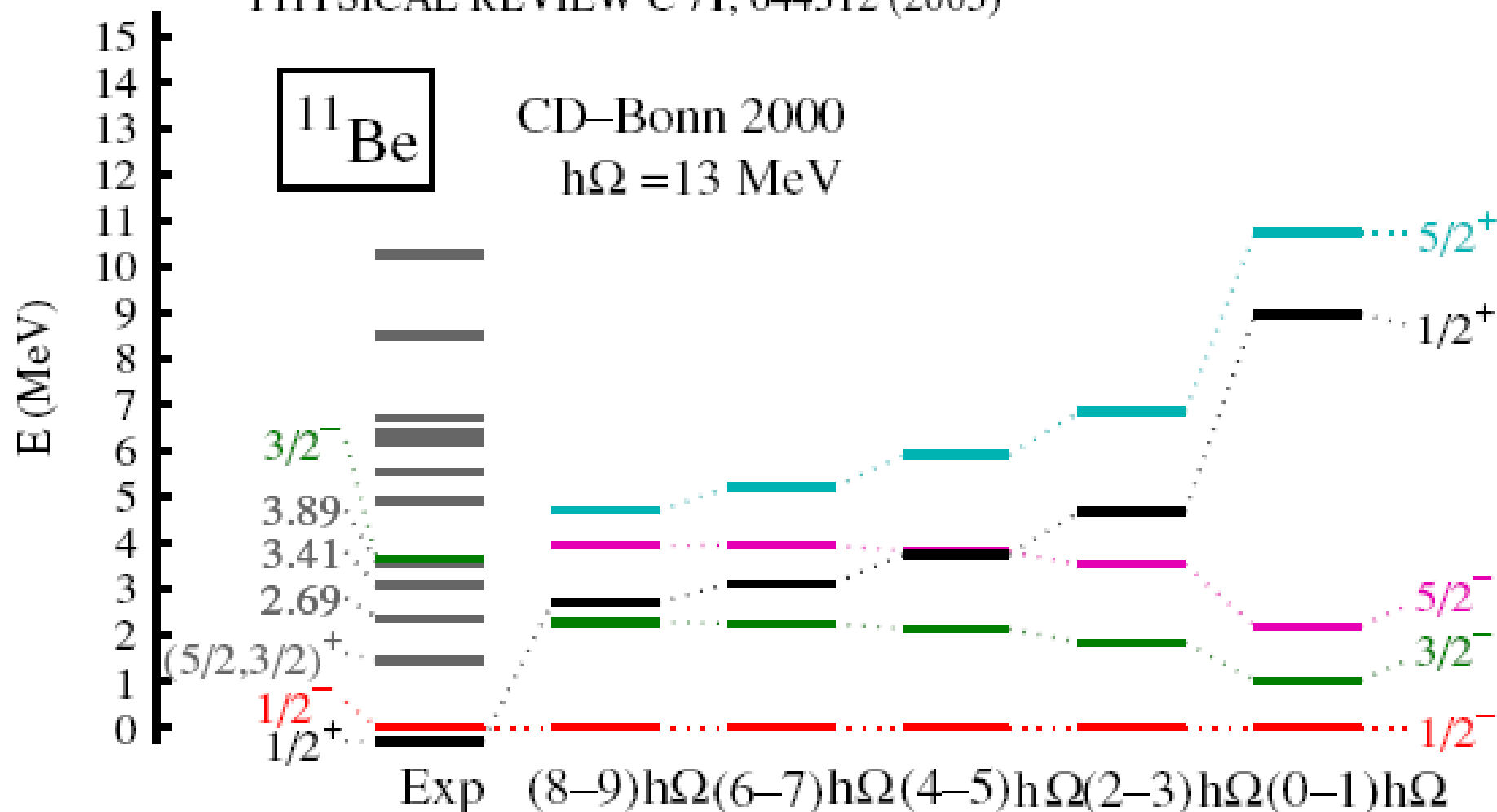
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We report the microscopic origins of the anomalously suppressed beta decay of ^{14}C to ^{14}N using the *ab initio* no-core shell model (NCSM) with the Hamiltonian from chiral effective field theory (EFT) including three-nucleon force (3NF) terms. The 3NF induces unexpectedly large cancellations within the *p*-shell between contributions to beta decay, which reduce the traditionally large contributions from the NN interactions by an order of magnitude, leading to the long lifetime of ^{14}C .



PHYSICAL REVIEW C 71, 044312 (2005)



