Extending the No Core Shell Model to Heavier Mass Nuclei

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ERICE School 2011 September 18, 2011

OUTLINE

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

II. Approaches for Extending the NCSM to Heavier Mass Nuclei

III. Summary and Outlook

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

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

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); talk by James Vary at this meeting on Friday, September 23.

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

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

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

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

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}

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

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

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

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

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

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

Effective Hamiltonian for NCSM

Solving $H^{\Omega}_{A,\,a=2}\Psi_{a=2} = E^{\Omega}_{A,\,a=2}\Psi_{a=2}$ in "infinite space" 2n+l = 450 relative coordinates

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

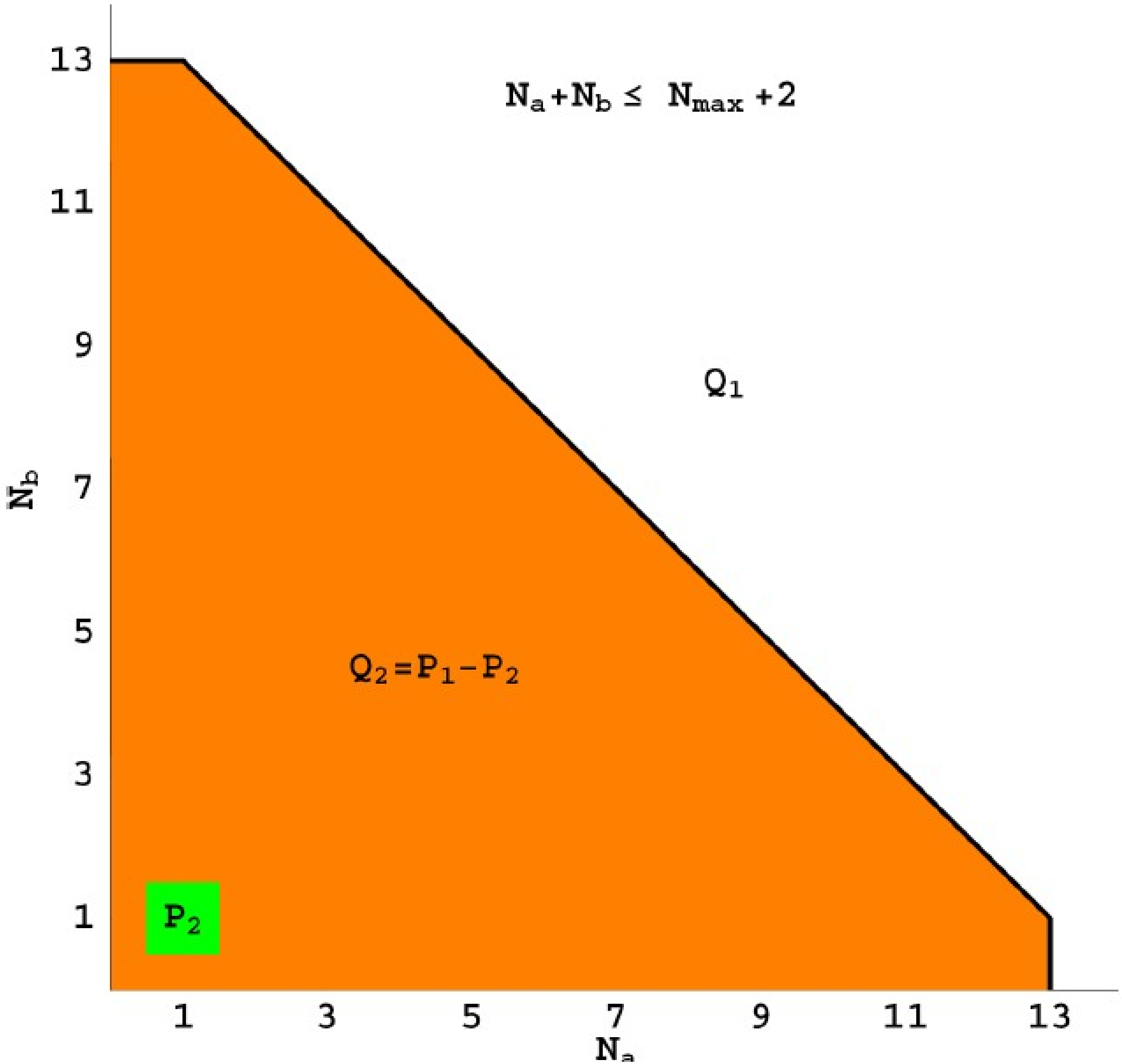
$$E^{\Omega}_{A,2} = U_2 H^{\Omega}_{A,2} U_2^{\dagger} \qquad U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} E^{\Omega}_{A,2,P} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

$$H^{N_{\max},\Omega,\mathrm{eff}}_{A,2} = \frac{U^{\dagger}_{2,P}}{\sqrt{U^{\dagger}_{2,P}U_{2,P}}} E^{\Omega}_{A,2,P} \frac{U_{2,P}}{\sqrt{U^{\dagger}_{2,P}U_{2,P}}}$$

Two ways of convergence:

1) For P → 1 and fixed a: $H^{\mathrm{eff}}_{A,a=2} \to H_A$

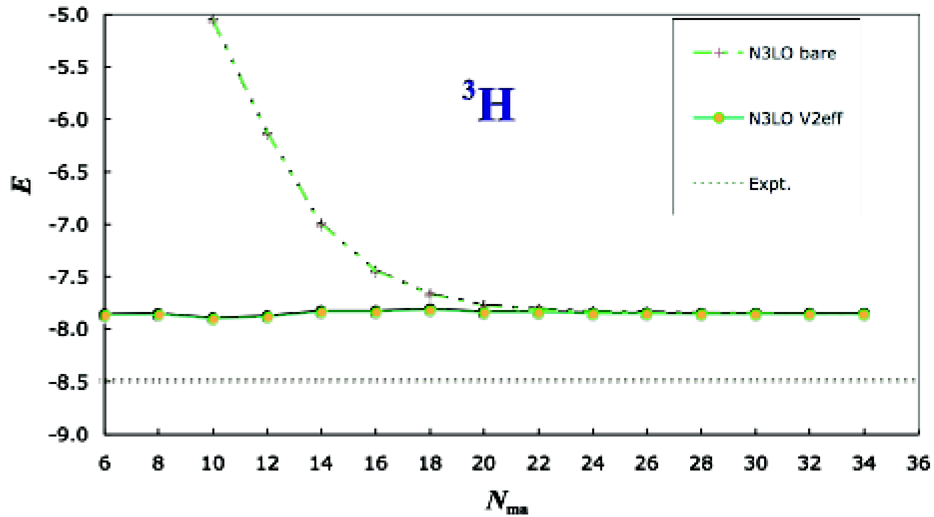
2) For a → A and fixed P: $H^{\mathrm{eff}}_{A,a} \to H_A$

