The No Core Shell Model: with and without a core (Extensions to Heavier Nuclei)

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INT-11-2a June 7, 2011

MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many-body theory

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)

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

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

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

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

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

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

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

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

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

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;

$$E^{\Omega}_{A,2} = U_2 H^{\Omega}_{A,2} U_2^{\dagger}$$

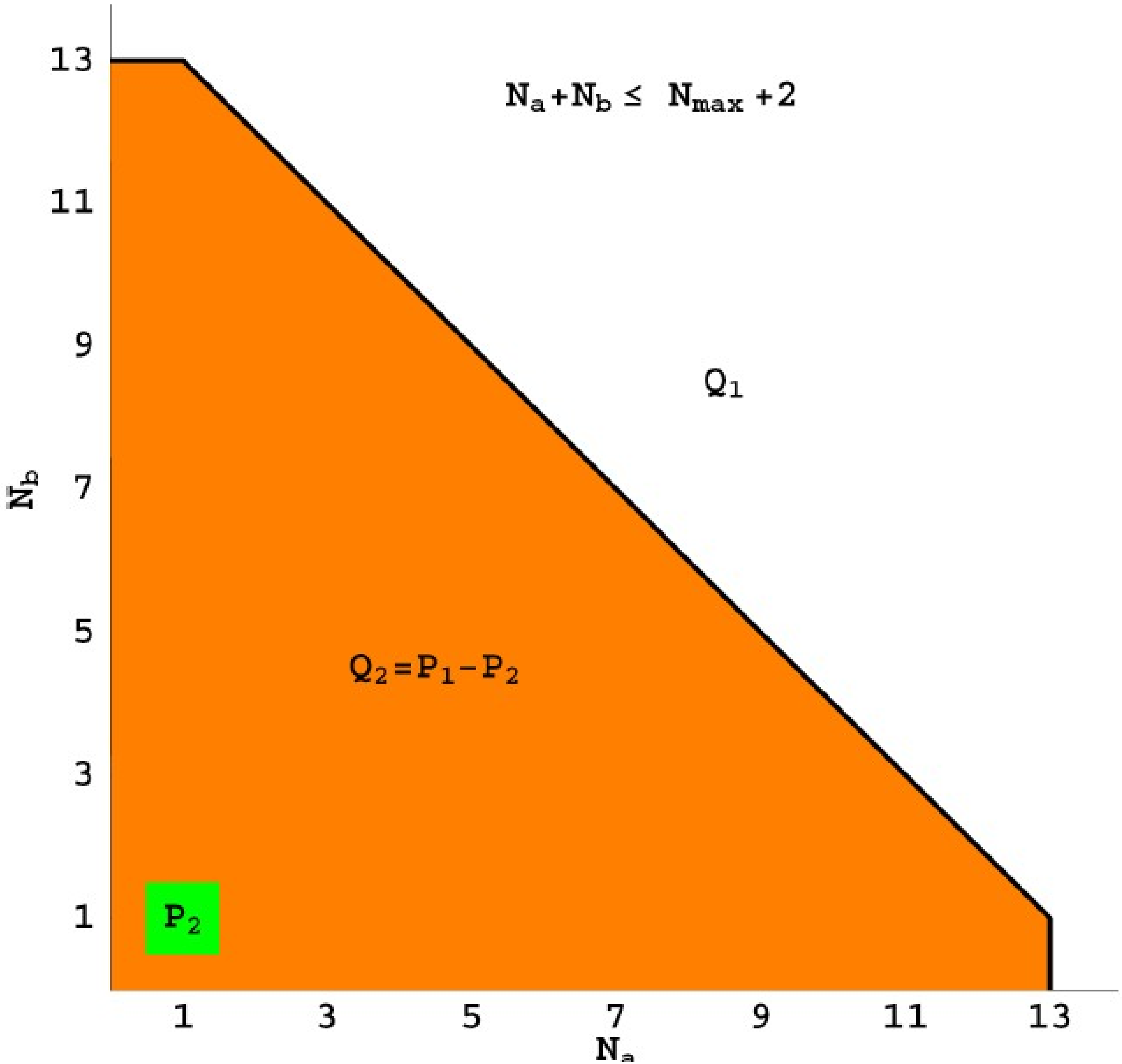
$$U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} E^{\Omega}_{A,2,P} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

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

Two ways of convergence:

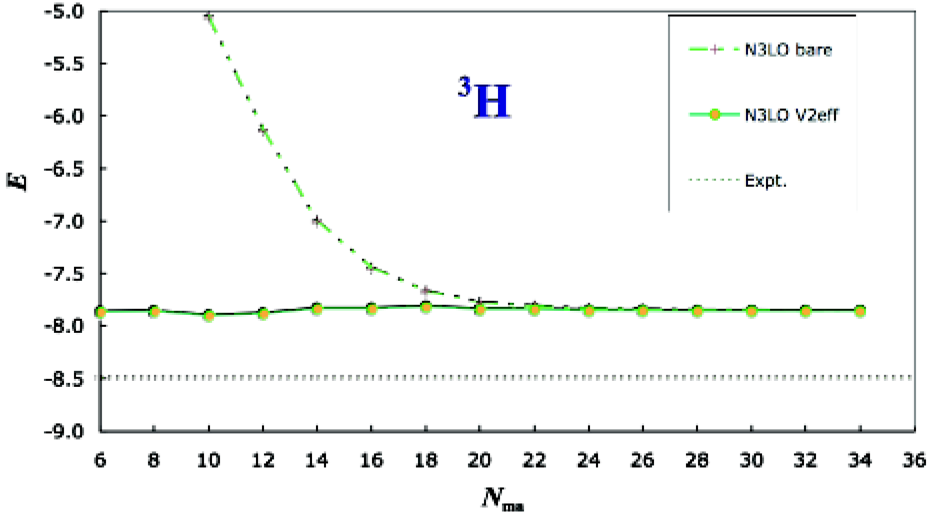
1) For P → 1 and fixed a: $H^{\mathrm{eff}}_{A,a=2} \to H_A$

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



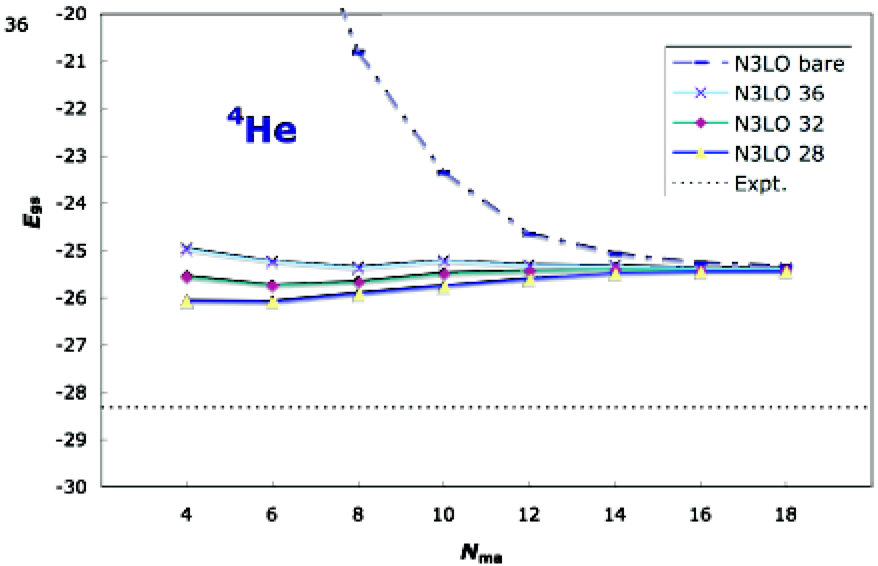
$N_a + N_b \leq N_{max} + 2$
Q_1
$Q_2 = P_1 - P_2$
P_2
N_b
N_a
1
3
5
7
9
11
13

