Ab Initio Shell Model with a Core: Extending the NCSM to Heavier Nuclei

Bruce R. Barrett
University of Arizona,
Tucson

THE UNIVERSITY OF ARIZONA.
Arizona's First University.

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MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many-body theory

$$H\,\Psi = E\,\Psi$$

We cannot, in general, solve the full problem in the complete Hilbert space, so we must truncate to a finite model space

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

Some current shell-model references

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

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

3. 3. I. Talmi, “Fifty Years of the Shell Model-The Quest for the

4. Effective Interaction,” *Advances in Nuclear Physics*, Vol. **27**,

5. ed. J. W. Negele and E. Vogt (Plenum, NY, 2003)

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

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., nucl-th arXiv: 0904.0463

From few-body to many-body

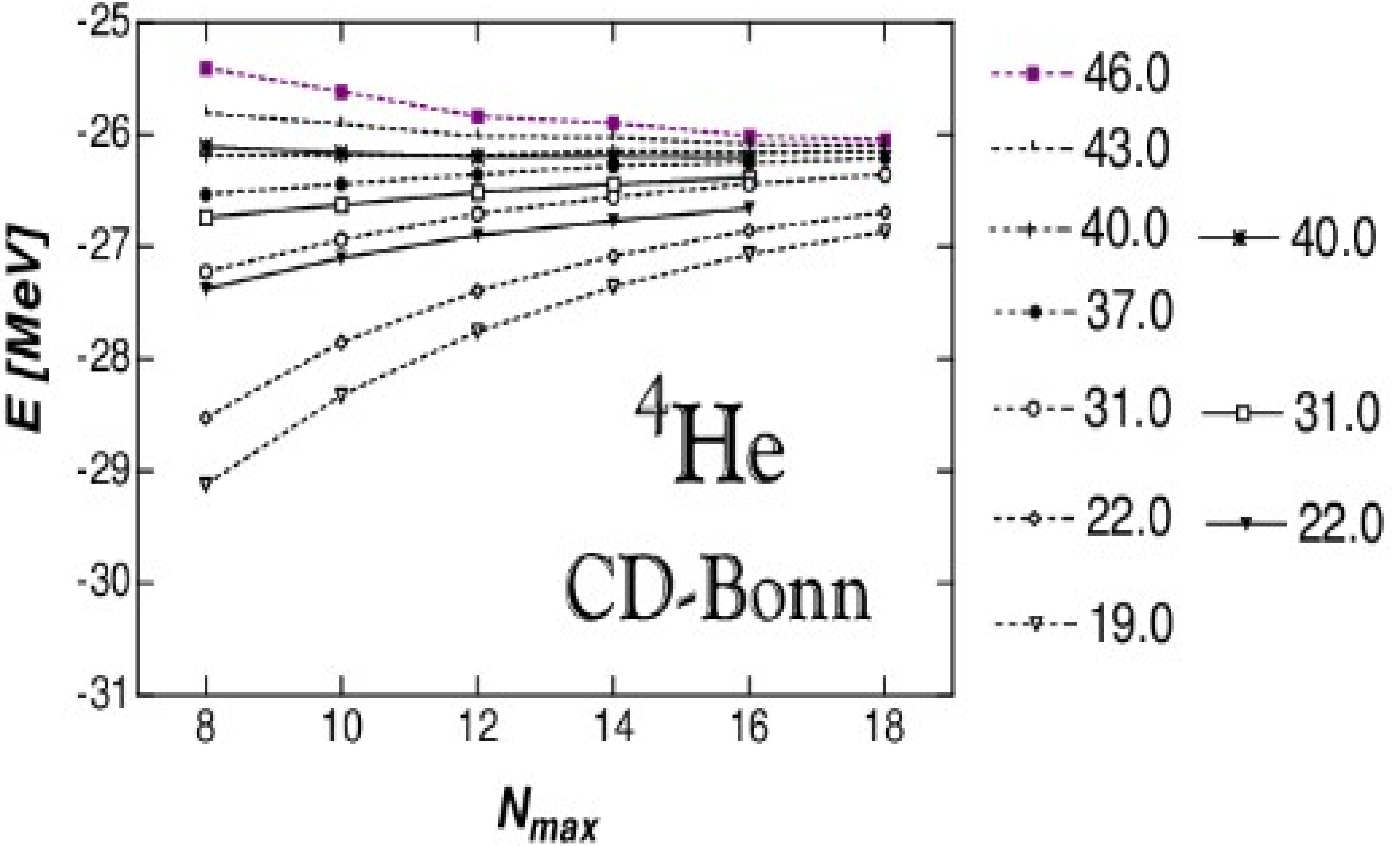
Ab initio
No Core Shell Model

Realistic NN & NNN forces

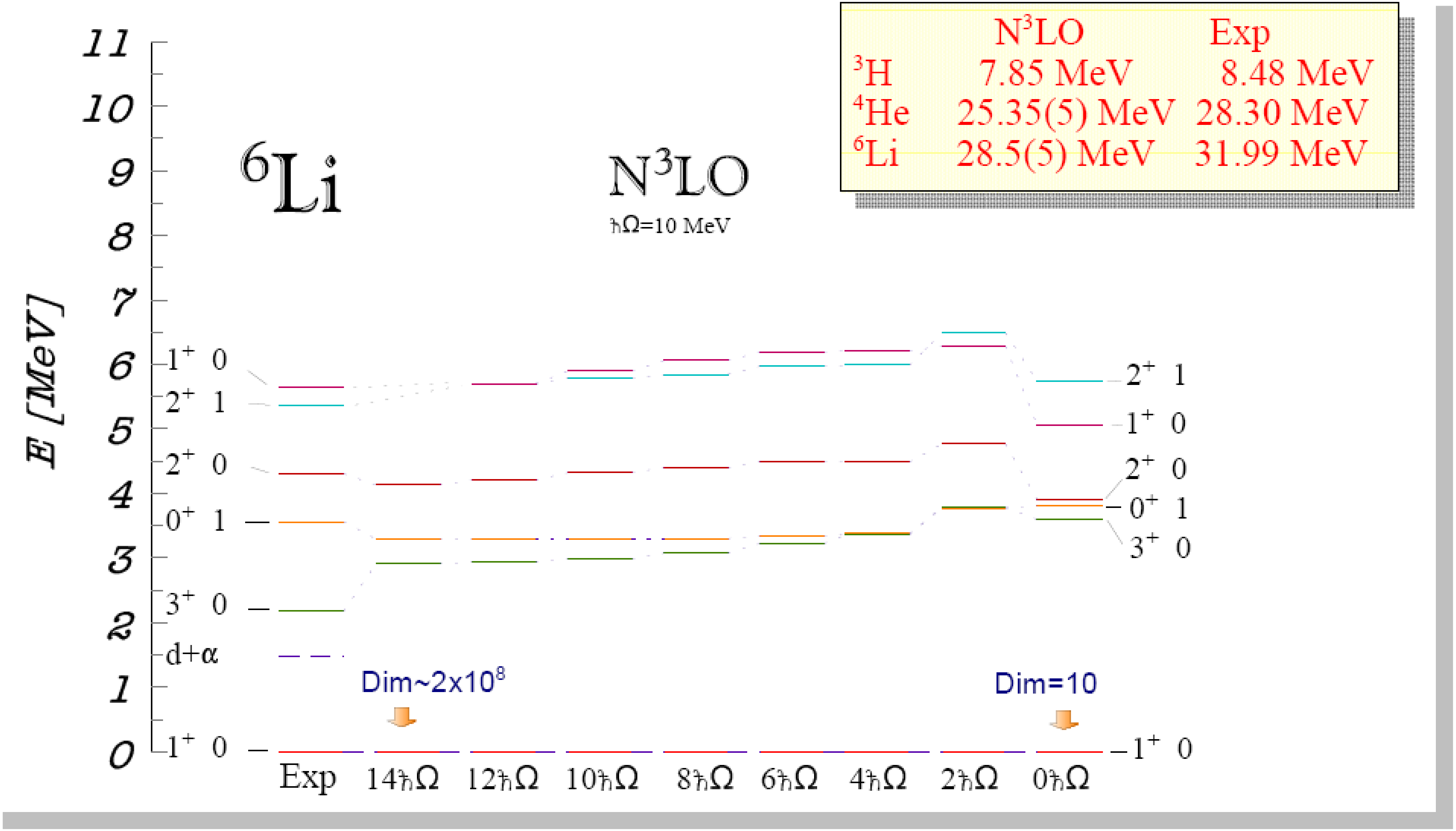
Effective interactions in cluster approximation