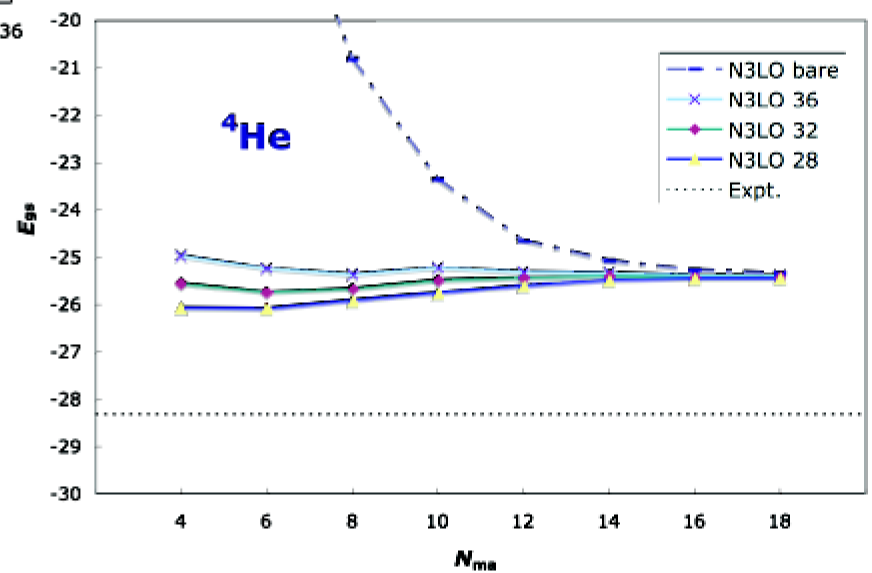


$N_a + N_b \leq N_{max} + 2$
Q_1
$Q_2 = P_1 - P_2$
P_2
N_b
N_a
1
3
5
7
9
11
13

- NCSM convergence test
  - Comparison to other methods

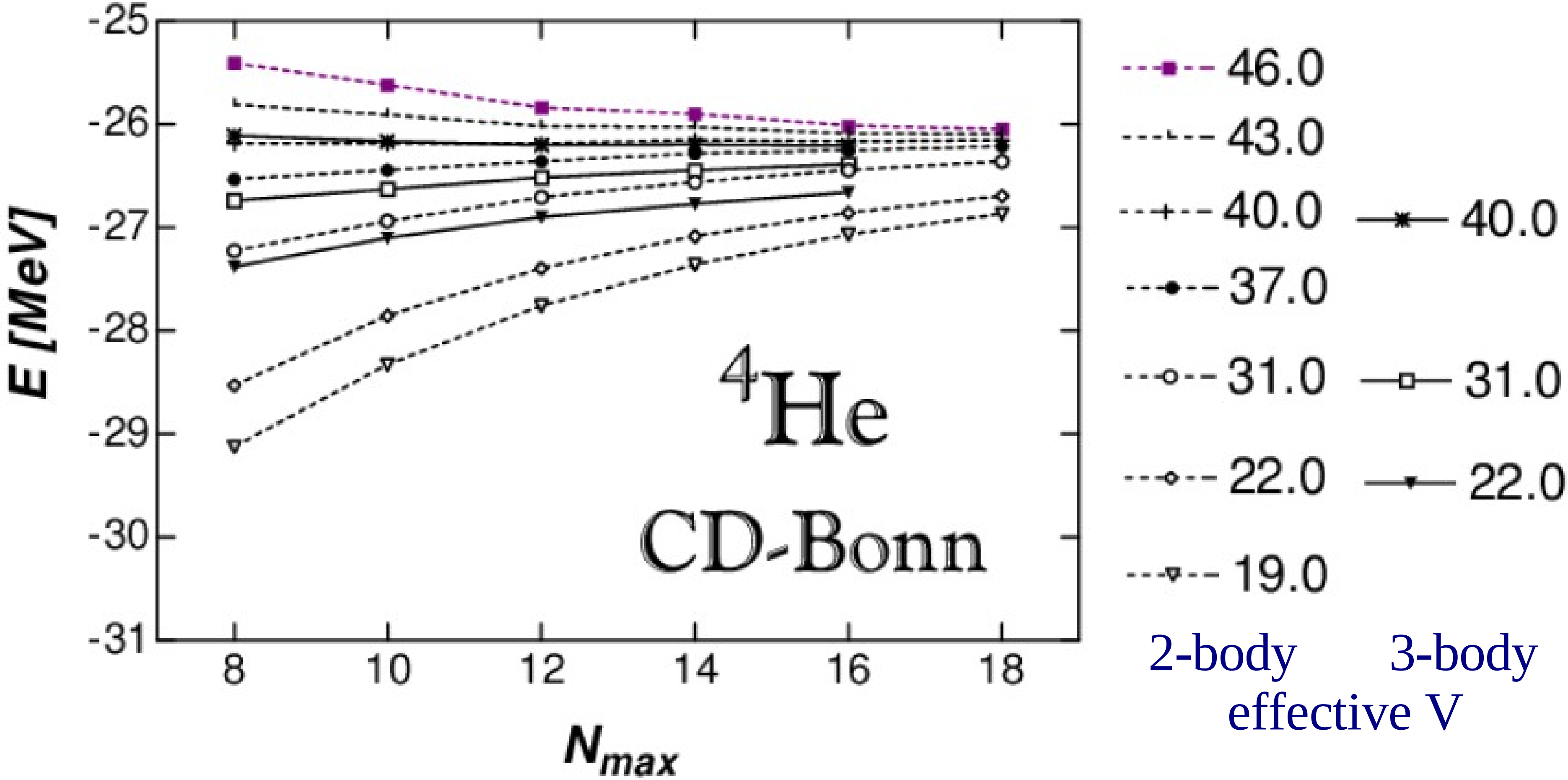
N^3LO NN	NCSM	FY	HH
^3H	7.852(5)	7.854	7.854
^4He	25.39(1)	25.37	25.38



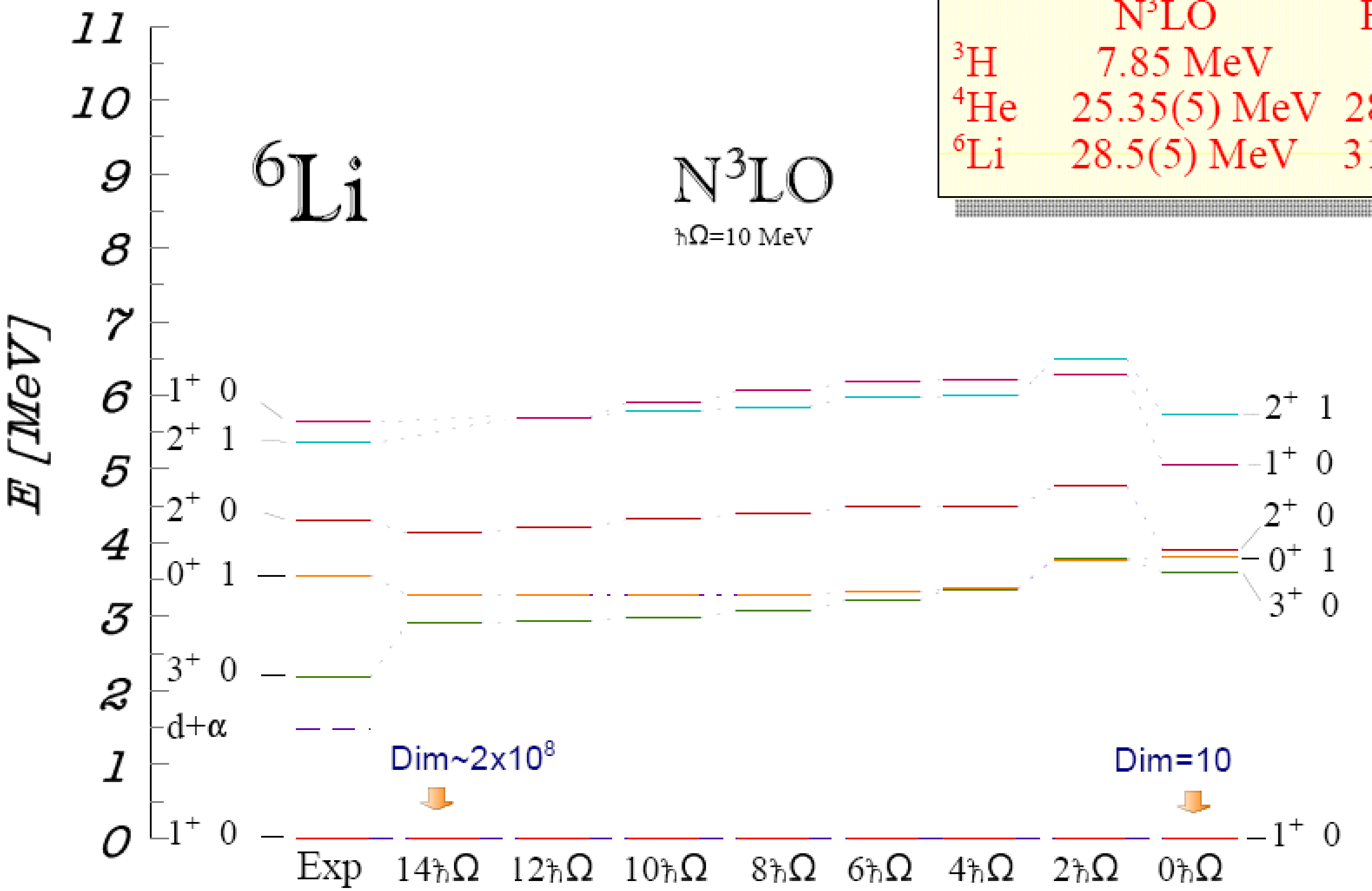


- Short-range correlations ⇒ effective interaction
- Medium-range correlations ⇒ multi-$h\Omega$ model space
- Dependence on
  - size of the model space (N_{max})
  - HO frequency ($h\Omega$)
- Not a variational calculation
- Convergence OK
- NN interaction insufficient to reproduce experiment