- NCSM convergence test
  - Comparison to other methods

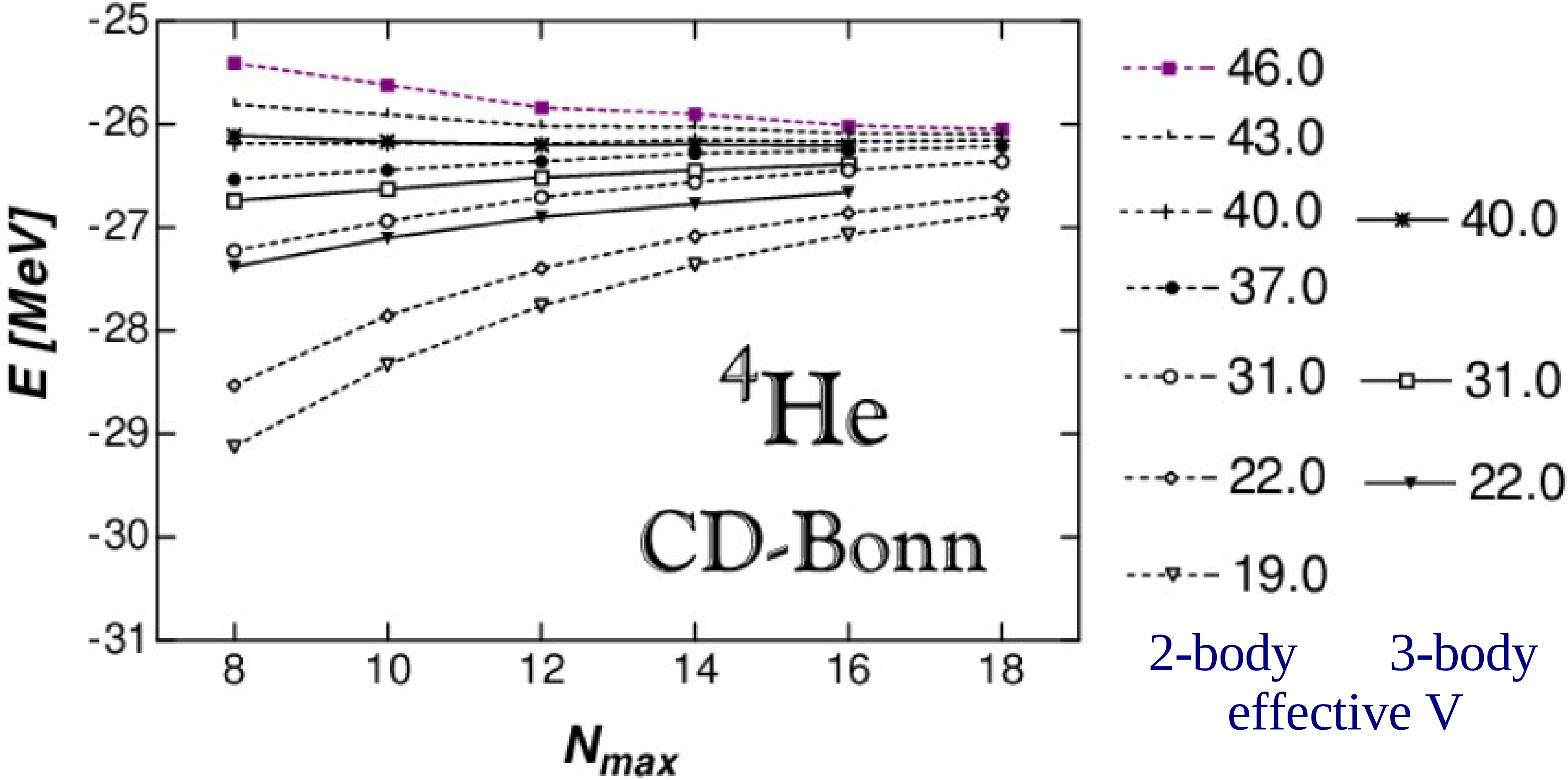


N^3LO NN	NCSM	FY	HH
^3H	7.852(5)	7.854	7.854
^4He	25.39(1)	25.37	25.38

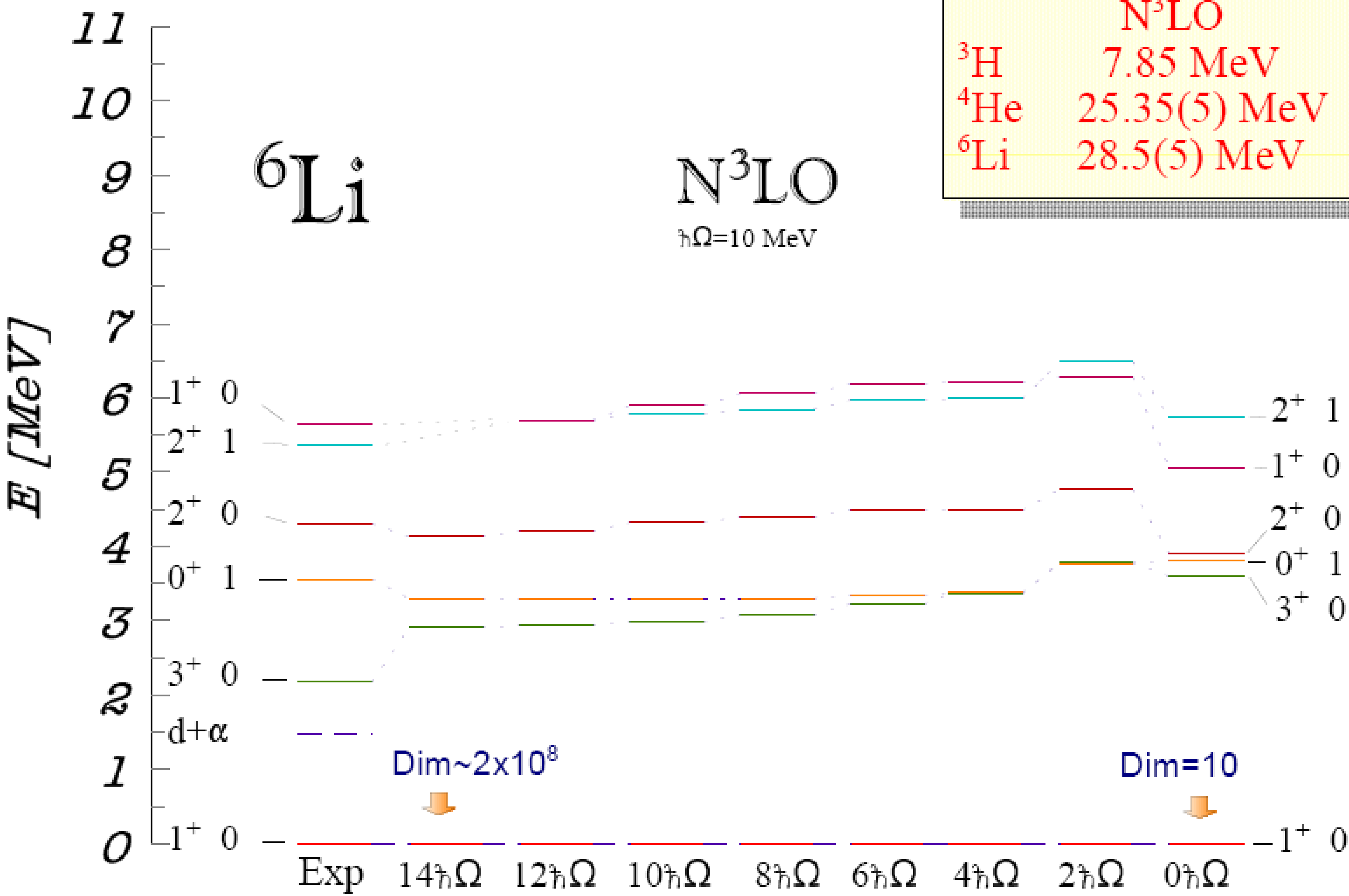
- Short-range correlations ⇒ effective interaction
- Medium-range correlations ⇒ multi-$\hbar\Omega$ model space
- Dependence on
  - size of the model space (N_{max})
  - HO frequency ($\hbar\Omega$)
- Not a variational calculation
- Convergence OK
- NN interaction insufficient to reproduce experiment