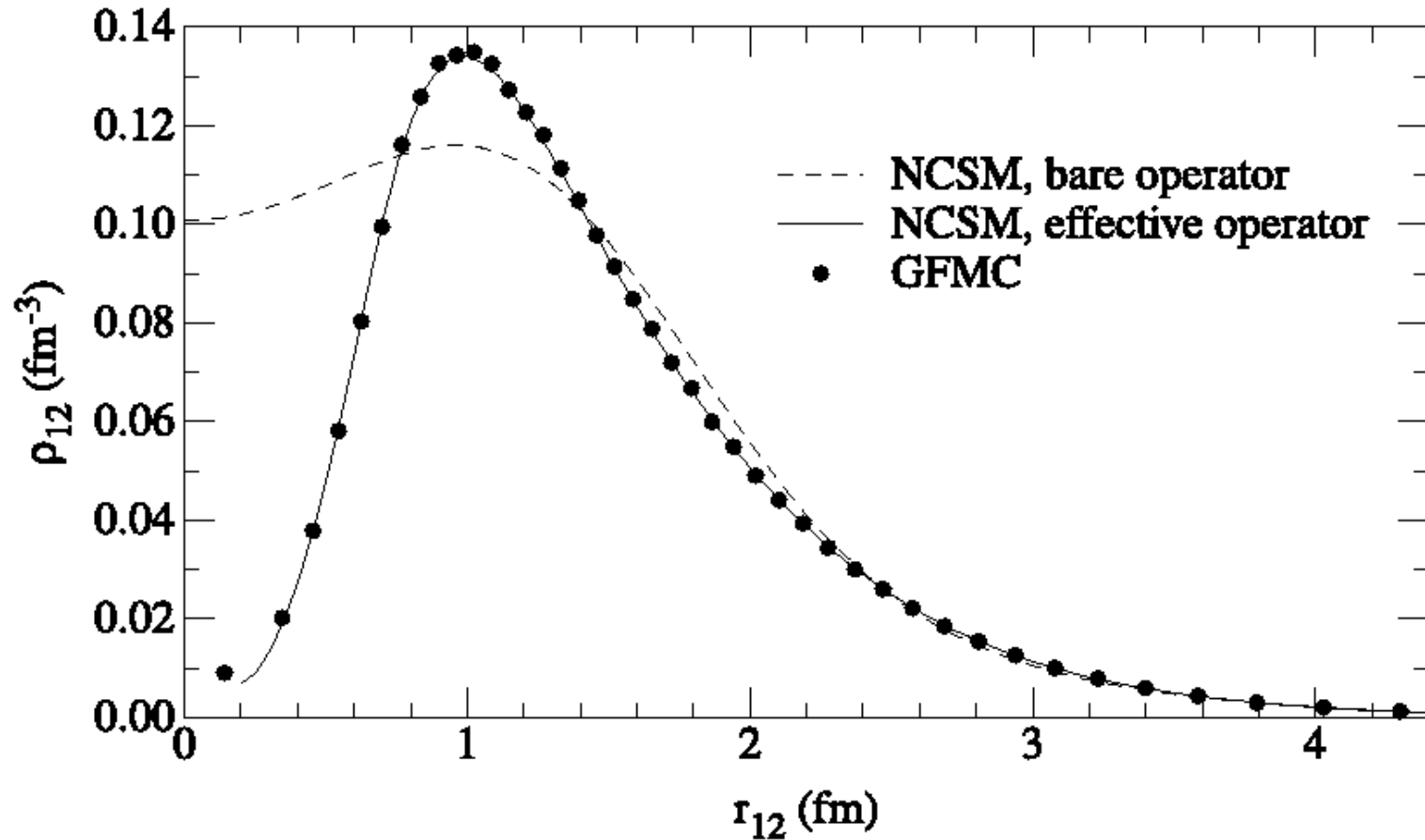


Figure 2. *NCSM and GFM C NN pair density in ⁴He.*

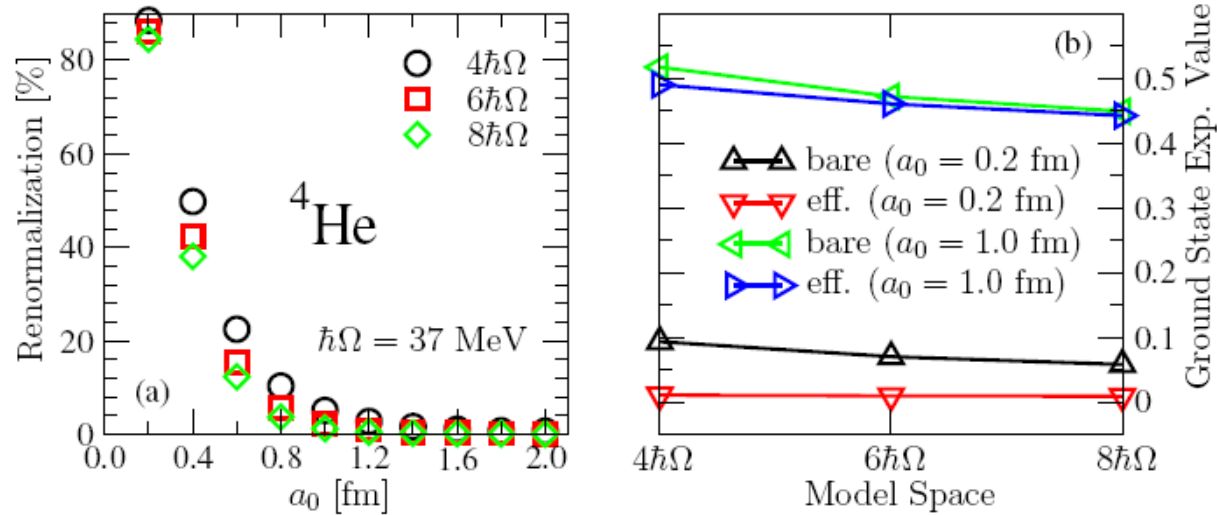
Nucleus	Observable	Model Space	Bare operator	Effective operator
${}^2\text{H}$	Q_0	$4\hbar\Omega$	0.179	0.270
${}^6\text{Li}$	$B(E2, 1^+0 \rightarrow 3^+0)$	$2\hbar\Omega$	2.647	2.784
${}^6\text{Li}$	$B(E2, 1^+0 \rightarrow 3^+0)$	$10\hbar\Omega$	10.221	-
${}^6\text{Li}$	$B(E2, 2^+0 \rightarrow 1^+0)$	$2\hbar\Omega$	2.183	2.269
${}^6\text{Li}$	$B(E2, 2^+0 \rightarrow 1^+0)$	$10\hbar\Omega$	4.502	-
${}^{10}\text{C}$	$B(E2, 2_1^+0 \rightarrow 0^+0)$	$4\hbar\Omega$	3.05	3.08
${}^{12}\text{C}$	$B(E2, 2_1^+0 \rightarrow 0^+0)$	$4\hbar\Omega$	4.03	4.05
${}^4\text{He}$	$\langle g.s. T_{rel} g.s. \rangle$	$8\hbar\Omega$	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
- $a \rightarrow A$ for fixed model space;
- $P \rightarrow \infty$ for fixed cluster.



Range dependence



$$O \sim \exp \left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{a_0^2} \right]$$

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

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

PHYSICAL REVIEW C 78, 044302 (2008)

Ab-initio shell model with a core

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(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](https://doi.org/10.1103/PhysRevC.78.044302)