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



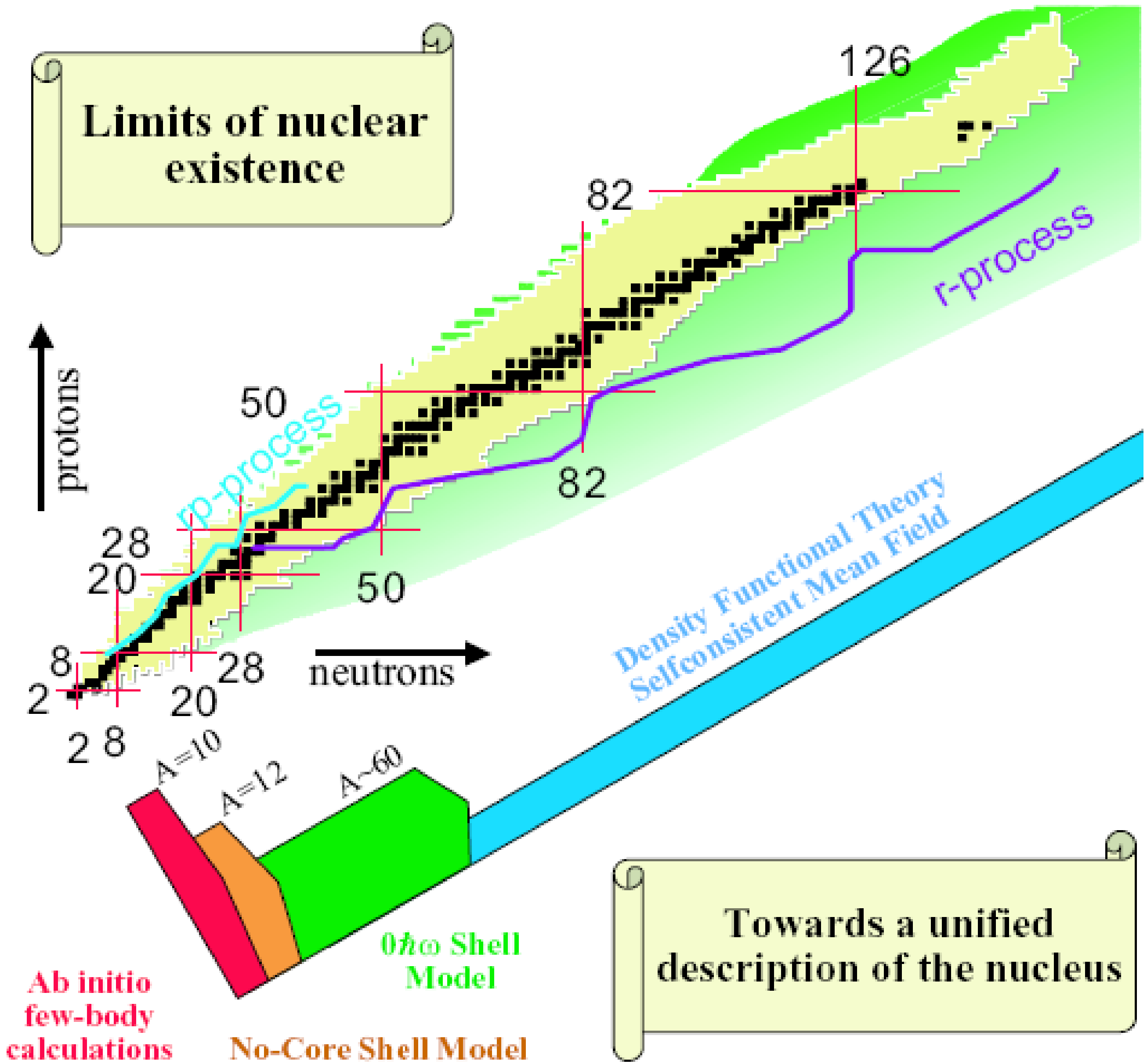
-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N_{max}
^{4}He
CD-Bonn
46.0
43.0
40.0
40.0
37.0
31.0
31.0
22.0
22.0
19.0
2-body
3-body
effective V



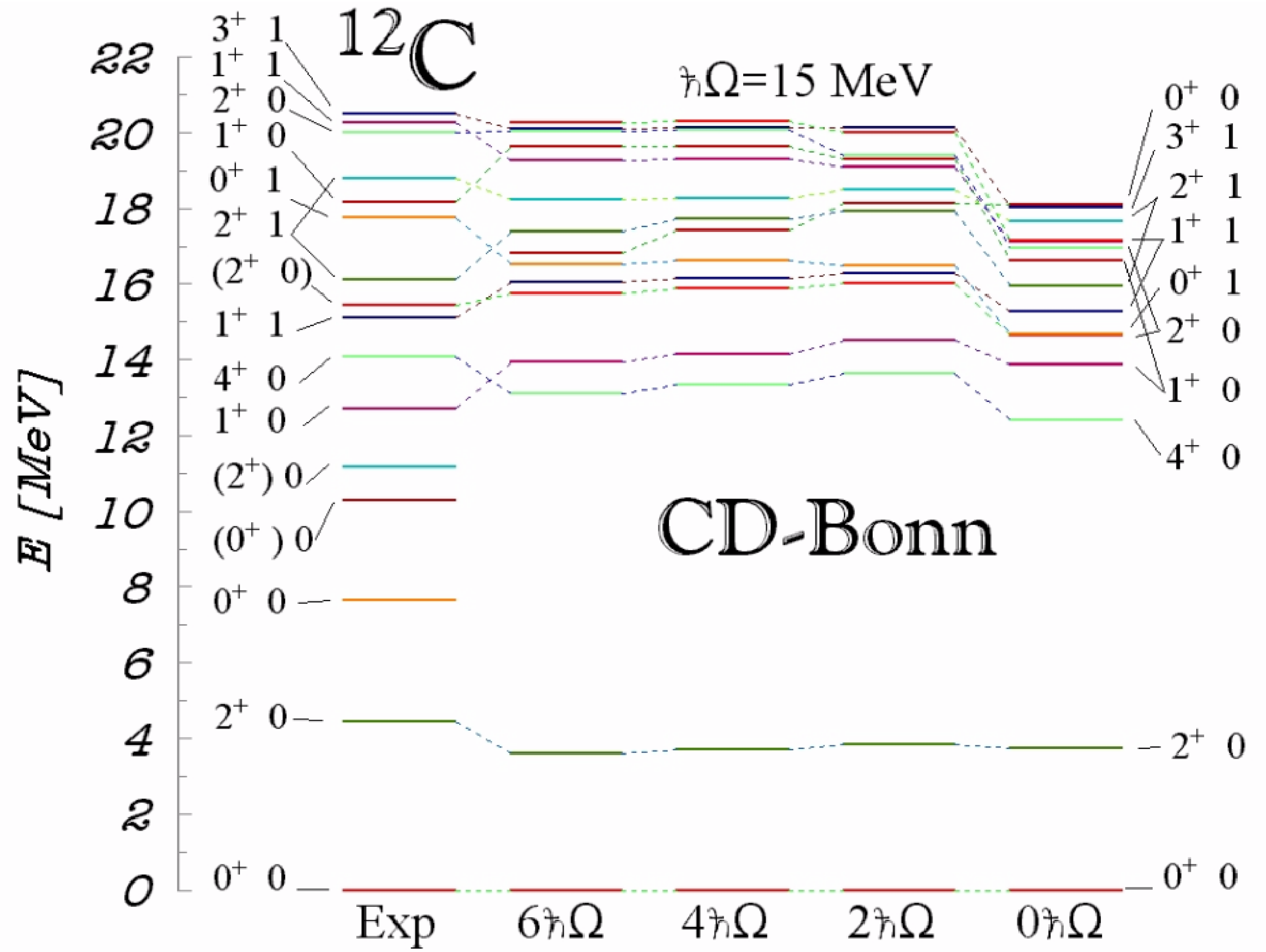
	N3LO	Exp
^{3}H	7.85 MeV	8.48 MeV
^{4}He	25.35(5) MeV	28.30 MeV
^{6}Li	28.5(5) MeV	31.99 MeV

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

II. Extending the NCSM to Heavier Mass Nuclei



Limits of nuclear existence
protons
neutrons
126
82
50
28
20
8
2
82
50
28
20
2 8
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
Ab initio few-body calculations
No-Core Shell Model
0ħω Shell Model
Towards a unified description of the nucleus