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

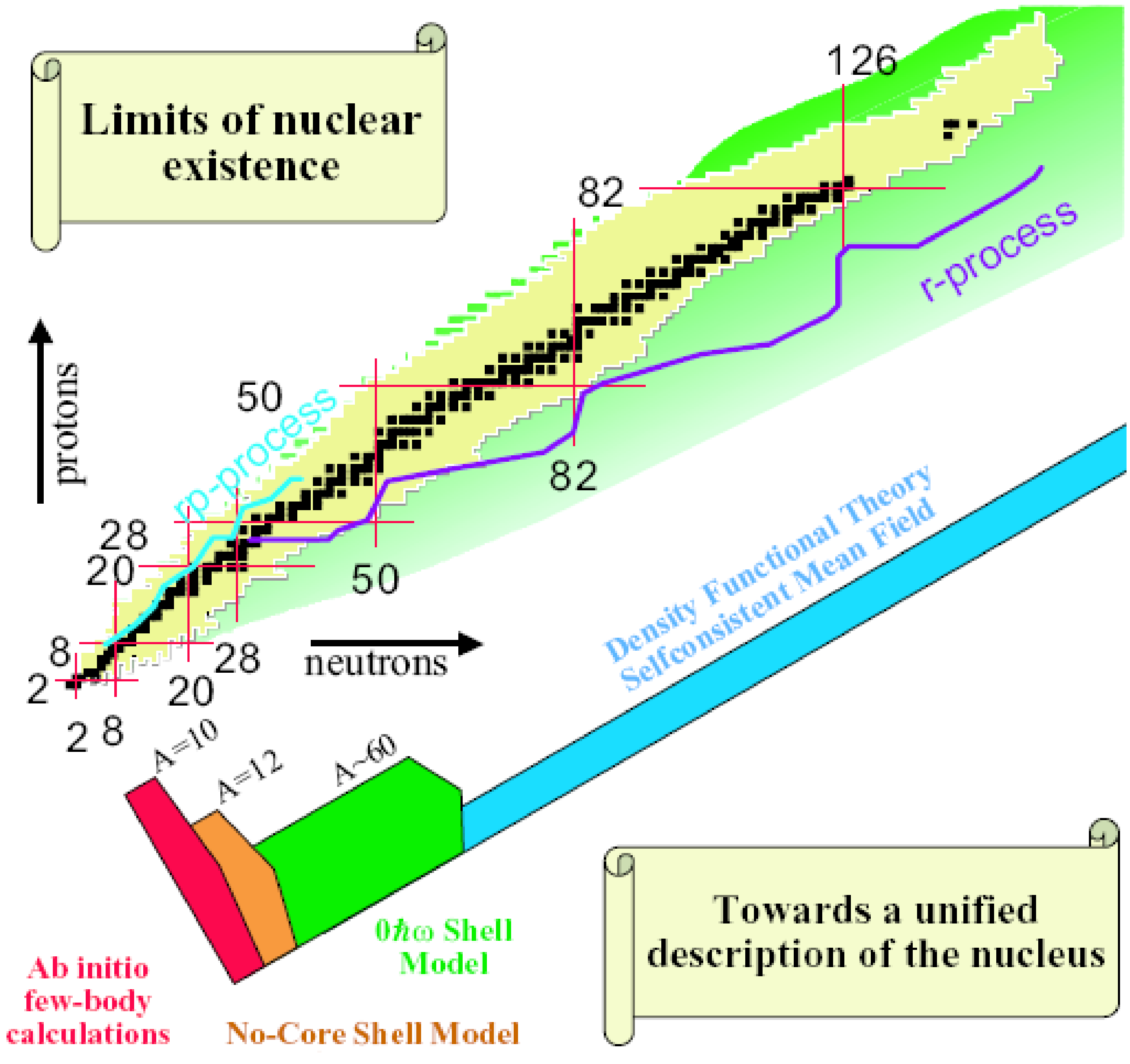


-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N_{max}
^{4}He
CD-Bonn
46.0
43.0
40.0
40.0
37.0
31.0
31.0
22.0
22.0
19.0
2-body
3-body
effective V



	N^{3}LO	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)



Limits of nuclear existence
126
82
50
28
20
8
2
2 8
20
28
50
82
protons
neutrons
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

Beyond the No Core Shell Model

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

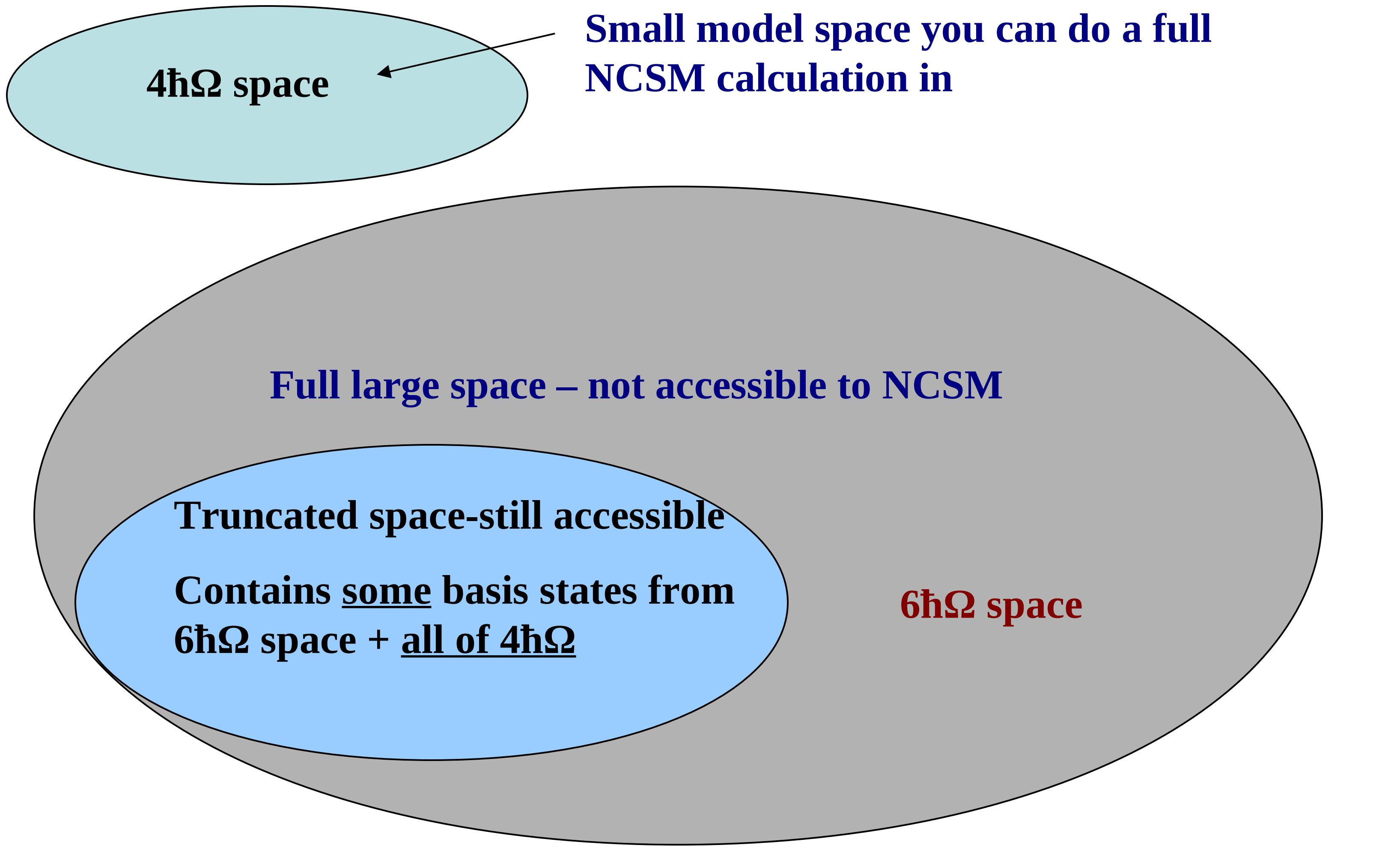
2. Importance Truncation

3. The *ab initio* Shell Model with a core

1. The NCSM in an Effective Field Theory Framework (talk by Bira van Kolck on Monday, June 6, 2001)

2. Importance Truncation

The idea of Importance Truncation



Formalism of Importance truncation.

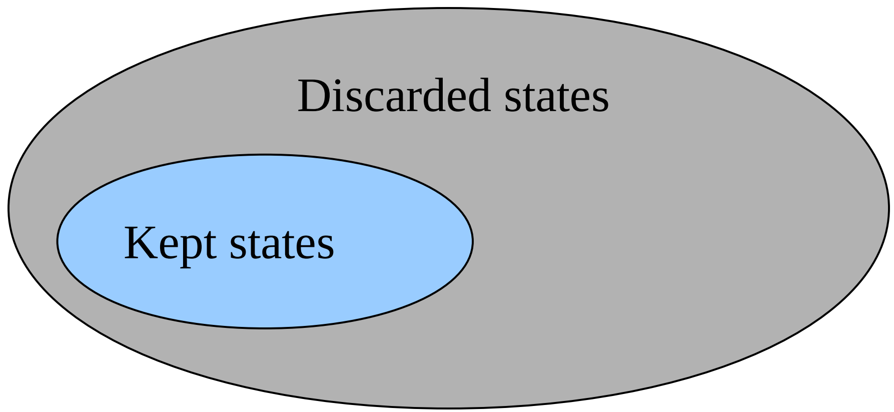
- First order multi-configurational perturbation theory gives...