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

From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

Effective interactions in
cluster approximation

Diagonalization of
many-body Hamiltonian

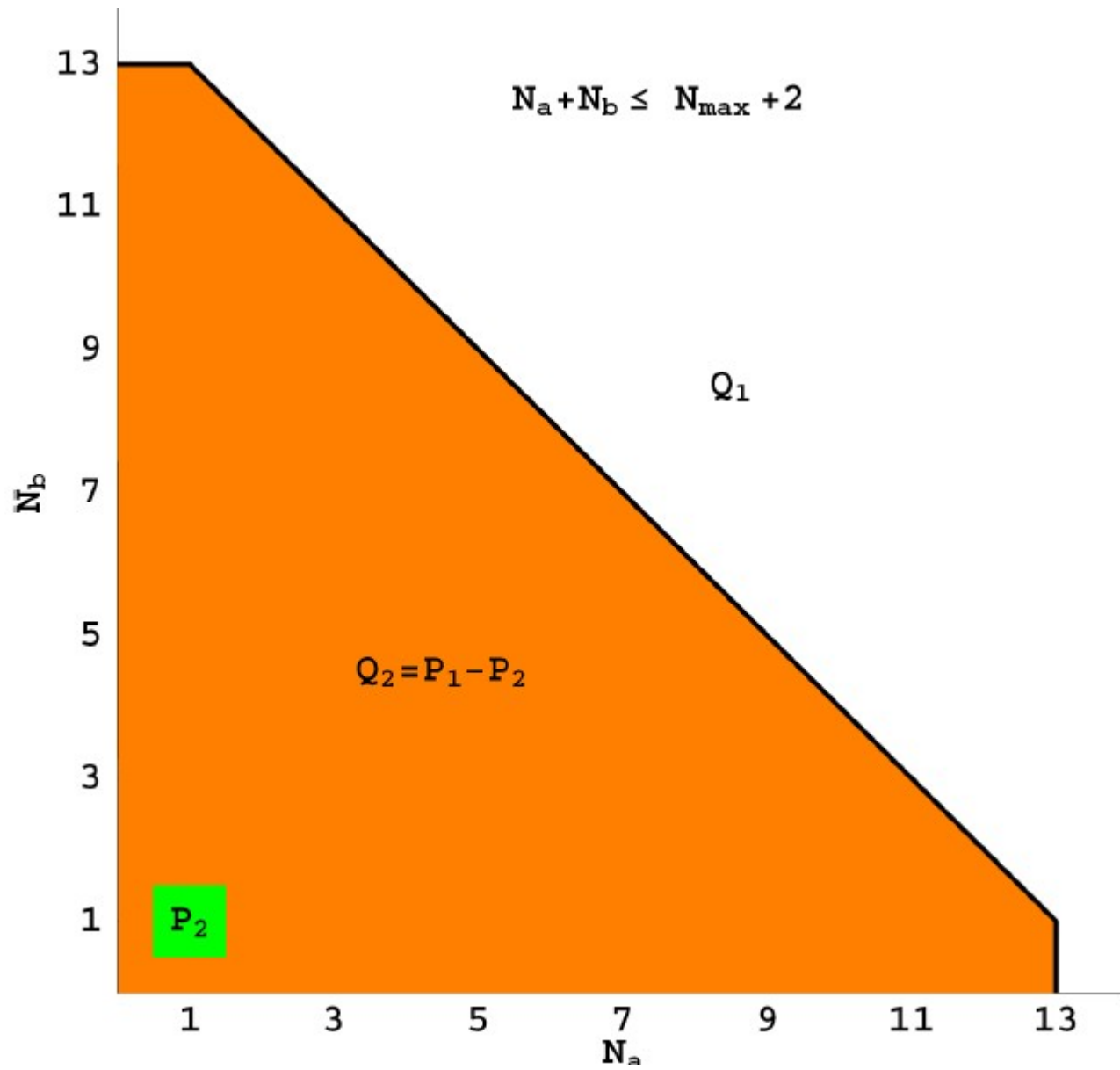
Core Shell Model

effective interactions for
valence nucleons

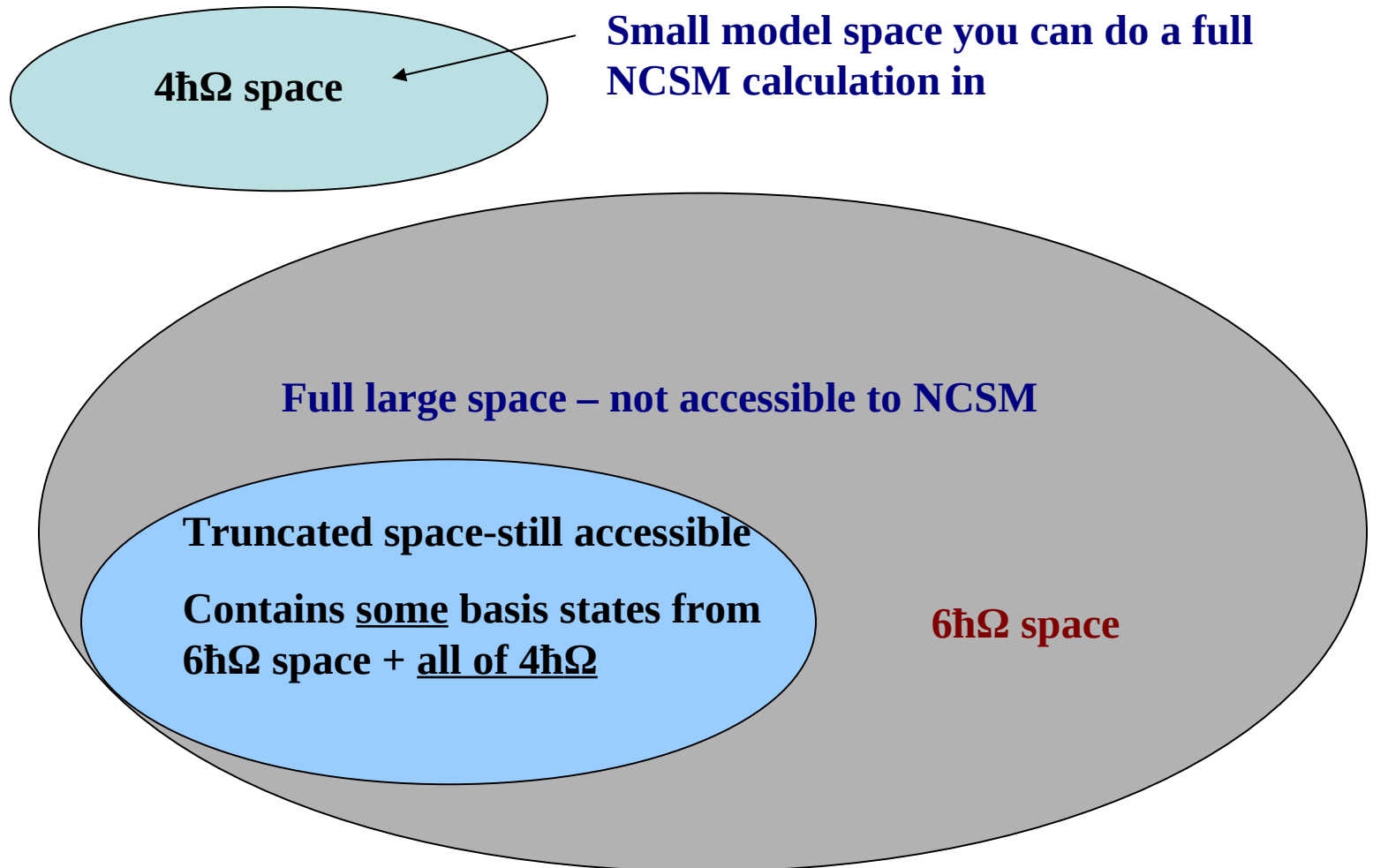
Diagonalization of the
Hamiltonian for valence
nucleons

Many-body experimental data





The idea of Importance Truncation





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

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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 ${}^2\text{H}$, ${}^3\text{H}$ and ${}^4\text{He}$ be exactly reproduced. The first $(0^+; 0)$ excited state of ${}^4\text{He}$ and the ground state of ${}^6\text{Li}$ are then obtained by means of NCSM calculations in several spaces and frequencies. After we remove the harmonic-oscillator frequency dependence, we predict for ${}^4\text{He}$ an energy level for the first $(0^+; 0)$ excited state in remarkable agreement with the experimental value. The corresponding ${}^6\text{Li}$ 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

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

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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:

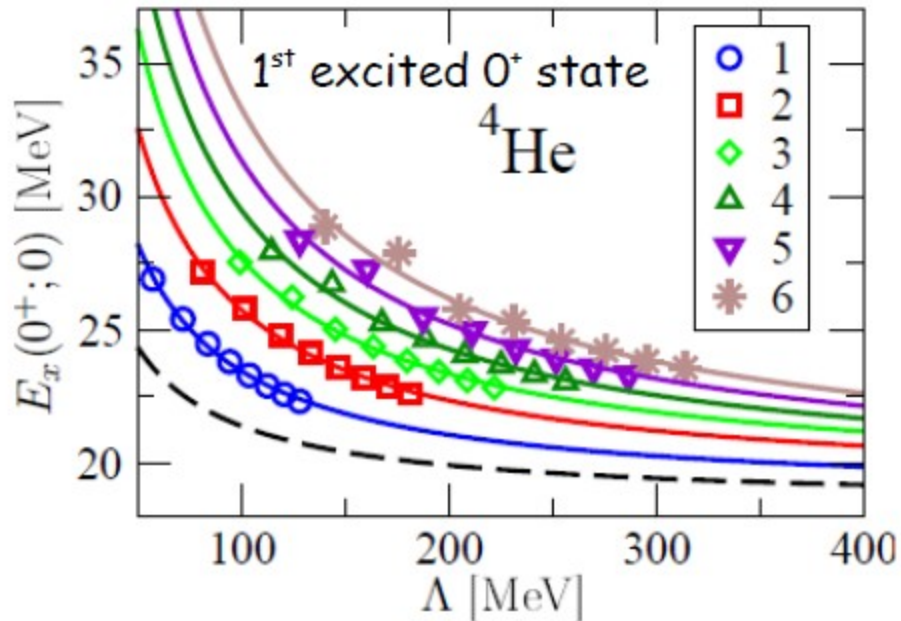
1. Flexible many-body method/easy to implement
2. Equivalent SD and Jacobi formulations
3. Can handle both NN and NNN interactions
4. In principle applies to any nucleus/extensions to heavier nuclei

Pionless EFT for nuclei within the NCSM:

Without pions--> Breakdown momentum roughly 100 MeV/c

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

Stetcu et. al., 2007



-> calculation at **Leading order** :
two N-N contact interactions in
the $^3S_1, ^1S_0$ channel and a three-
body contact interaction in the 3-
nucleon $S_{1/2}$ 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

$$H_{int} = \frac{1}{A} \sum_{i>j=1}^A \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i>j=1}^A V_{ij} + \sum_{i>j>k=1}^A V_{ijk} + \dots$$

$$H = H_{int} + \frac{\vec{P}_{CM}^2}{2mA} + \frac{1}{2}mA\omega^2 \vec{R}_{CM}^2$$

$$= \sum_{i=1}^A \left(\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 r_i^2 \right) + \sum_{i<j=1}^A \left(V_{ij} - \frac{m\omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right) + \sum_{i<j<k=1}^A V_{ijk} + \dots$$

$$h_{12} = \frac{p_1^2}{2m} + \frac{1}{2}m\omega r_1^2 + \frac{p_2^2}{2m} + \frac{1}{2}m\omega r_2^2 + V_{12} - \frac{m\omega^2}{2A} (\vec{r}_1 - \vec{r}_2)^2$$

$$h_{12} = h_{rel} + h_{CM}$$

NCSM: unitary transformation h_{rel}

Renormalization for trap $\Omega = \omega \sqrt{\frac{A-2}{A}}$

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:

$$V_{LO}(\vec{p}, \vec{p}') = C_0$$

$$V_{NLO}(\vec{p}, \vec{p}') = C_2(p^2 + p'^2)$$

$$V_{N^2LO}(\vec{p}, \vec{p}') = C_4(p^2 + p'^2)^2$$

C_0, C_2, C_4, \dots

Constants to be determined in each model space so that select observables are preserved

LO RENORMALIZATION

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

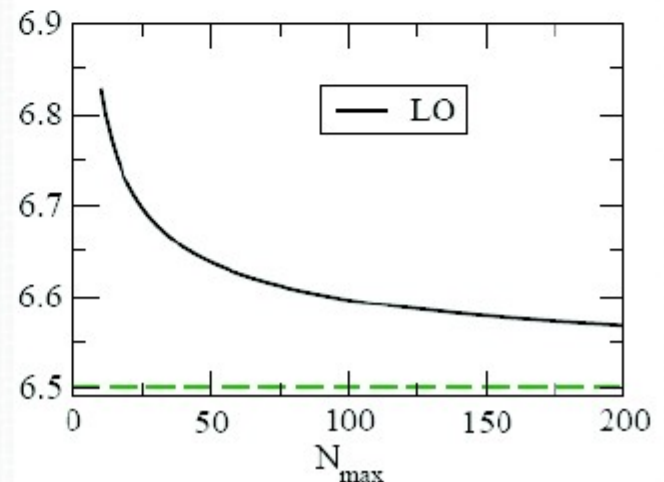
$$\left[b^2 p^2 + \frac{r^2}{b^2} + 2\mu C_0(N_{\max}) b^2 \delta^{(3)}(\vec{r}) \right] \Psi(\vec{r}) = 2 \frac{E}{\omega} \Psi(\vec{r})$$

$$\frac{1}{C_0(N_{\max})} = - \sum_{n=0}^{N_{\max}/2} \frac{|\varphi_n(0)|^2}{2n + 3/2 - \epsilon}$$