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

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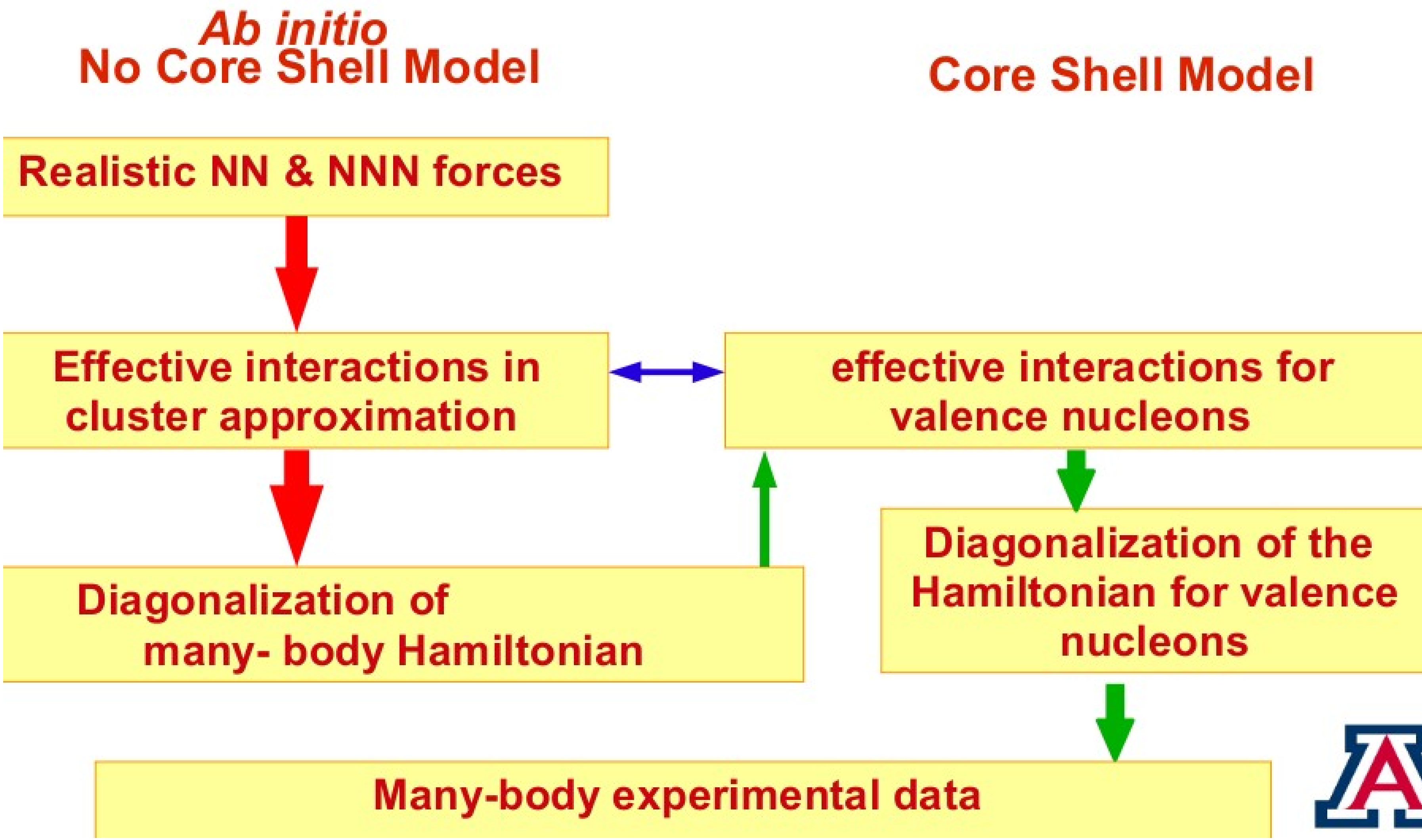
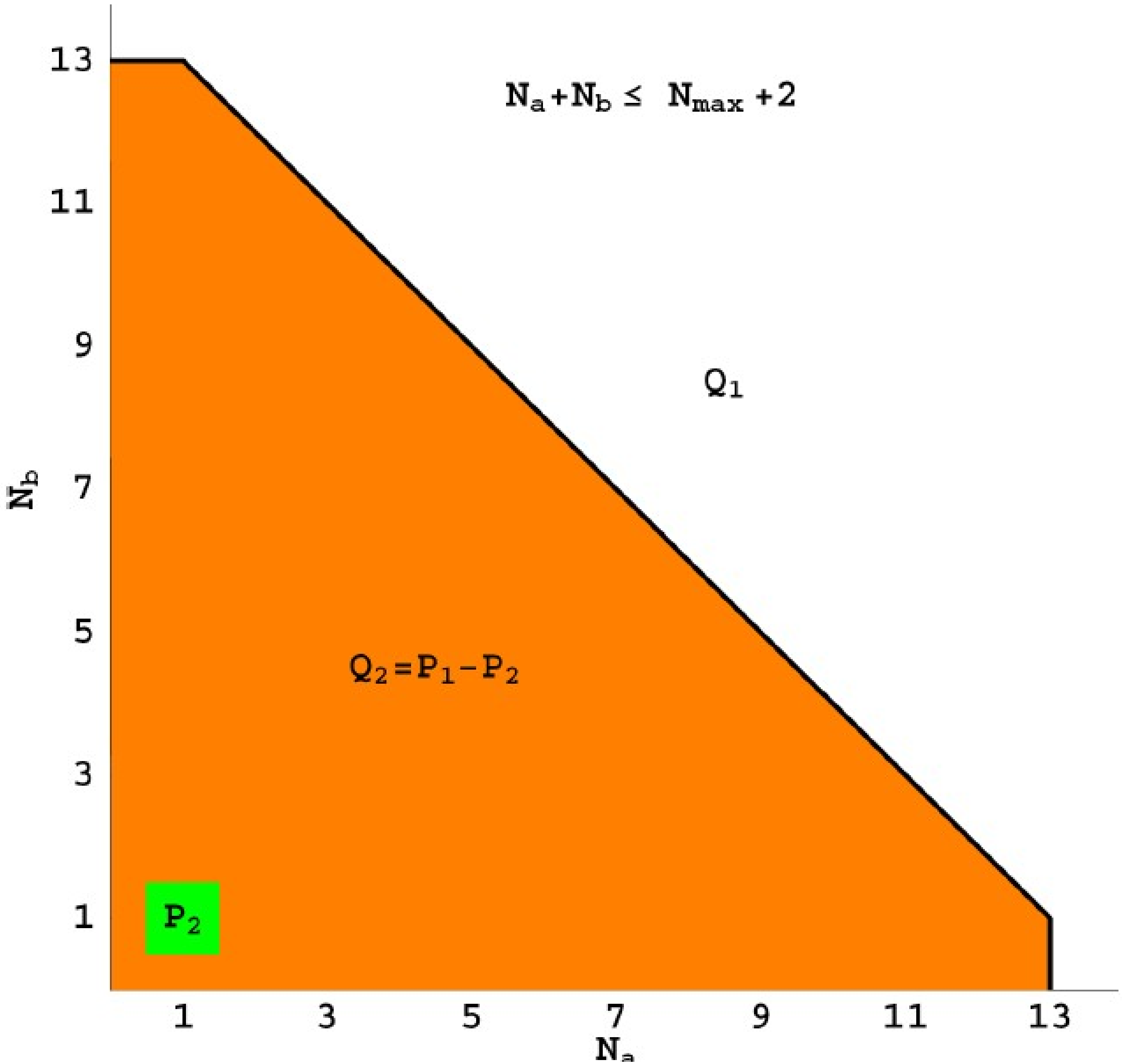
(Received 20 June 2008; published 10 October 2008)

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

From few-body to many-body





13
11
9
7
5
3
1
N_b
$N_a + N_b \leq N_{max} + 2$
Q_1
$Q_2 = P_1 - P_2$
P_2
1
3
5
7
9
11
13
N_a

Two-body VCE for ^{6}Li

$$\mathcal{H}^{0,N_{\max}}_{A=6,a_1=6} = V_0^{6,4} + V_1^{6,5} + V_2^{6,6}$$

Need NCSM results in N_{max} space for ^{4}He | ^{5}He ^{5}Li | ^{6}He ^{6}Li ^{6}Be

With effective interaction for A=6 !!! $H^{N_{\max},\Omega,\mathrm{eff}}_{A=6,2}$

Core Energy: $V_0^{6,4}$ = -51.644 MeV

$$V_1^{6,5} = \mathcal{H}^{0,N_{\max}}_{6,5} - V_0^{6,4} \quad \langle ab;JT|V_1^{6,5}|cd;JT\rangle = (\epsilon_a + \epsilon_b)\delta_{a,c}\delta_{b,d}$$

Single Particle Energies: $\varepsilon_{p3/2}$ = 14.574 MeV $\quad \varepsilon_{p1/2}$ = 18.516 MeV

$$V_2^{6,6} = \mathcal{H}^{0,N_{\max}}_{6,6} - \mathcal{H}^{0,N_{\max}}_{6,5}$$

TBMEs:

$\langle p_{3/2}p_{3/2}|V_2^{6,6}|p_{3/2}p_{3/2}\rangle_{J=3,T=0}$ = -1.825 MeV

$\langle p_{3/2}p_{3/2}|V_2^{6,6}|p_{3/2}p_{3/2}\rangle_{J=2,T=1}$ = 2.762 MeV

2-body Valence Cluster approximation for A=6

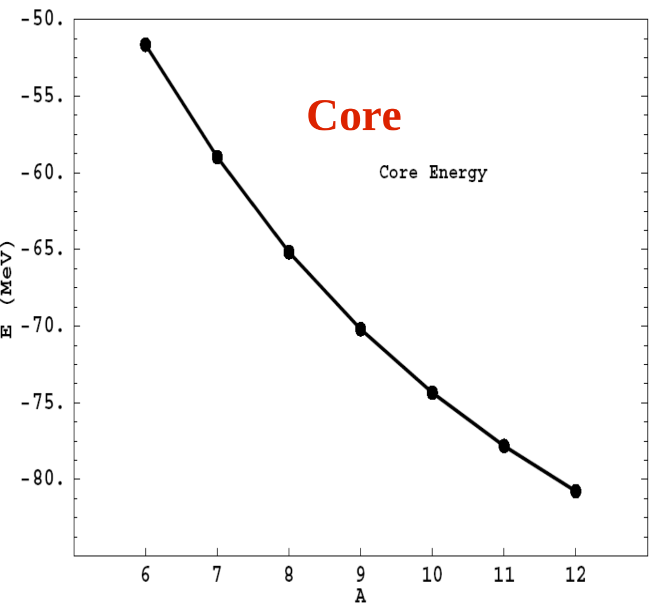
$$\mathcal{H}_{A,a_1=6}^{0,N_{\max}} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$