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

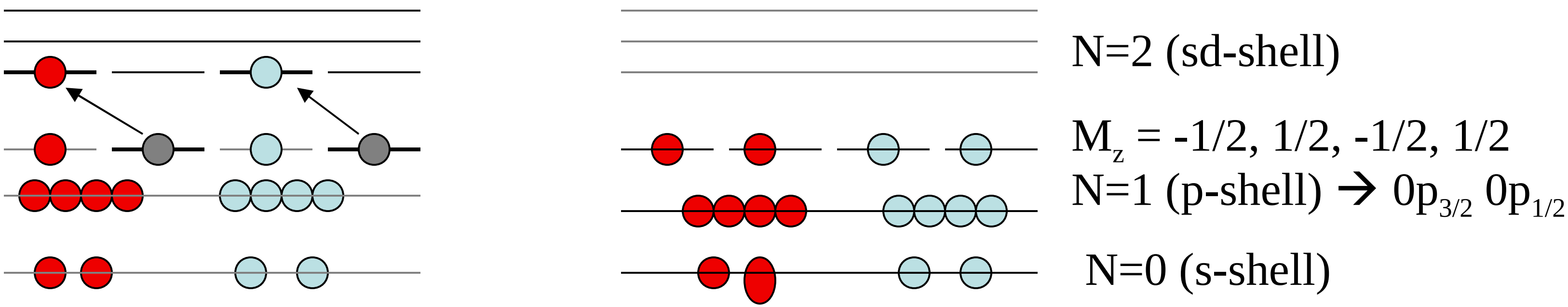
$$W = H - H_0$$

Importance truncation schematically

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



$\langle \Phi_\nu |$. $|\Psi_{ref}\rangle$



O16 – one possible configuration

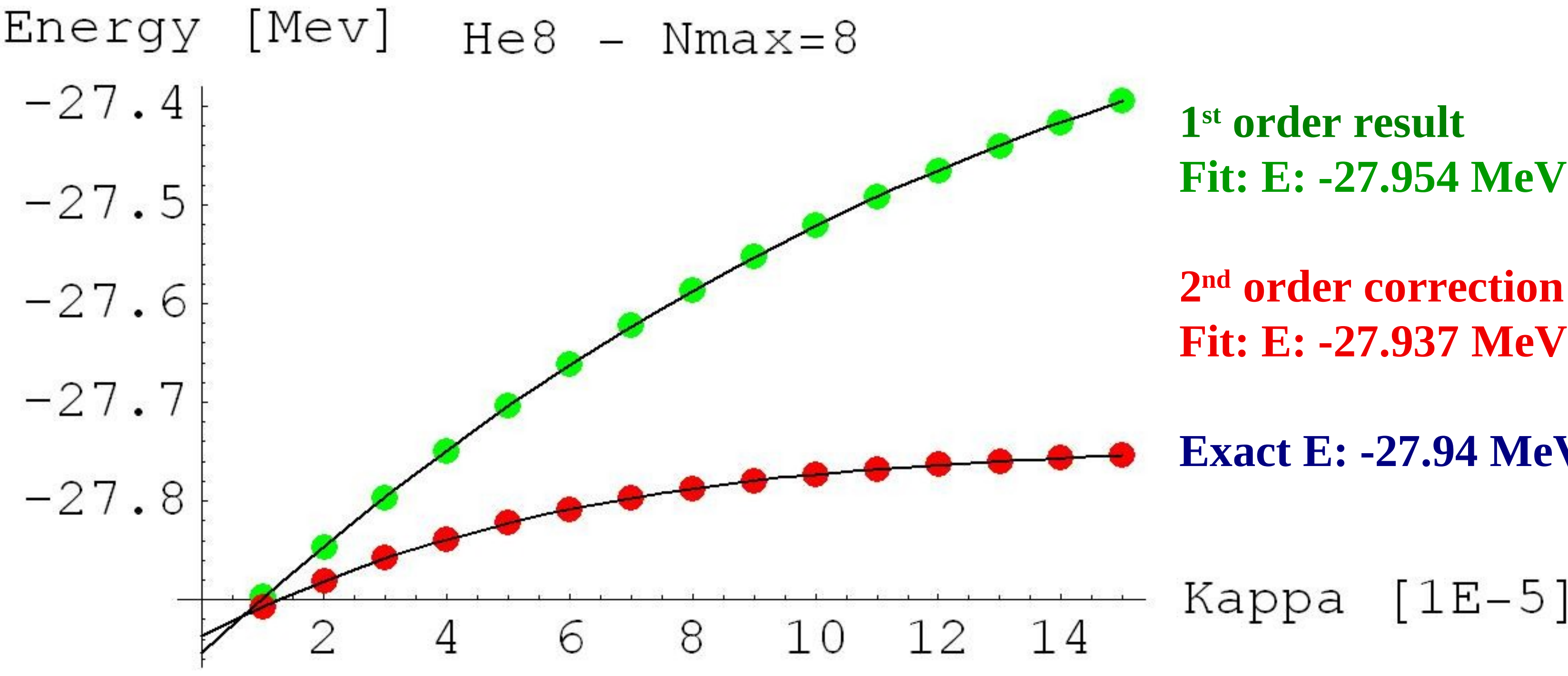
O16 - 0ħΩ configuration

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.

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

^{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 *ab initio* Shell Model with a Core

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

Ab-initio shell model with a core

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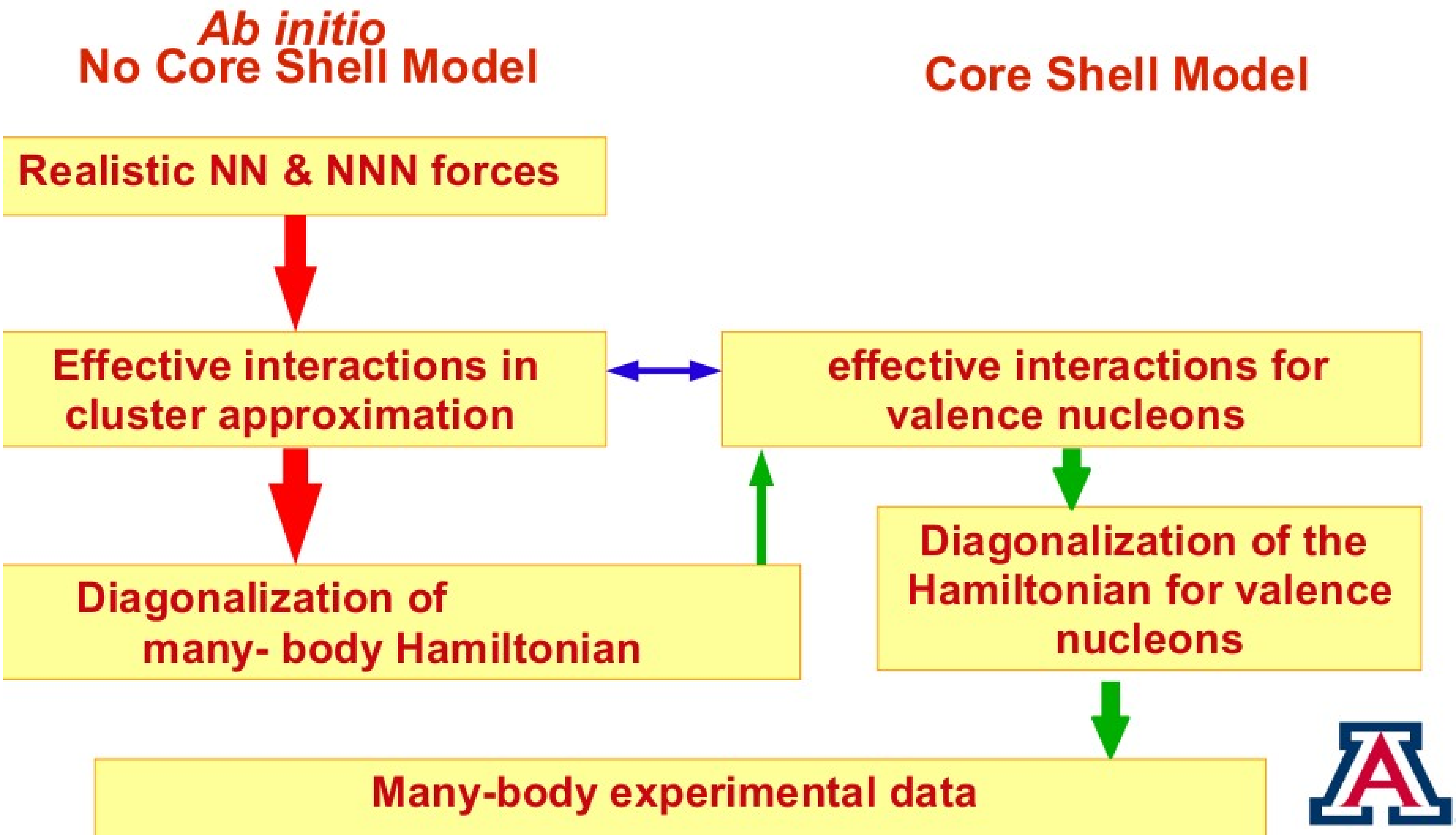
(Received 20 June 2008; published 10 October 2008)

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.