Fix from Busch's formula

Stetcu et. al, 2007

Energy of third
excited state at
unitarity

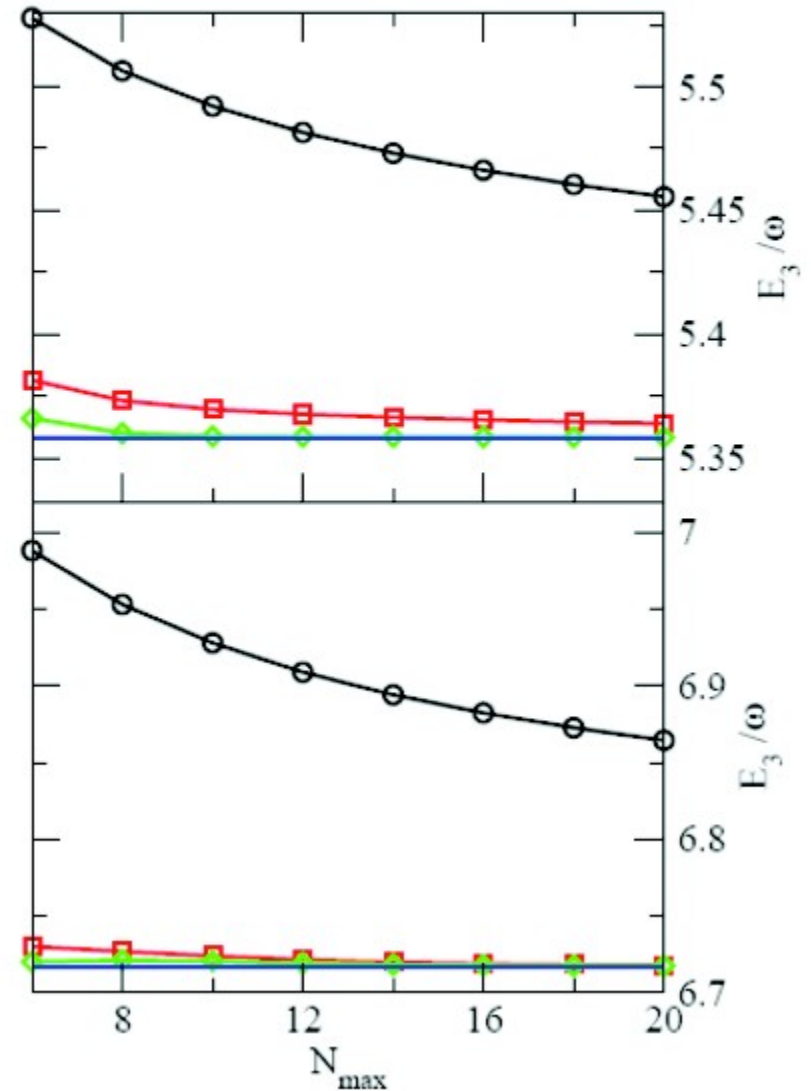
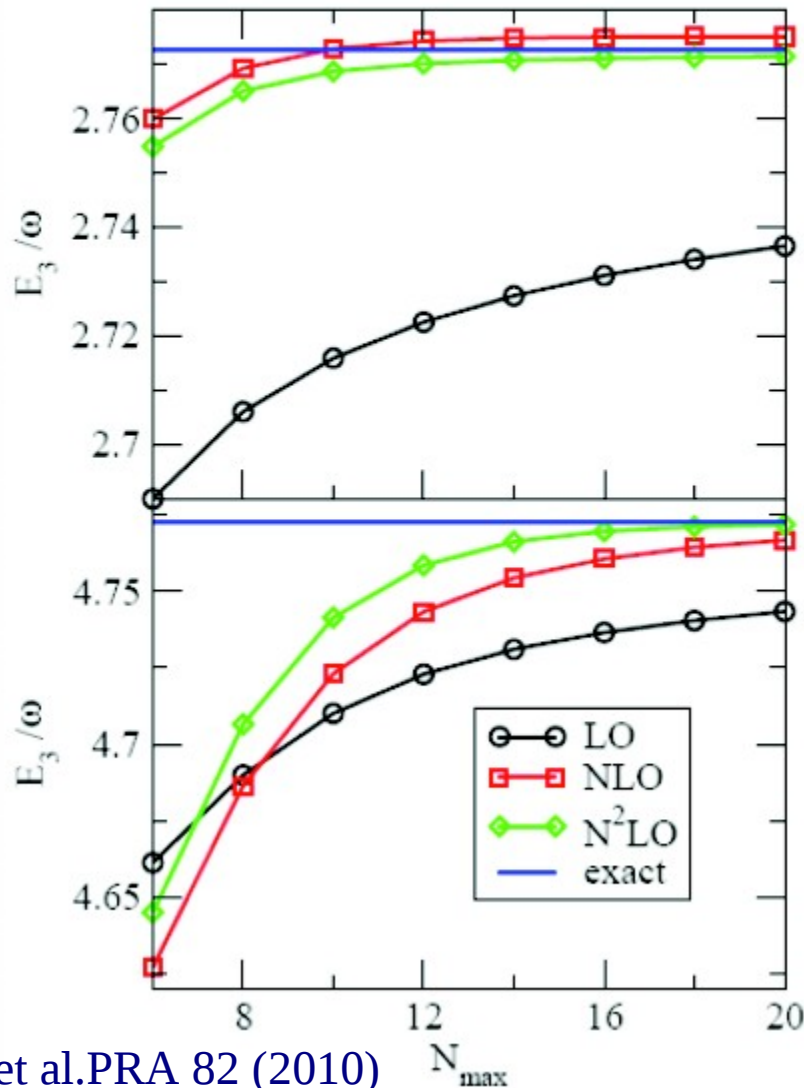


THREE-BODY PROBLEM UP TO N²LO (UNITARITY)

$$E = E_{c.m.} + (s_{l,n} + 1 + 2q)\omega$$

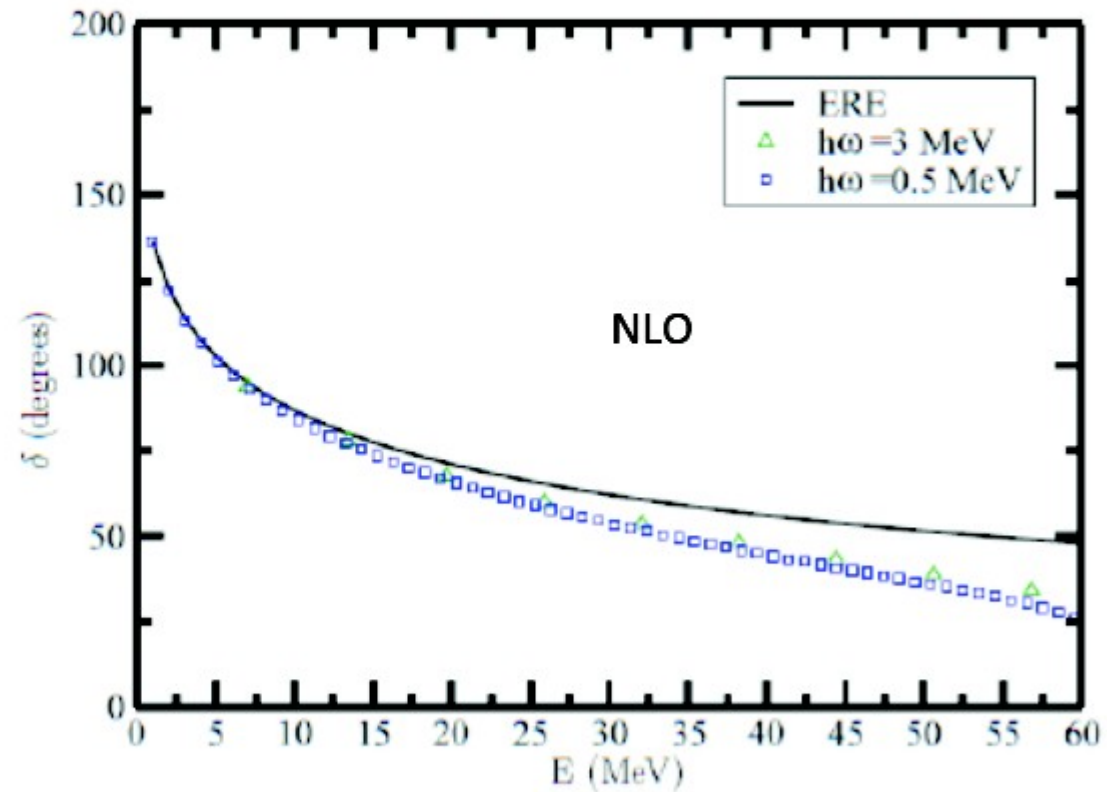
Werner and Castin, PRL 97 (2006)