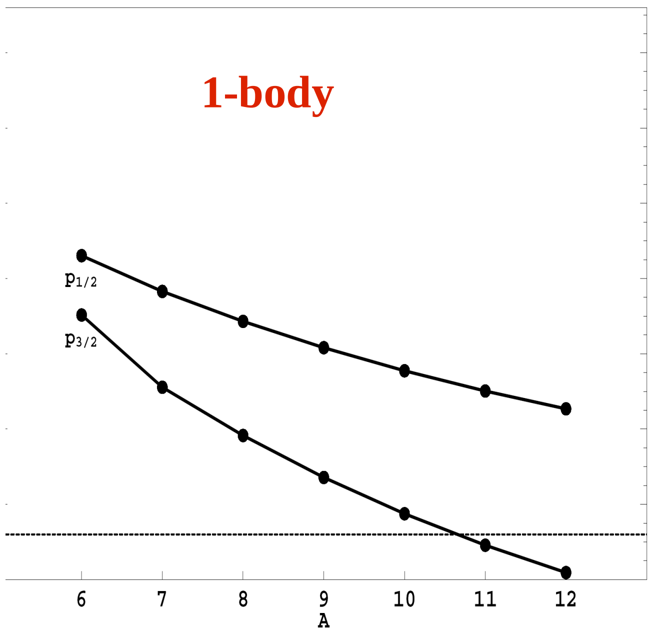
Need NCSM results in N_{max} space for **^{4}He** **^{5}He ^{5}Li** **^{6}He ^{6}Li ^{6}Be**

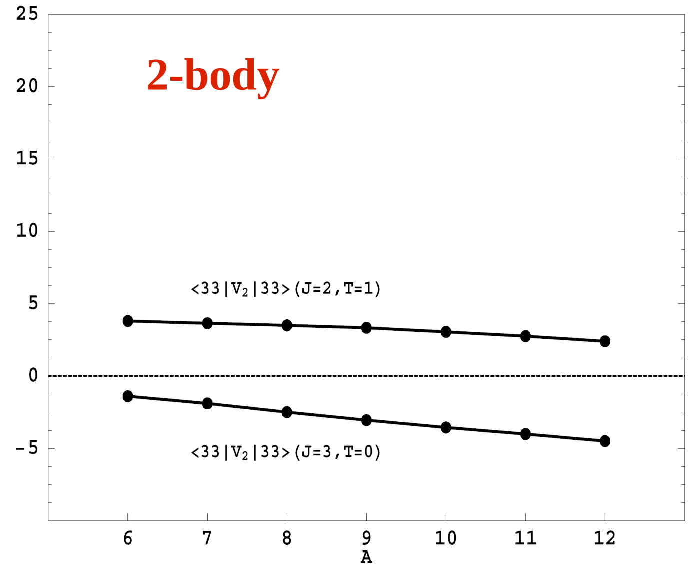
$N_{max} = 6$

With effective interaction for A !!!

$$H_{A,2}^{N_{\max},\Omega,\mathrm{eff}}$$







2-body Valence Cluster approximation for A=7

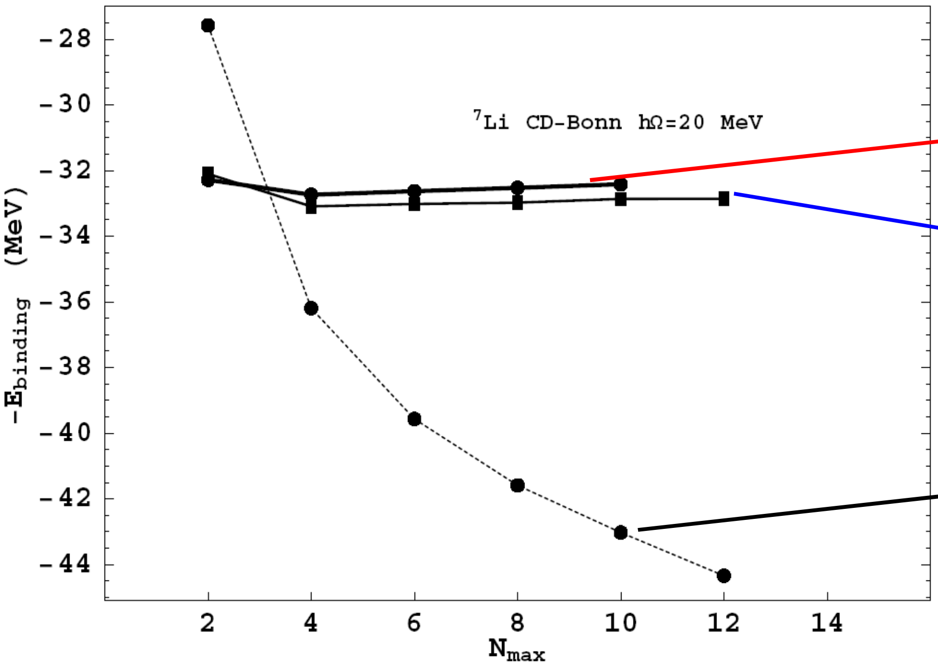
$$\mathcal{H}^{0,N_{\max}}_{A,a_1=6} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$

Need NCSM results in N_{max} space for

^{4}He **^{5}He ^{5}Li** **^{6}He ^{6}Li ^{6}Be**

With effective interaction for A=7 !!!

$$H^{N_{\max},\Omega,\text{eff}}_{A,2}$$



Exact NCSM

SSM with A-dependent core

SSM with inert core

3-body Valence Cluster approximation for A>6

$$\mathcal{H}^{0,N_{\max}}_{A,a_1=7} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6} + V_3^{A,7}$$

Need NCSM results in N_{max} space for

^4He

^5He ^5Li

^6He ^6Li ^6Be

^7He ^7Li ^7B ^7Be

With effective interaction for A !!!