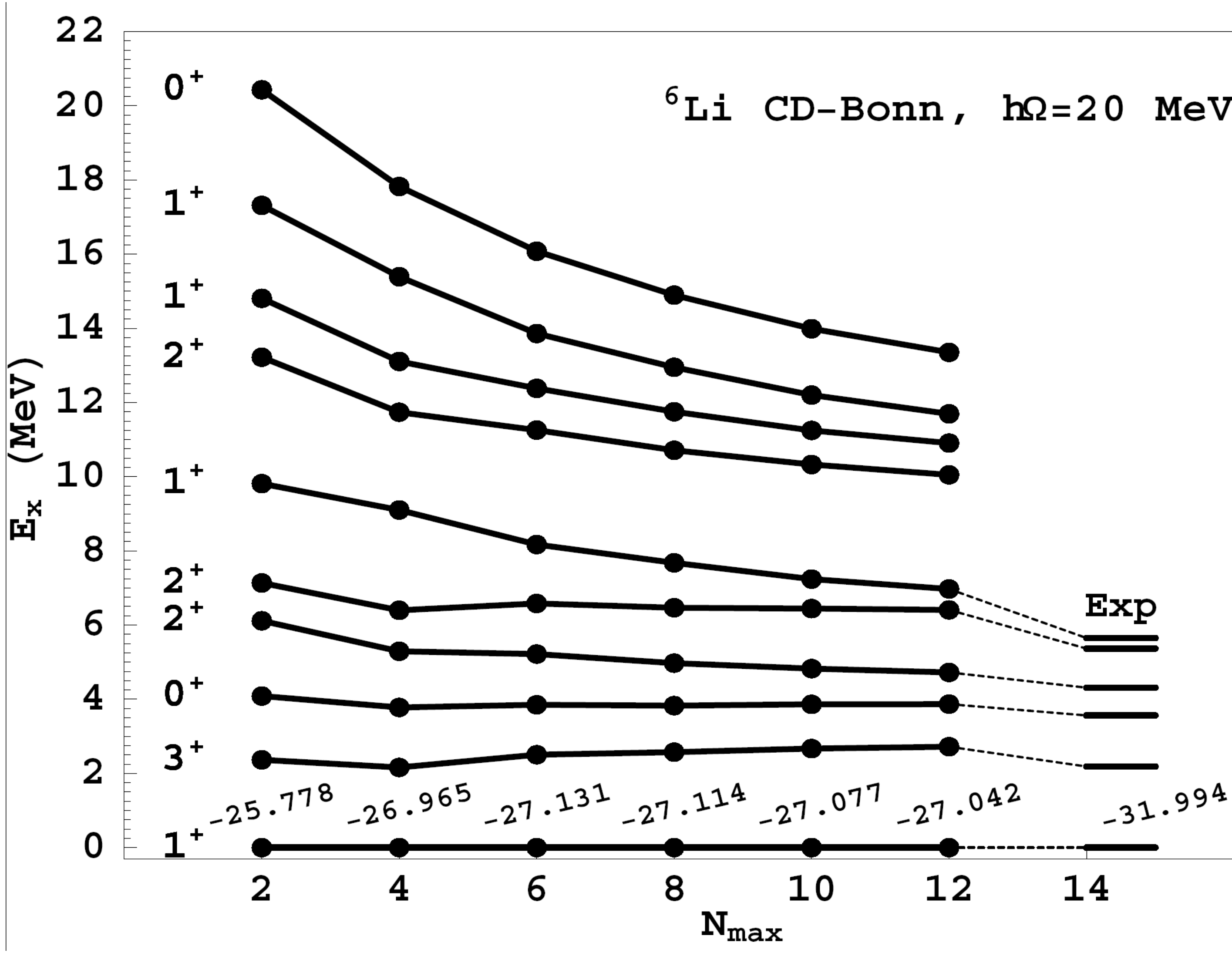
DOI: 10.1103/PhysRevC.78.044302 PACS number(s): 21.10.Hw, 21.60.Cs, 23.20.Lv, 27.20.+n