3 $s = \frac{1}{2}$ fermions

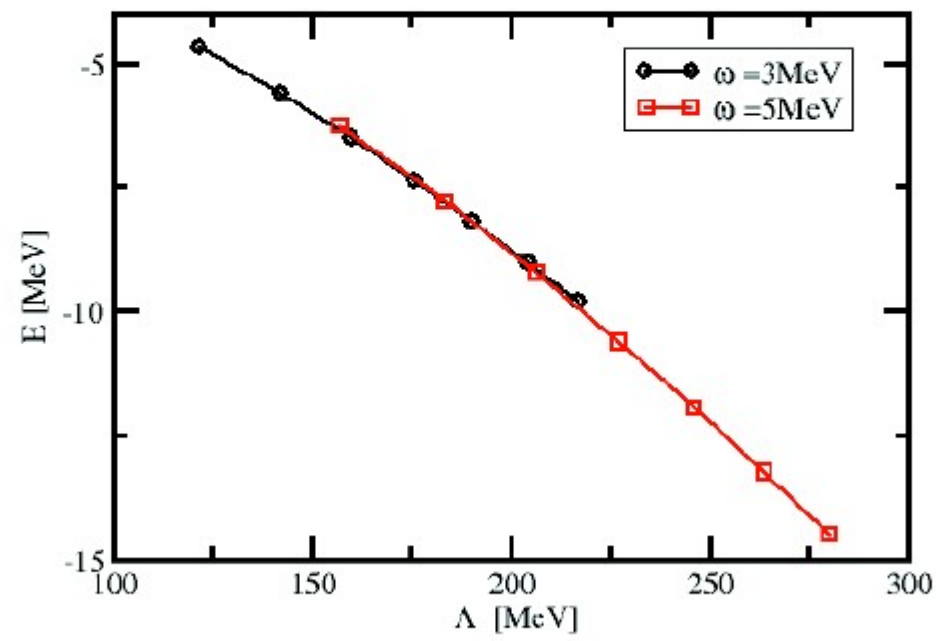


TRAPPED NUCLEONS

Triplet S NN phase shift



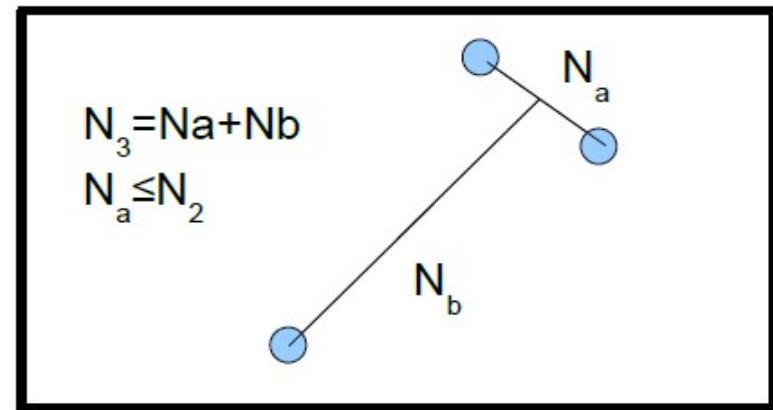
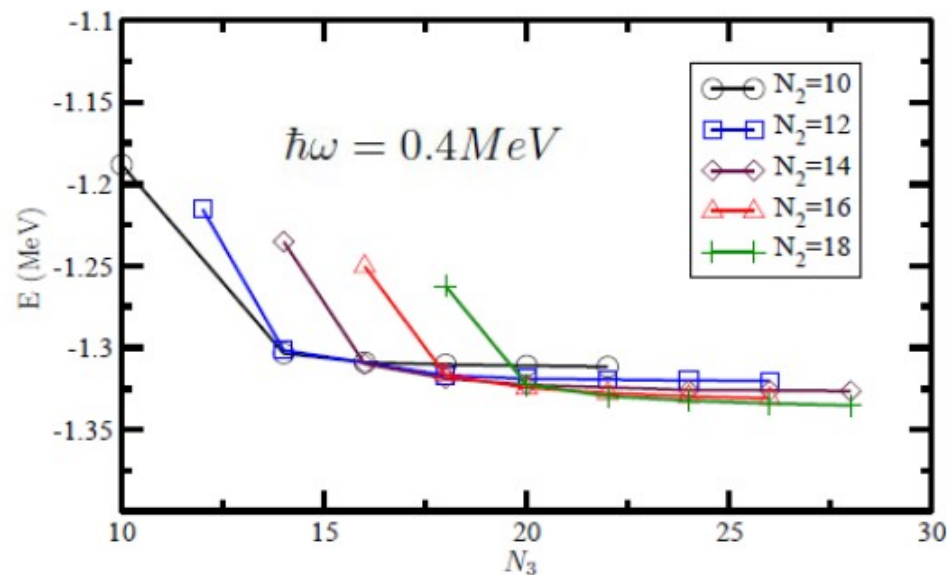
TRITON IN LO W/O A THREE-BODY FORCE



Rotureau et. al., in preparation

3 nucleons at Leading-Order 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 N_2 increases
- > as expected no need for a three body force at Leading Order.