$$H_{A,2}^{N_{\max},\Omega,\text{eff}}$$

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

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

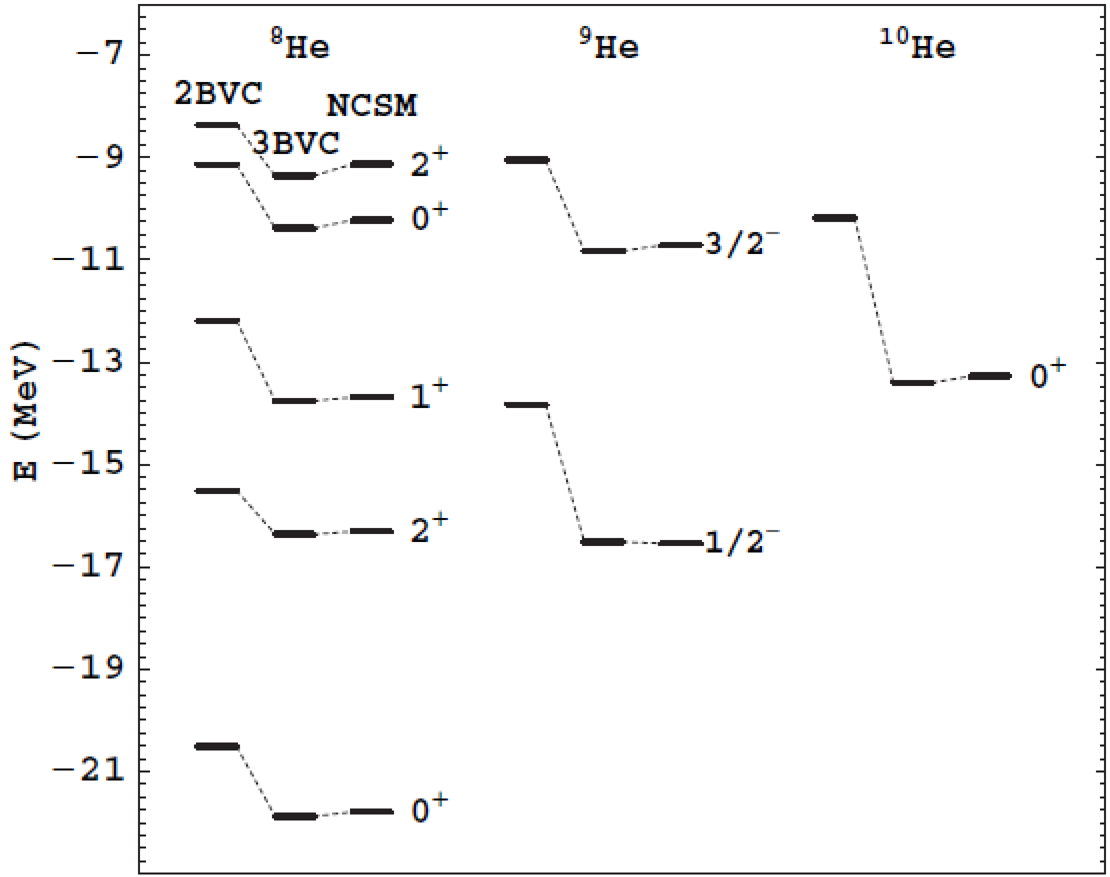
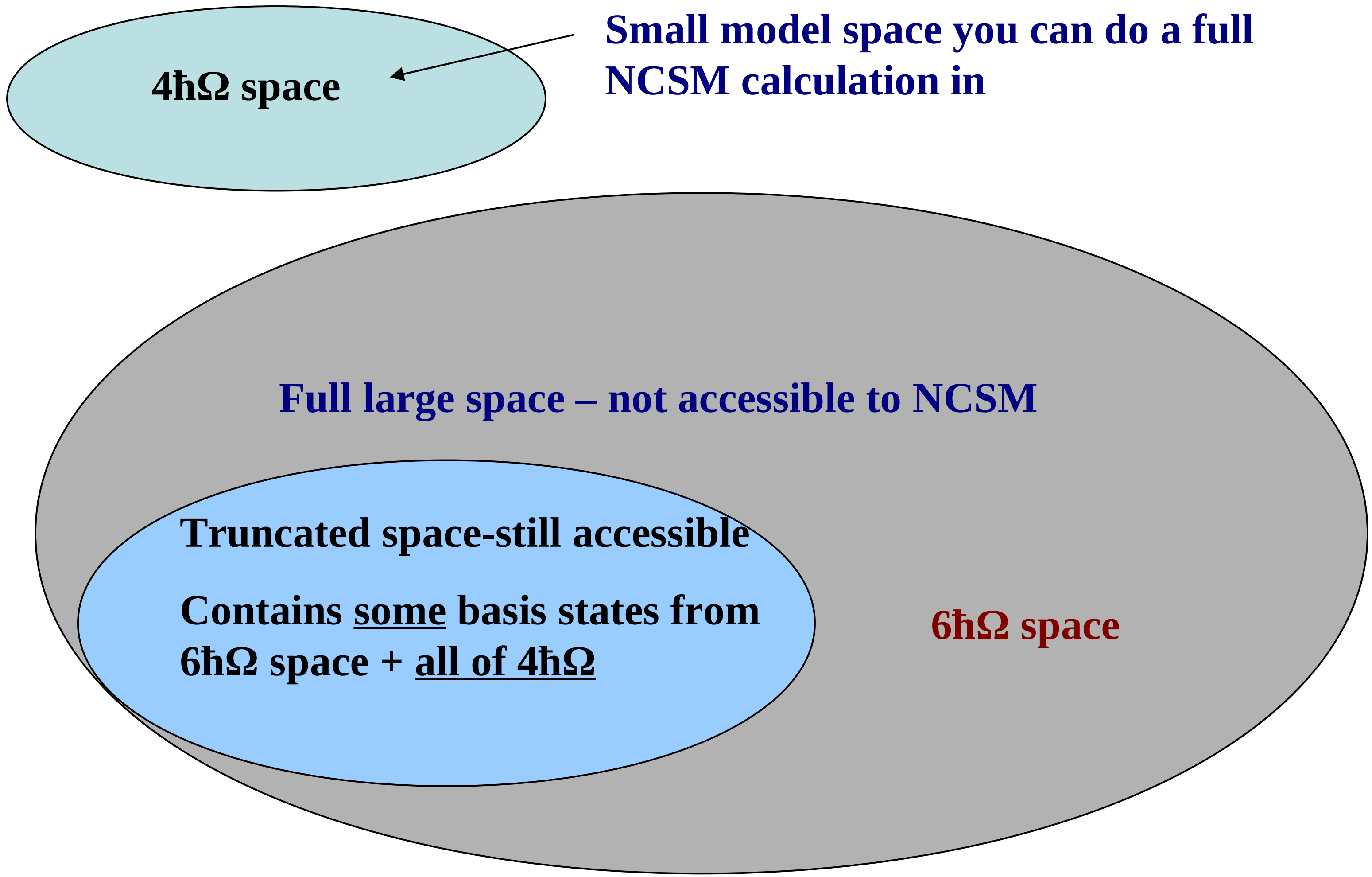


FIG. 9. Comparison of spectra for ^{8}He, ^{9}He, and ^{10}He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$ and $\hbar\Omega = 20$ MeV using the CD-Bonn interaction.

2. Importance Truncation

The idea of Importance Truncation



Formalism of Importance truncation.

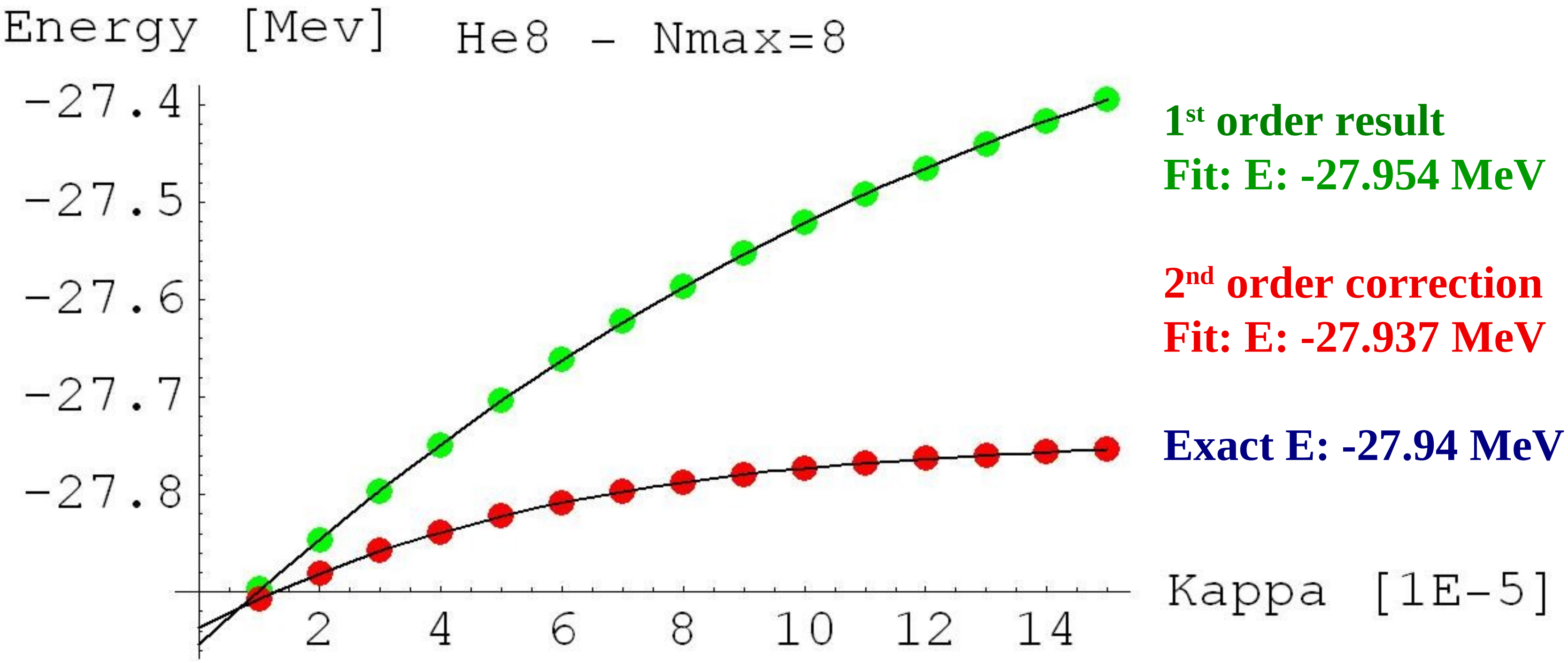
- First order multi-configurational perturbation theory gives...

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

$$= -\sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}} |\Phi_\nu\rangle.$$

$$W = H - H_0$$

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



1st order result
Fit: E: -27.954 MeV

2nd order correction
Fit: E: -27.937 MeV

Exact E: -27.94 MeV

Interaction: ^{8}He SRG N3LO

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

Available online at www.sciencedirect.com
ScienceDirect
Physics Letters B 653 (2007) 358–362
PHYSICS LETTERS B
www.elsevier.com/locate/physletb

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}H, ^{3}H and ^{4}He be exactly reproduced. The first $(0^+;0)$ excited state of ^{4}He and the ground state of ^{6}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}He an energy level for the first $(0^+;0)$ excited state in remarkable agreement with the experimental value. The corresponding ^{6}Li binding energy is about 70% of the experimental value, consistent with the expansion parameter of the EFT.