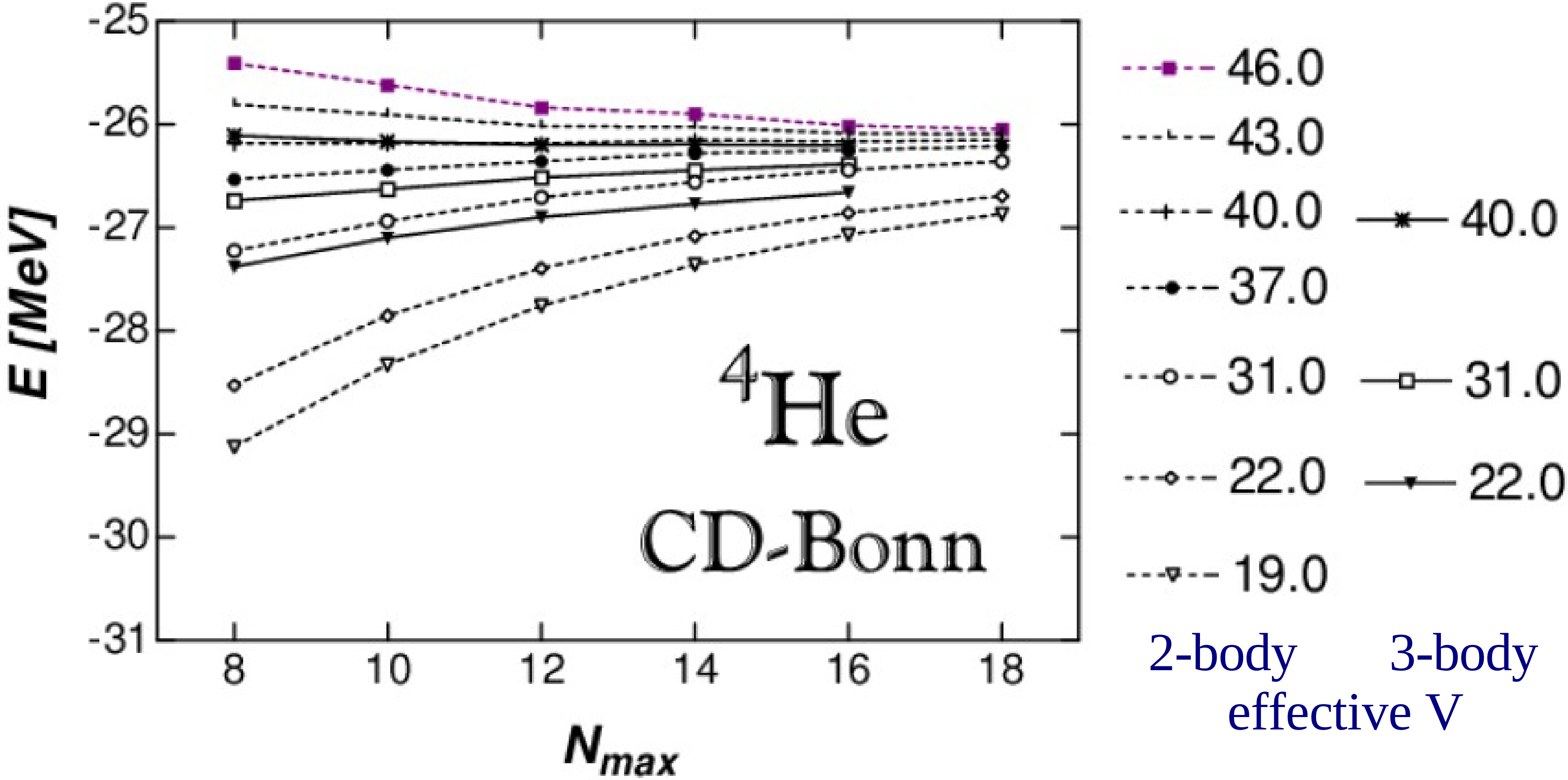
From few-body to many-body



NCSM results for ^{6}Li with CD-Bonn NN potential

Dimensions p-space: 10; N_{max}=12: 48 887 665; N_{max} = 14: 211 286 096





-25
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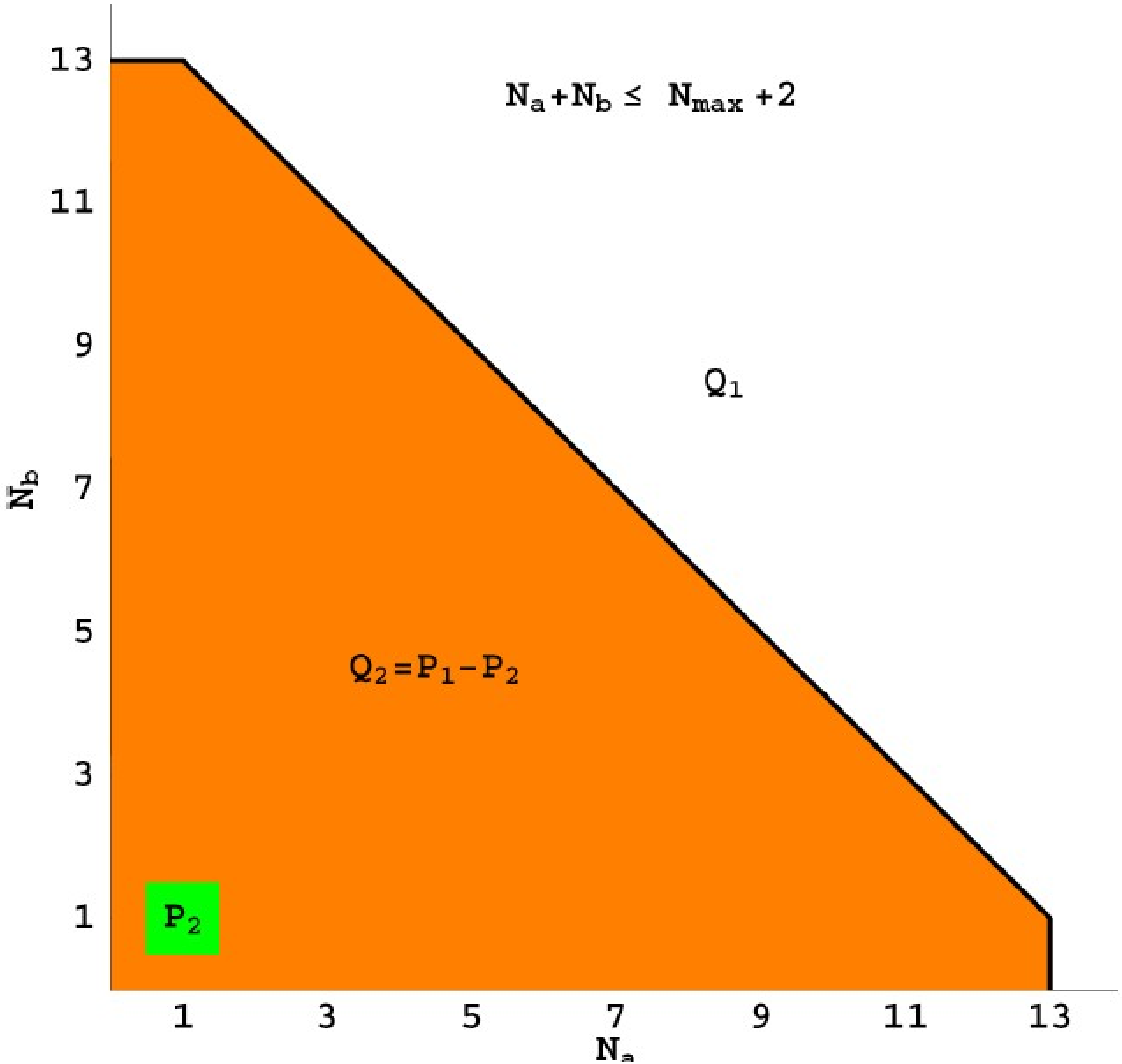
31.0
22.0
2-body
3-body
effective V



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

Effective Hamiltonian for SSM

Two ways of convergence:

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

2) For $a_1 \to A$ and fixed P_1: $H^{eff}_{A,a1} \to H_A$

$P_1 + Q_1 = P$; 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;

$$\mathcal{H}_{A,a_1}^{0,N_{\max}} = \sum_{k}^{a_v} V_k^{A,A_c+k}$$

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 $\varepsilon_{p1/2}$ = 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

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

Need NCSM results in N_{max} space for

^{4}He

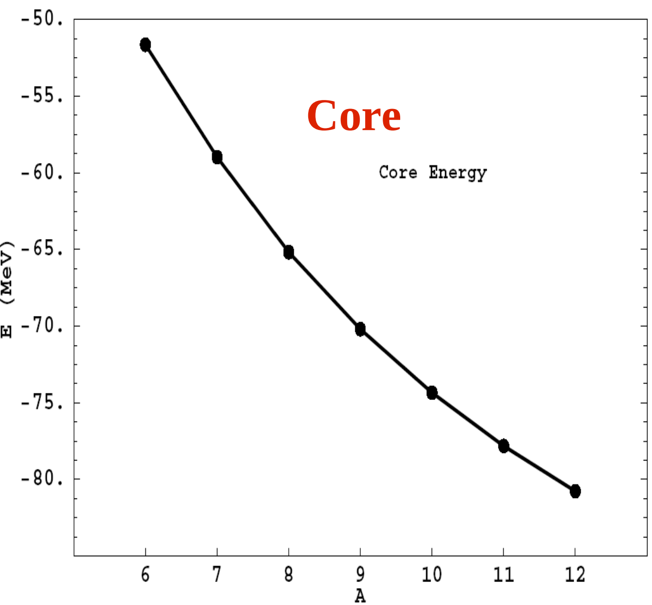
^{5}He ^{5}Li

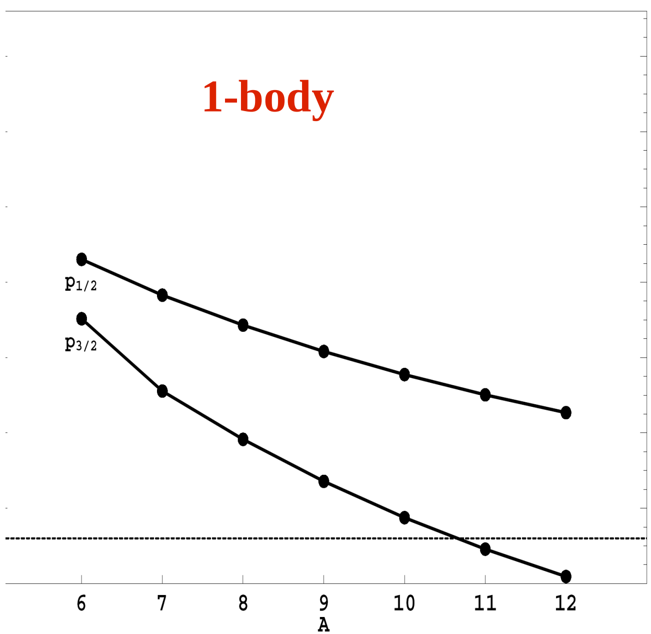
^{6}He ^{6}Li ^{6}Be

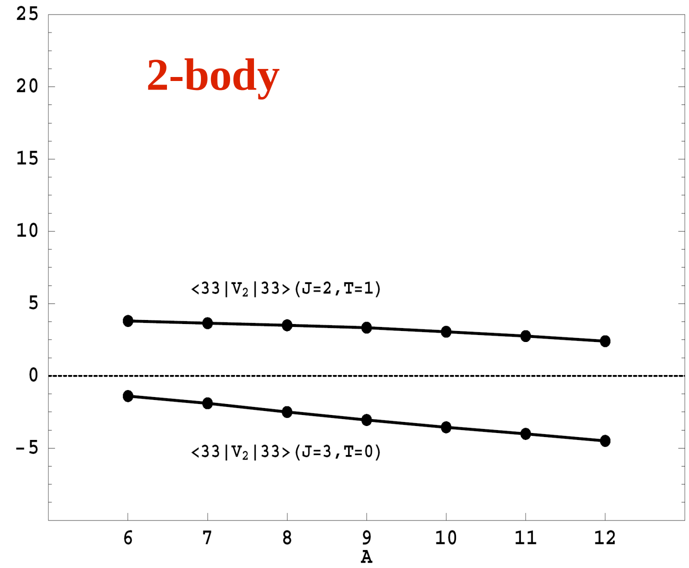
$N_{max} = 6$

With effective interaction for A !!!