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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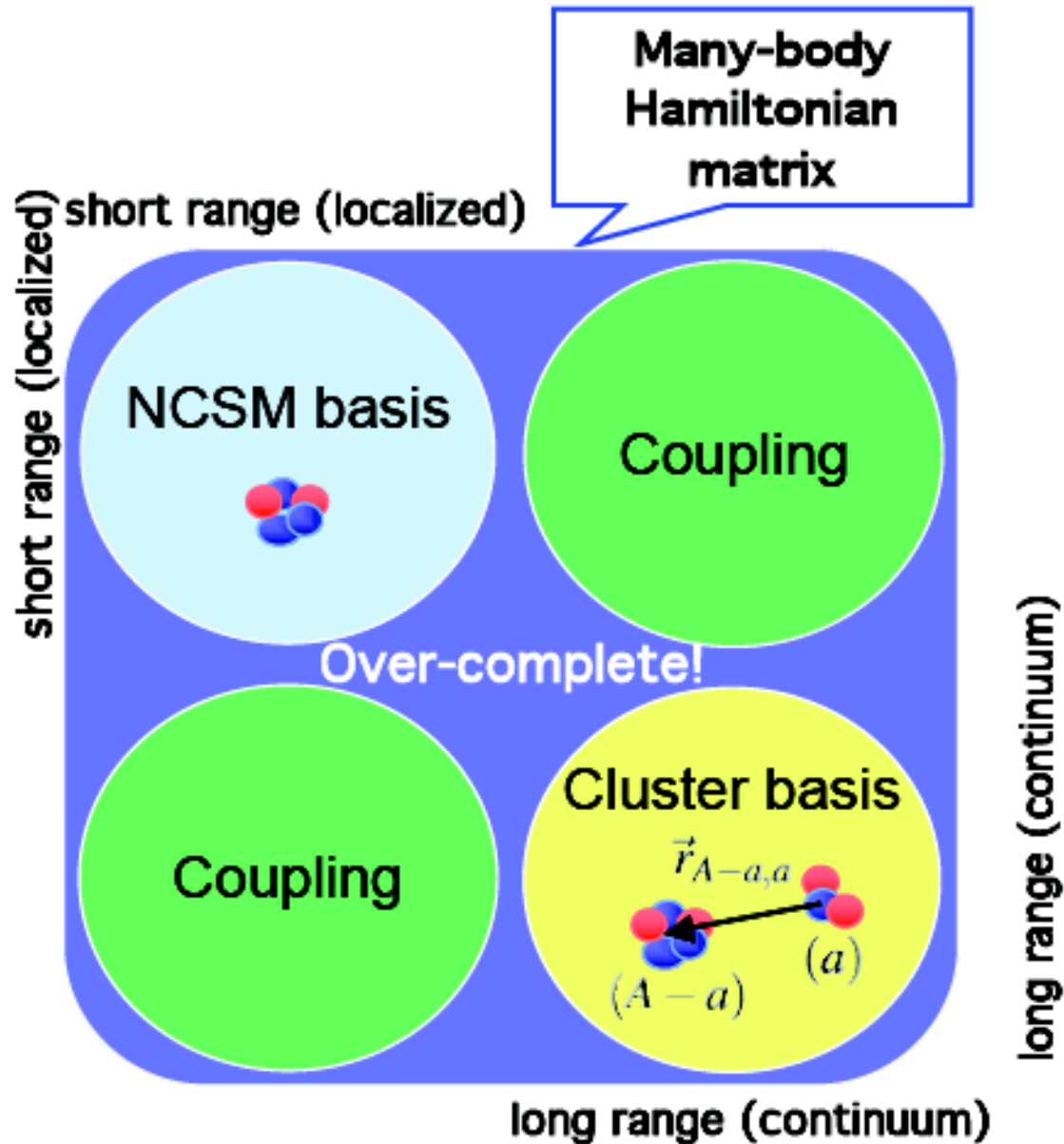
Sofia Quaglioni, Lawrence Livermore National Laboratory

Jimmy Rotureau, University of Arizona

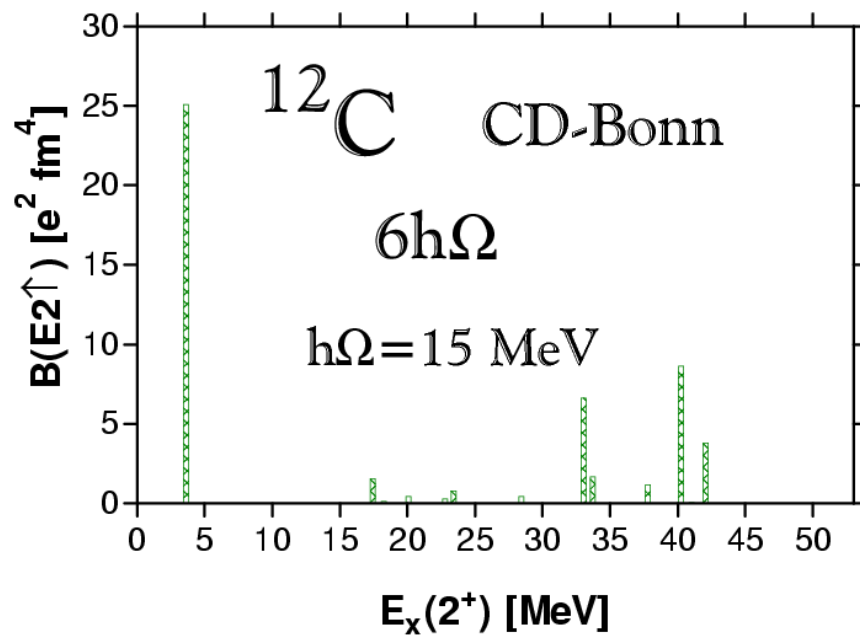
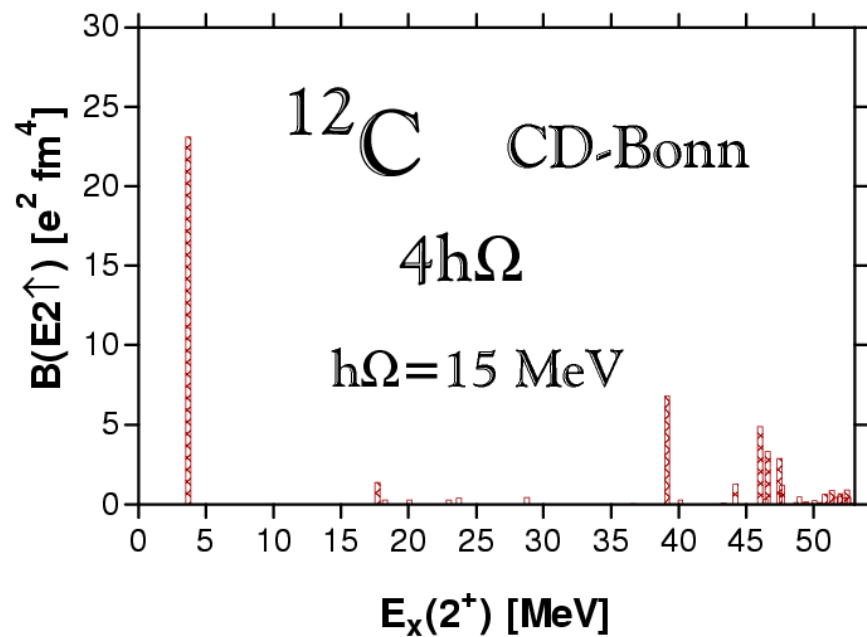
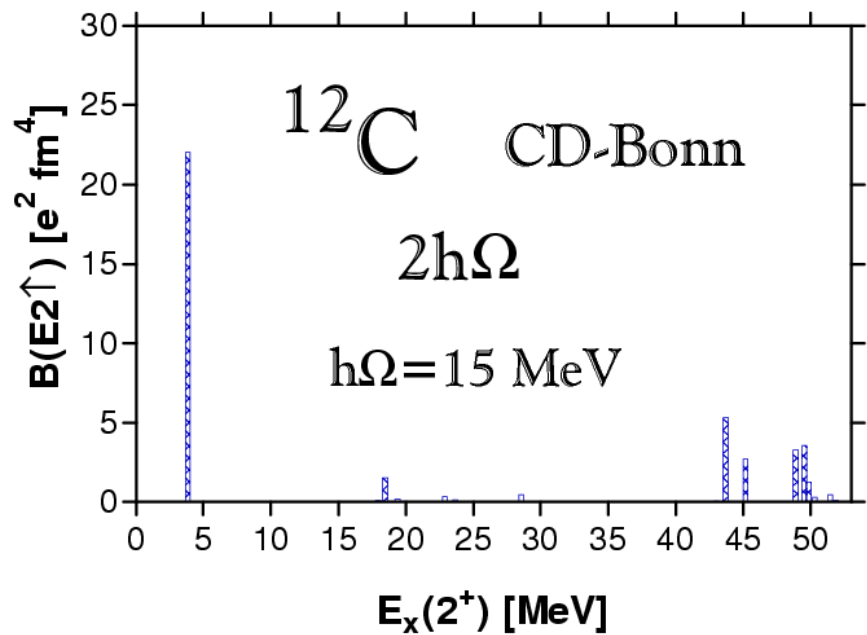
Ionel Stetcu, University of Washington