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

IOP PUBLISHING JOURNAL OF PHYSICS G: NUCLEAR AND PARTICLE PHYSICS

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

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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

Effective Field Theory (1/3)

i) Separation of scale :

M_{QCD} ~ 1 GeV (mass of nucleon)

M_{nucl} ~ 100 MeV (typical momentum in a nucleus)

M_{struct} ~ 10 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)

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

-> 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"):

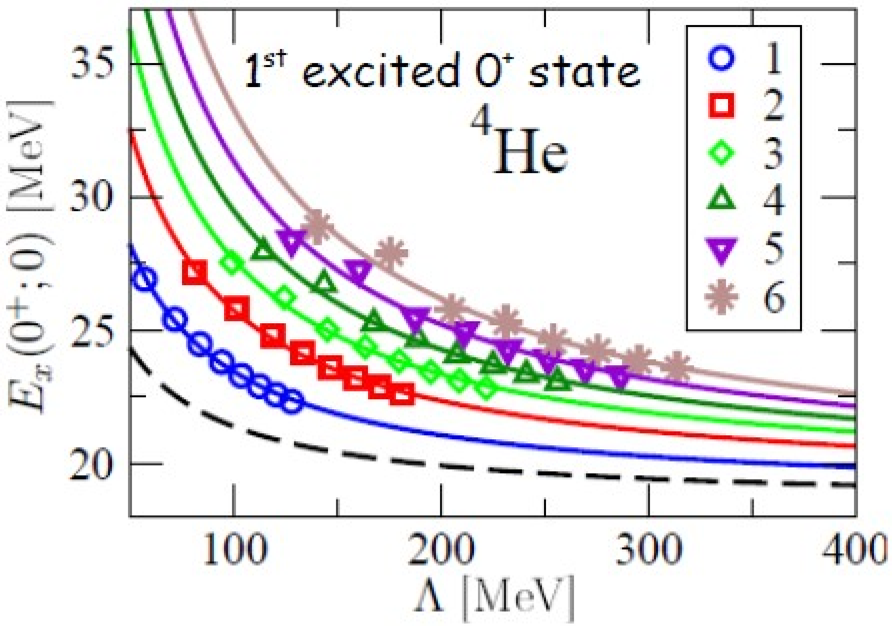
-> hierarchy between the different contributions

-> 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

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

Stetcu et. al., 2007
PLB 653, pp. 358-362



-> 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 ^{4}He.

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)

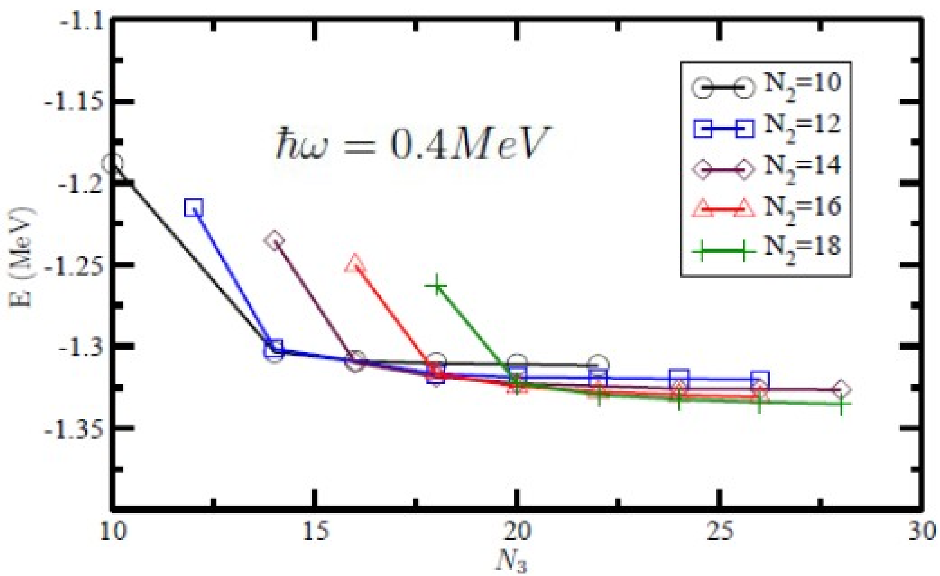
phase shift (scattering physics)

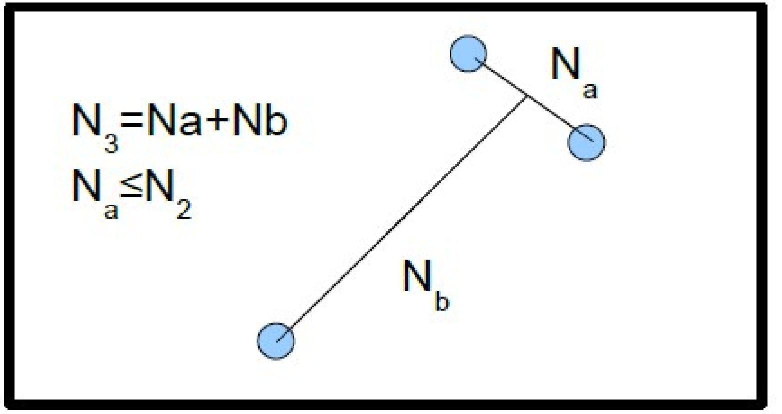
$$k\,\cot\delta = -\frac{1}{a_2} + \frac{1}{2} r_2 k^2 + \ldots ,$$

Effective Range Expansion

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.

J. Rotureau, ORNL,
March 2011

SUMMARY AND OUTLOOK

The NCSM is an *ab initio* method for calculating nuclear structure, which has been successfully applied to 0p-shell nuclei.

However, applications beyond the 0p-shell become increasing difficult due to the rapid growth of the model spaces needed for performing NCSM calculations.

A number of new techniques are being developed to extend the NCSM beyond the 0p-shell, *e.g.*, *ab initio* shell model with a core, importance truncation, NCSM in an EFT framework, *etc*. But, much work remains to be done on these approaches.

However, many significant and useful applications of the NCSM in 0p-shell nuclei and in reaction theory are currently possible and are underway.

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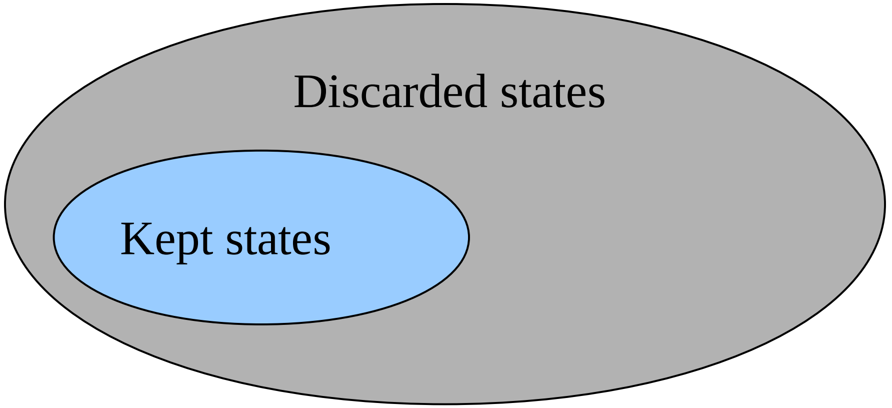
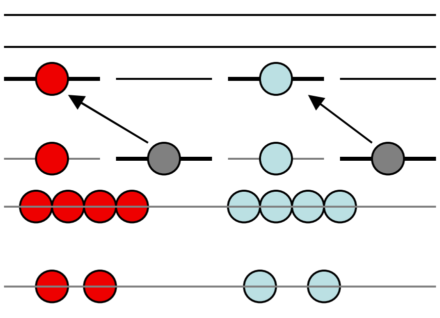
Importance truncation schematically

$$\kappa_\nu = \frac{|\langle \Phi_\nu | H | \Psi_{ref} \rangle|}{\epsilon_\nu - \epsilon_{ref}}$$

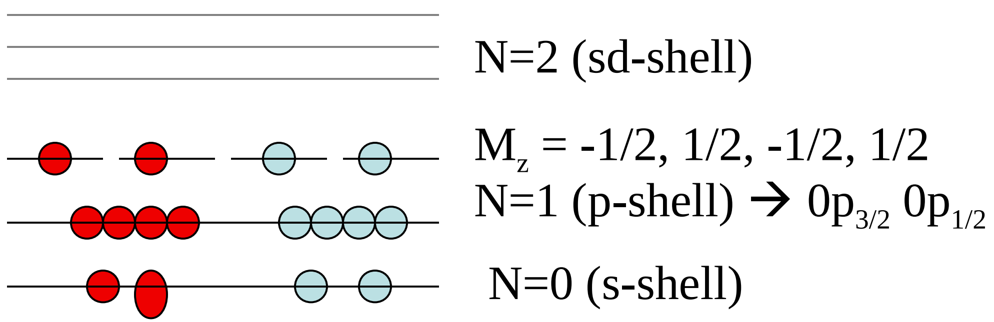


$\langle \Phi_\nu |$



O16 – one possible
configuration

$| \Psi_{ref} \rangle$



O16 - 0ħΩ
configuration

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.