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







2-body Valence Cluster approximation for A=7

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

Need NCSM results in N_{max} space for

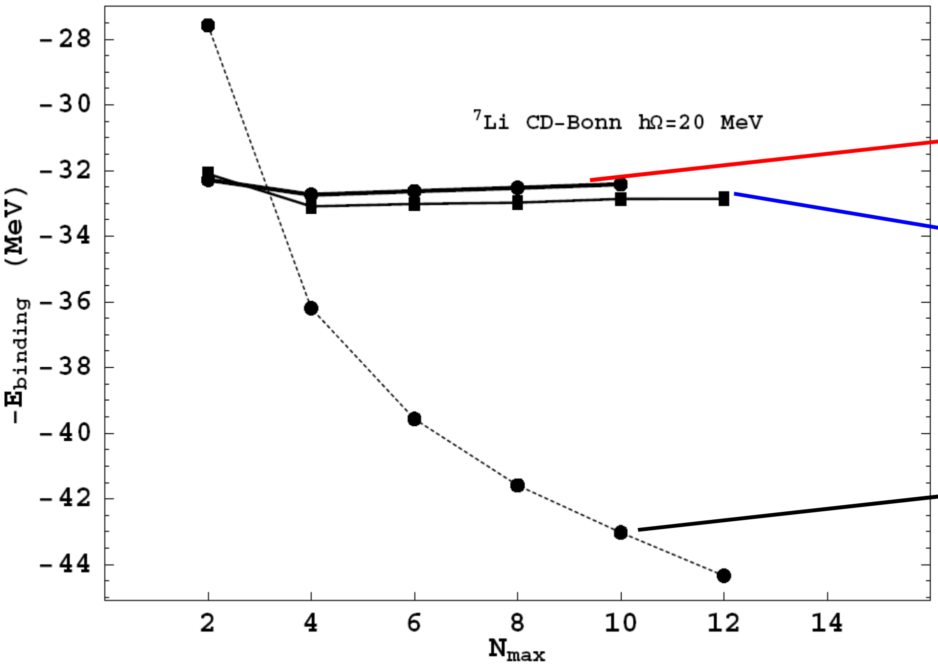
^4He

^5He ^5Li

^6He ^6Li ^6Be

With effective interaction for A=7 !!!

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



Exact NCSM

SSM with A-dependent core

SSM with inert core

3-body Valence Cluster approximation for A>6

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

Need NCSM results in N_{max} space for

^{4}He | **^{5}He ^{5}Li** | **^{6}He ^{6}Li ^{6}Be** | **^{7}He ^{7}Li ^{7}B ^{7}Be**

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

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

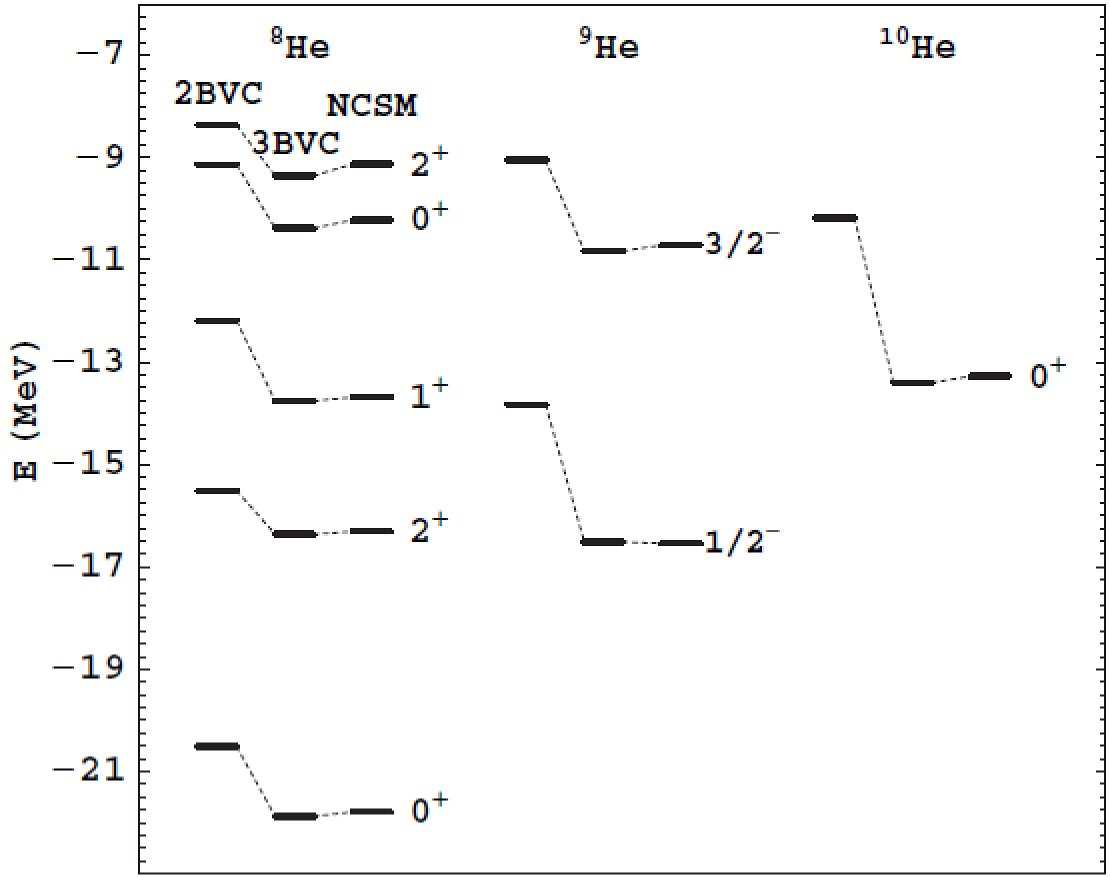


FIG. 9. Comparison of spectra for ^{8}He, ^{9}He, and ^{10}He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$ and $\hbar\Omega = 20$ MeV using the CD-Bonn interaction.

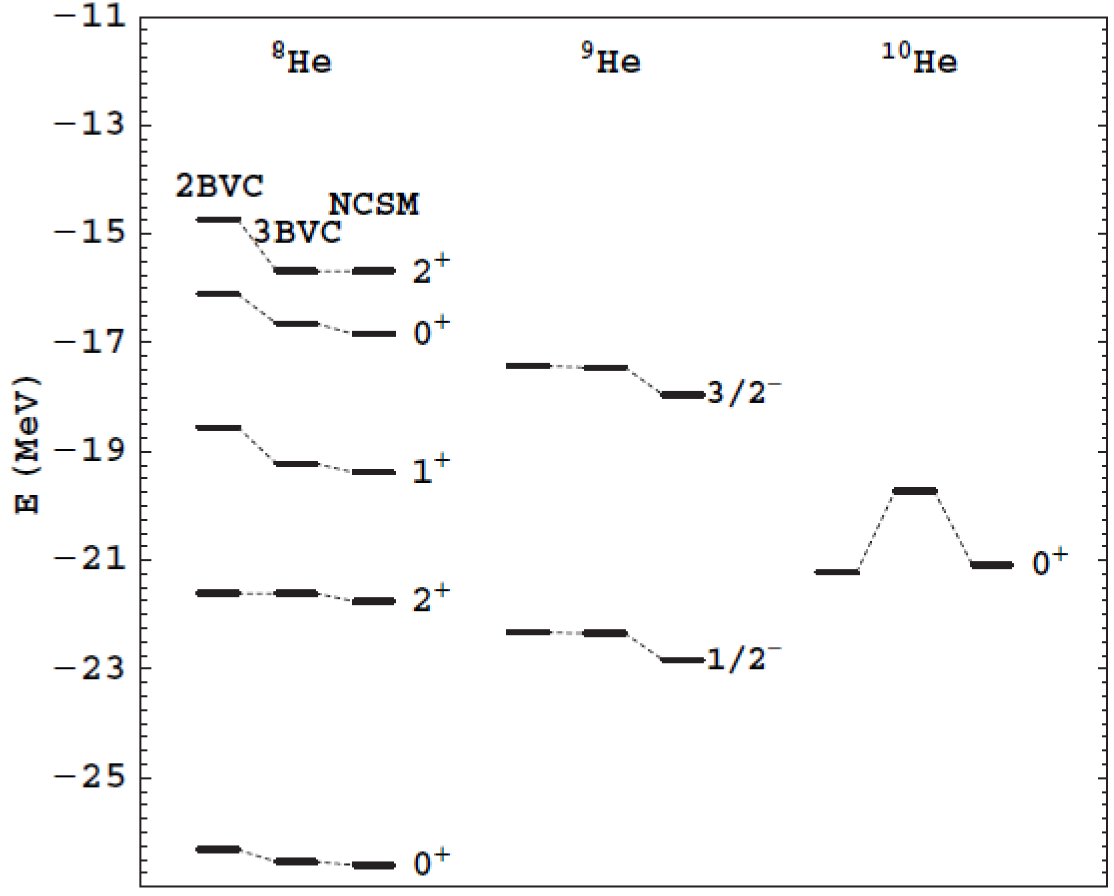
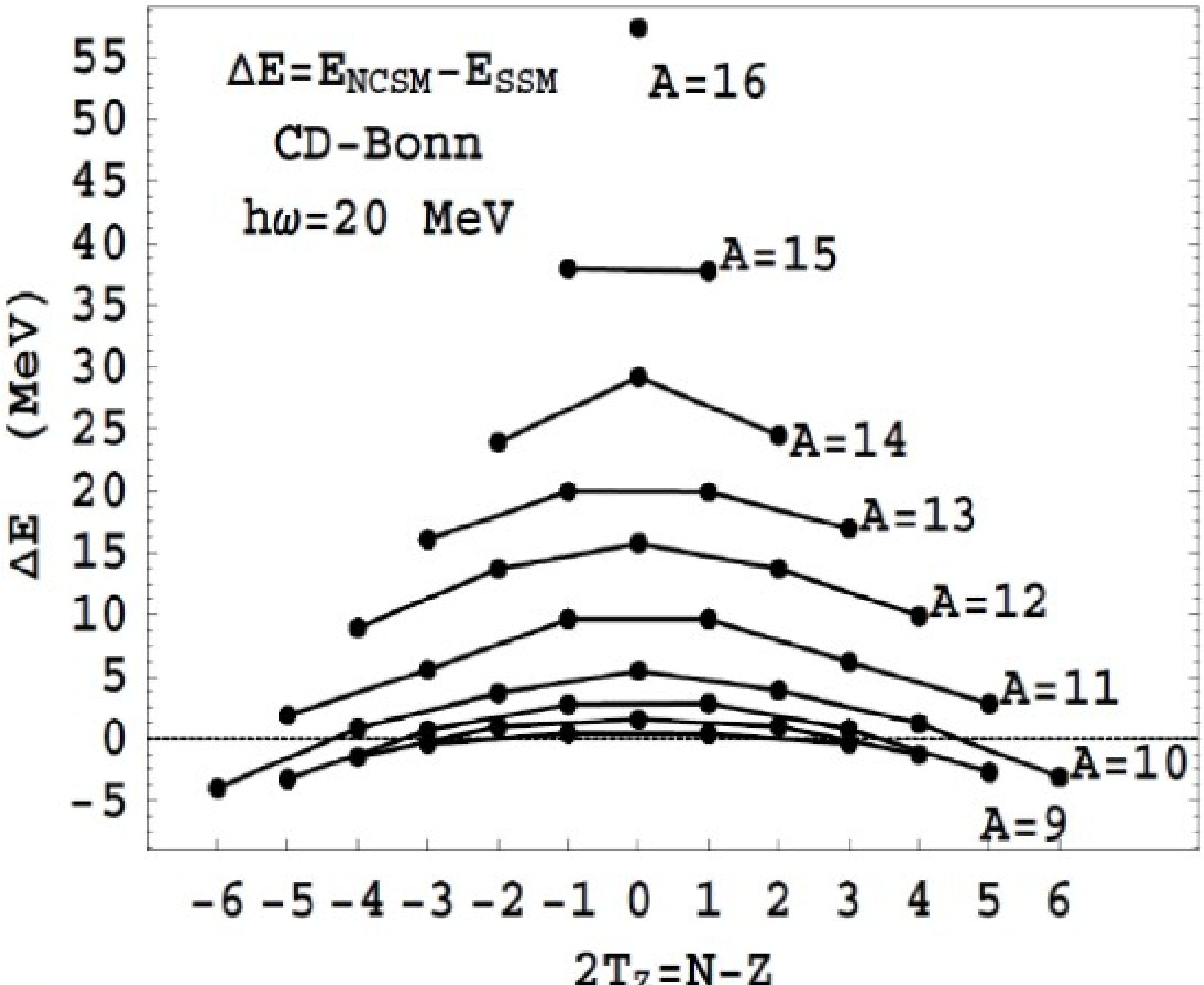