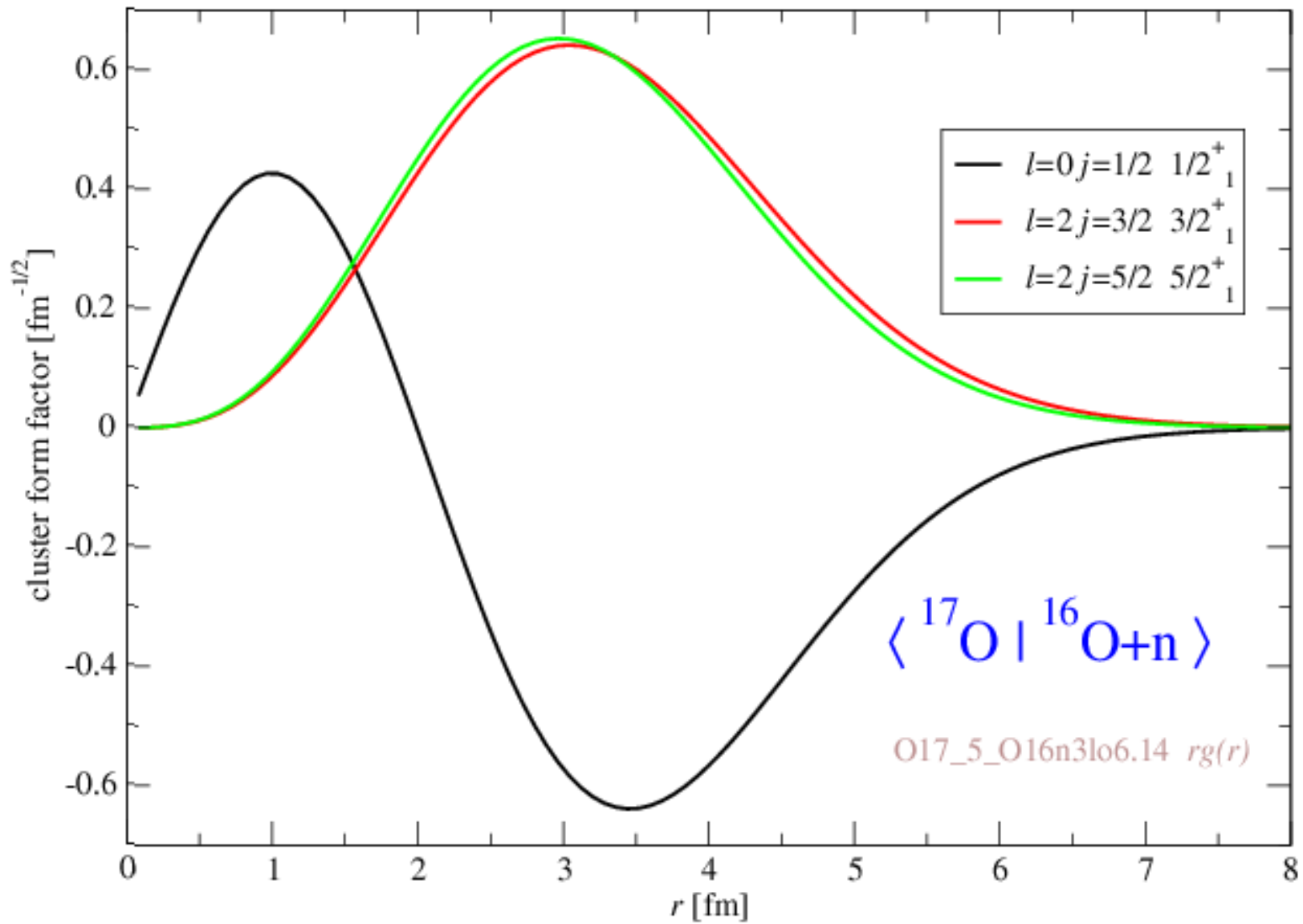
Ubirajara van Kolck, University of Arizona

James P. Vary, Iowa State University



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





P. Navrátil

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 the nucleons within an HO trap.

$$h_2 = \frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2 r^2 + V_2(r)$$

$$\frac{\Gamma(3/4 - \varepsilon/2)}{\Gamma(1/4 - \varepsilon/2)} = \frac{b}{2a_2} \quad \left(b = \frac{1}{\sqrt{\mu\omega}} \right)$$

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

Strong-Interaction Theory

1. Strong Interaction ----> Standard Model
2. Standard Model -----> Quarks exchanging gluons

However, at the energy level of low-energy nuclear physics the quark degrees of freedom are frozen out in favor of nucleon and meson degrees of freedom.

II. Many-Body Techniques for Solving the A-Nucleon Problem

1. Light Nuclei: ab initio approaches: s- and p-shell nuclei

Green Function Monte Carlo (GFMC) (R. Wiringa, et al.),
No-Core Shell Model (NCSM), Faddeev-Yakubovsky,
UCOM, $V_{\text{low-k}}$, SRG, ...

2. sd- and pf-shell nuclei:

NCSM, extended NCSM, Standard Shell Model (SSM),
Coupled Cluster (CC), Shell Model Monte Carlo (SMMC) (sign
problem defeated?), Monte Carlo Shell Model (MCSM) (Otsuka, et al.) ...

3. Heavier Nuclei:

Density Functional Theory (DFT) (SciDAC project: UNEDF); CC; Monte
Carlo approaches, ...

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)