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

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

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

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

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

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

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

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

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

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

LO RENORMALIZATION

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

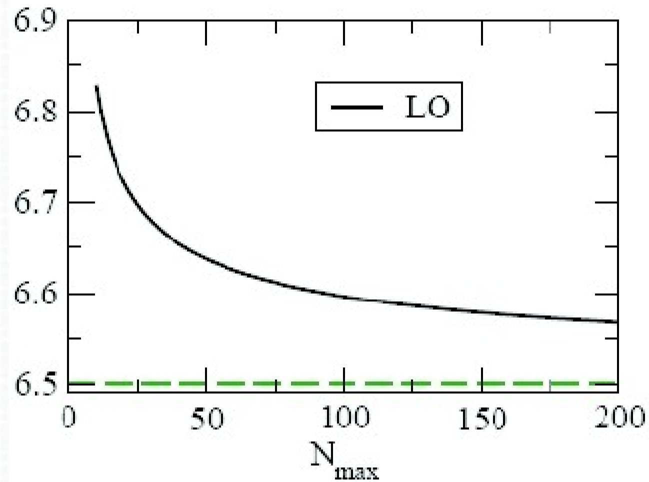
$$\left[b^2 p^2 + \frac{r^2}{b^2} + 2\mu C_0(N_{\max}) b^2 \delta^{(3)}(\vec{r}) \right] \Psi(\vec{r}) = 2\frac{E}{\omega}\Psi(\vec{r})$$

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

Fix from Busch's formula

Stetcu et. al, 2007

Energy of third excited state at unitarity



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.

$BE_{th} \approx 25.91$ MeV $\qquad$ $BE_{exp} \approx 28.296$ MeV

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

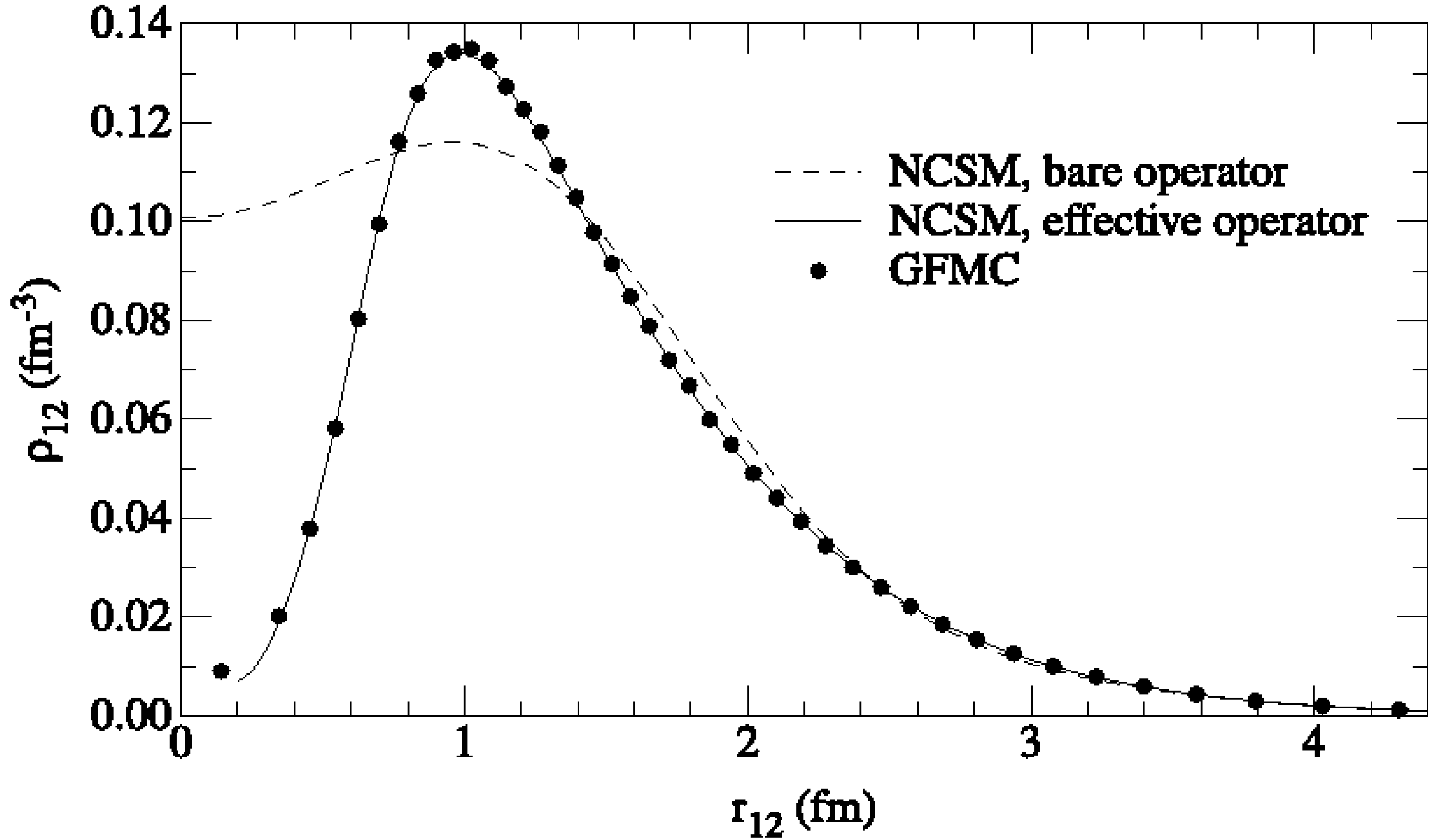


Figure 2. *NCSM and GFMC NN pair density in ^4He.*

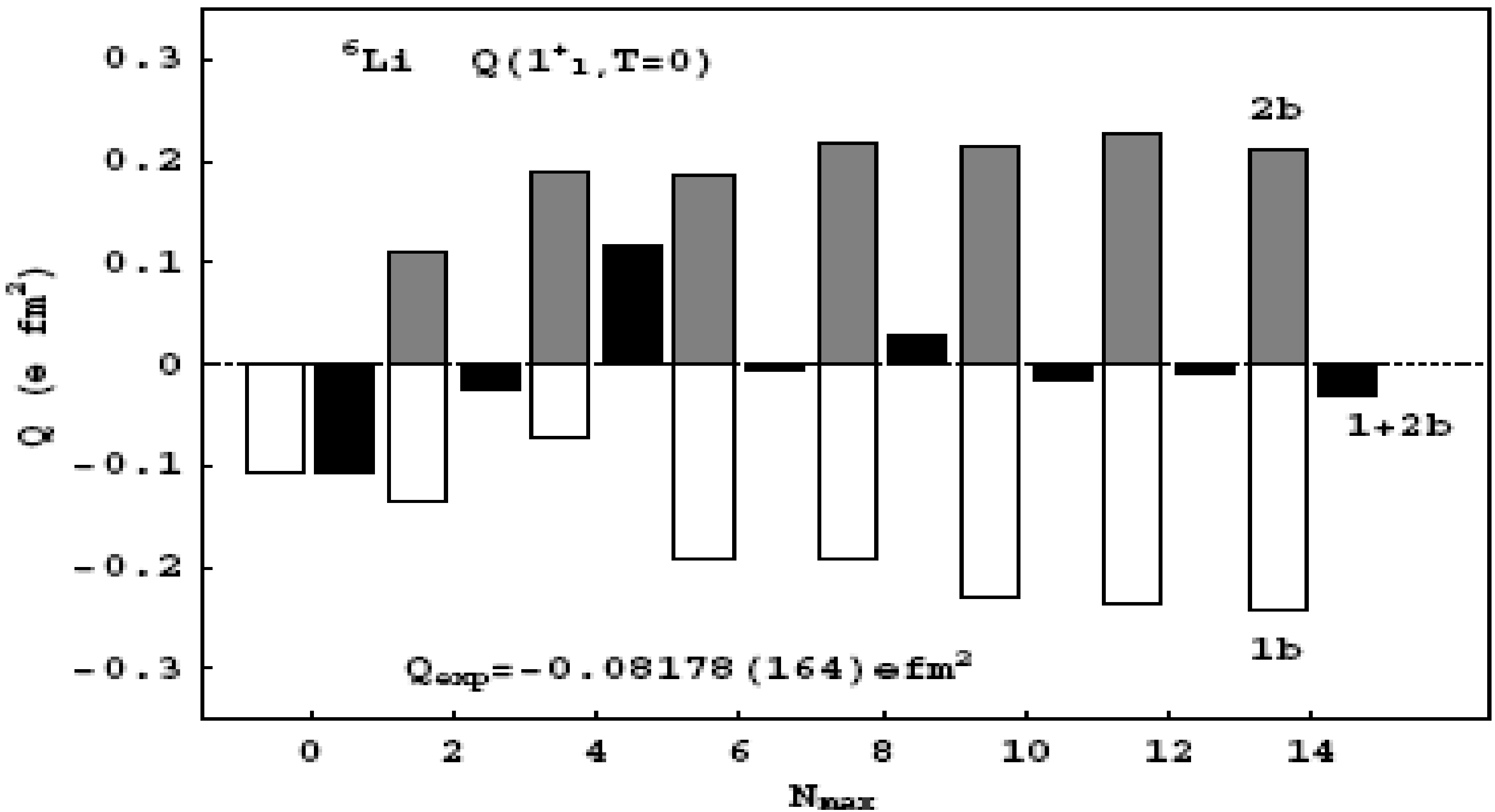


FIG. 6: The quadrupole moment of the ground state for ^{6}Li ($1^+(T = 0)$) is shown in terms of one- and two-body contributions as a function of increasing model space size.