FIG. 8. Comparison of spectra for ^{8}He, ^{9}He, and ^{10}He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$ and $\hbar\Omega = 14$ MeV using the INOY interaction.



ΔE=E_NCSM-E_SSM
CD-Bonn
hω=20 MeV
A=16
A=15
A=14
A=13
A=12
A=11
A=10
A=9
ΔE (MeV)
55
50
45
40
35
30
25
20
15
10
5
0
-5
-6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6
2T_Z=N-Z

PHYSICAL REVIEW C **80**, 024315 (2009)

Effective operators from exact many-body renormalization

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(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.

DOI: 10.1103/PhysRevC.80.024315 PACS number(s): 27.20.+n, 21.10.Hw, 21.60.Cs, 23.20.Lv

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

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

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

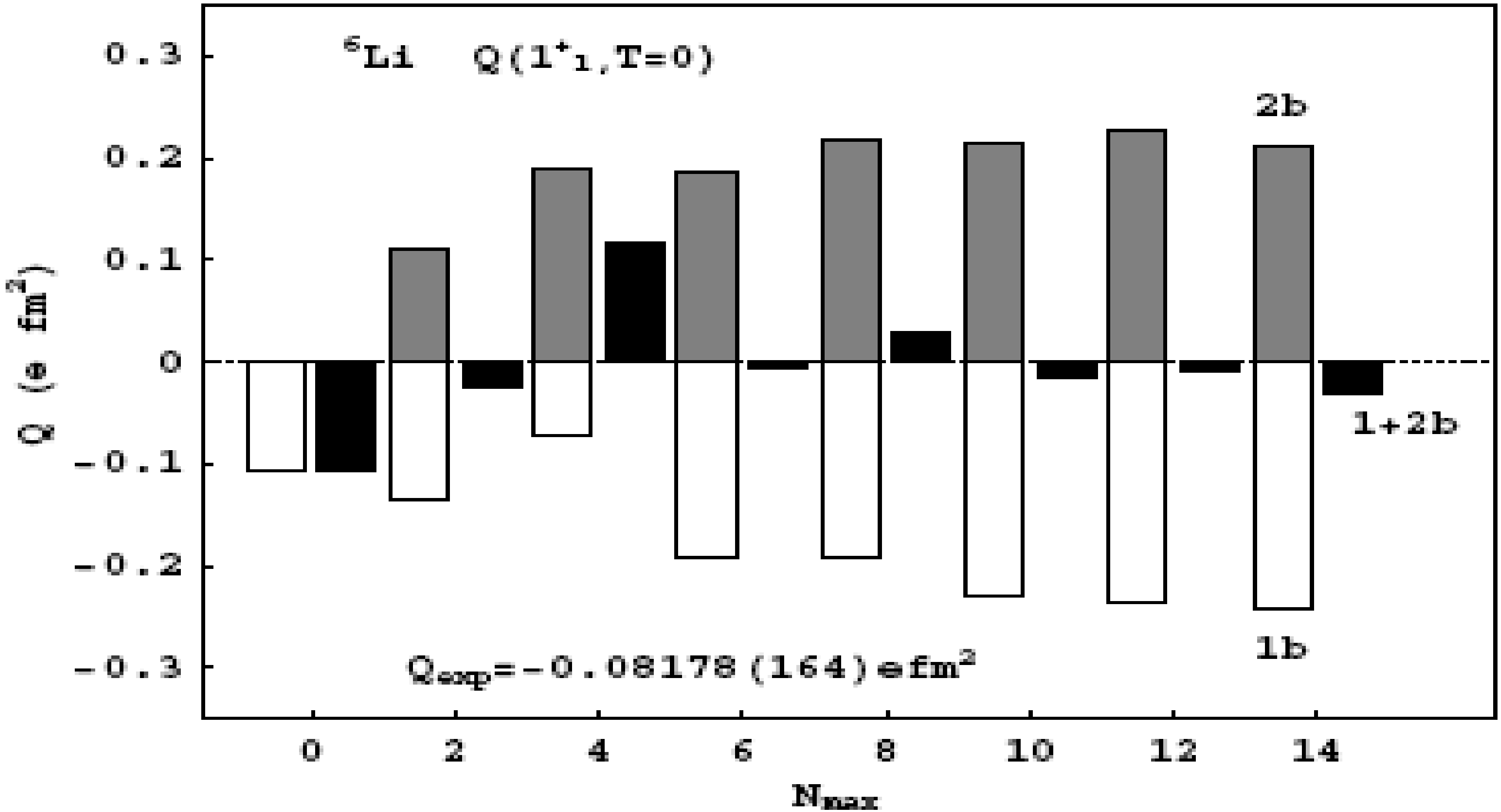

FIG. 6: The quadrupole moment of the ground state for ^{6}Li ($1^+(T = 0)$) is shown in terms of one- and two-body contributions as a function of increasing model space size.

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^{eff}

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

OUTLOOK

1. Extend the *ab initio* Shell Model with a core approach to nuclei in the sd-shell (and later to pf-shell nuclei).

2. This will require converged results for nuclei with A= 16, 17, 18 and 19.

3. The Importance Truncation method will be used to obtain the converged results for these sd-shell nuclei.

4. SSM calculations will then be performed using the core and 1-, 2- and 3-body terms determined by the *ab initio* Shell Model with a core approach.

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2-body Valence Cluster approximation for A=7

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