Diagonalization of many- body Hamiltonian

Many-body experimental data



-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



P. Navrátil and E. Caurier, Phys. Rev. C **6 9**, 014311 (2004)

From few-body to many-body

Ab initio No Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation

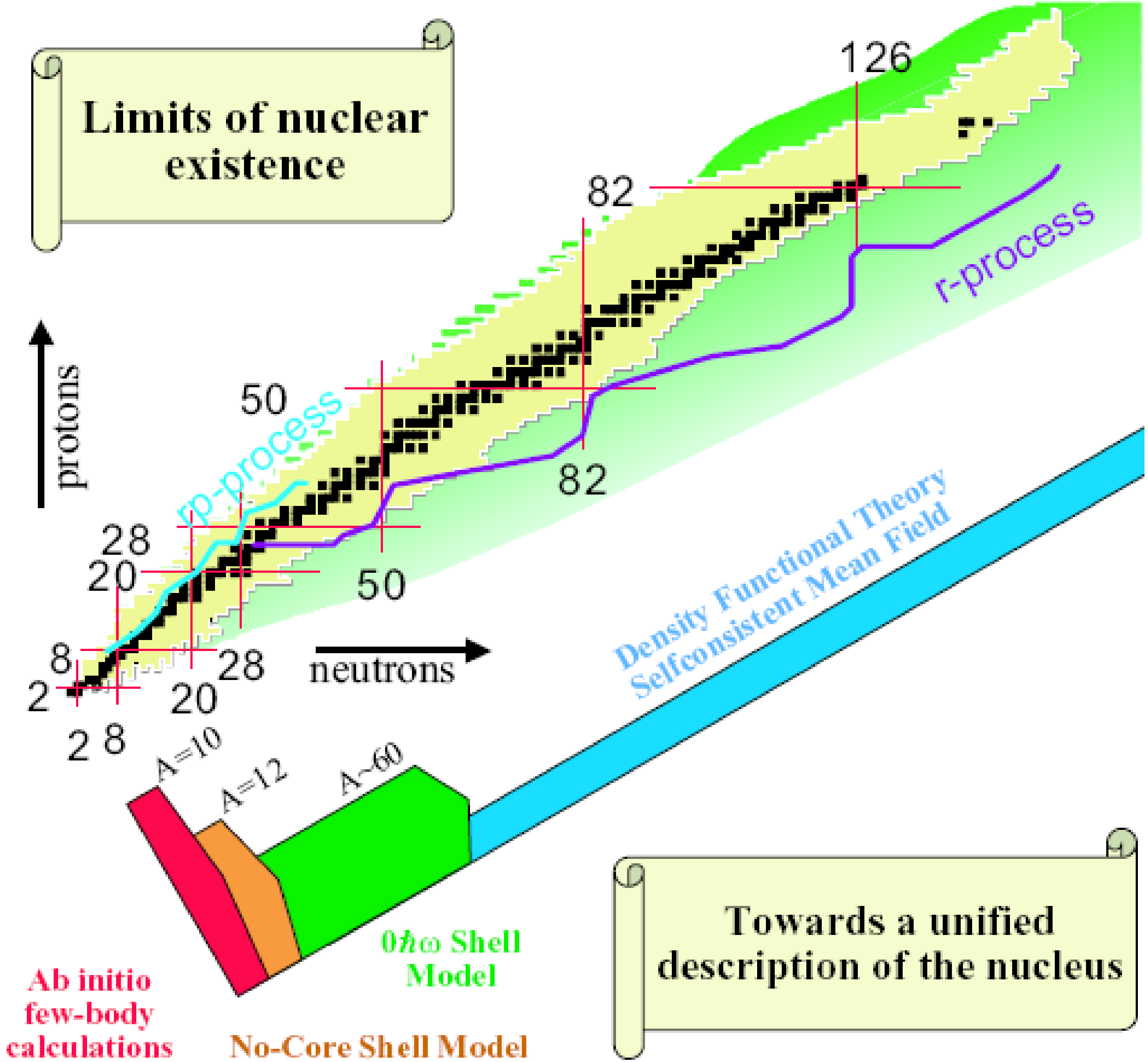
Diagonalization of many- body Hamiltonian

Core Shell Model

Phenomenological effective interactions

Diagonalization of the Hamiltonian for valence nucleons

Many-body experimental data


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

From few-body to many-body

Ab initio
No Core Shell Model

Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation

effective interactions for valence nucleons

Diagonalization of many- body Hamiltonian

Diagonalization of the Hamiltonian for valence nucleons

Many-body experimental data

No Core Shell Model

Starting Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A} V_{NN}(\vec{r}_i - \vec{r}_j) \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

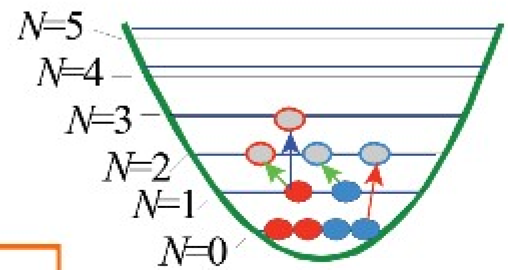
Realistic NN and NNN potentials

Coordinate space – Argonne V18, AV18',
Momentum space – CD-Bonn, chiral N^3LO,

NNN Tucson - Melbourne
NNN chiral N^2LO

Binding center-of-mass
HO potential (Lipkin 1958)

$$\frac{1}{2} A m \Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m \Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$



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

$\langle HO|V_{NN}(\quad,A)|HO\rangle$

Cluster Expansion:
Two-body cluster approximation

$$H_2^{\Omega} = \sum_{i=1}^{2} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m \Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{2} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

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;

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

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

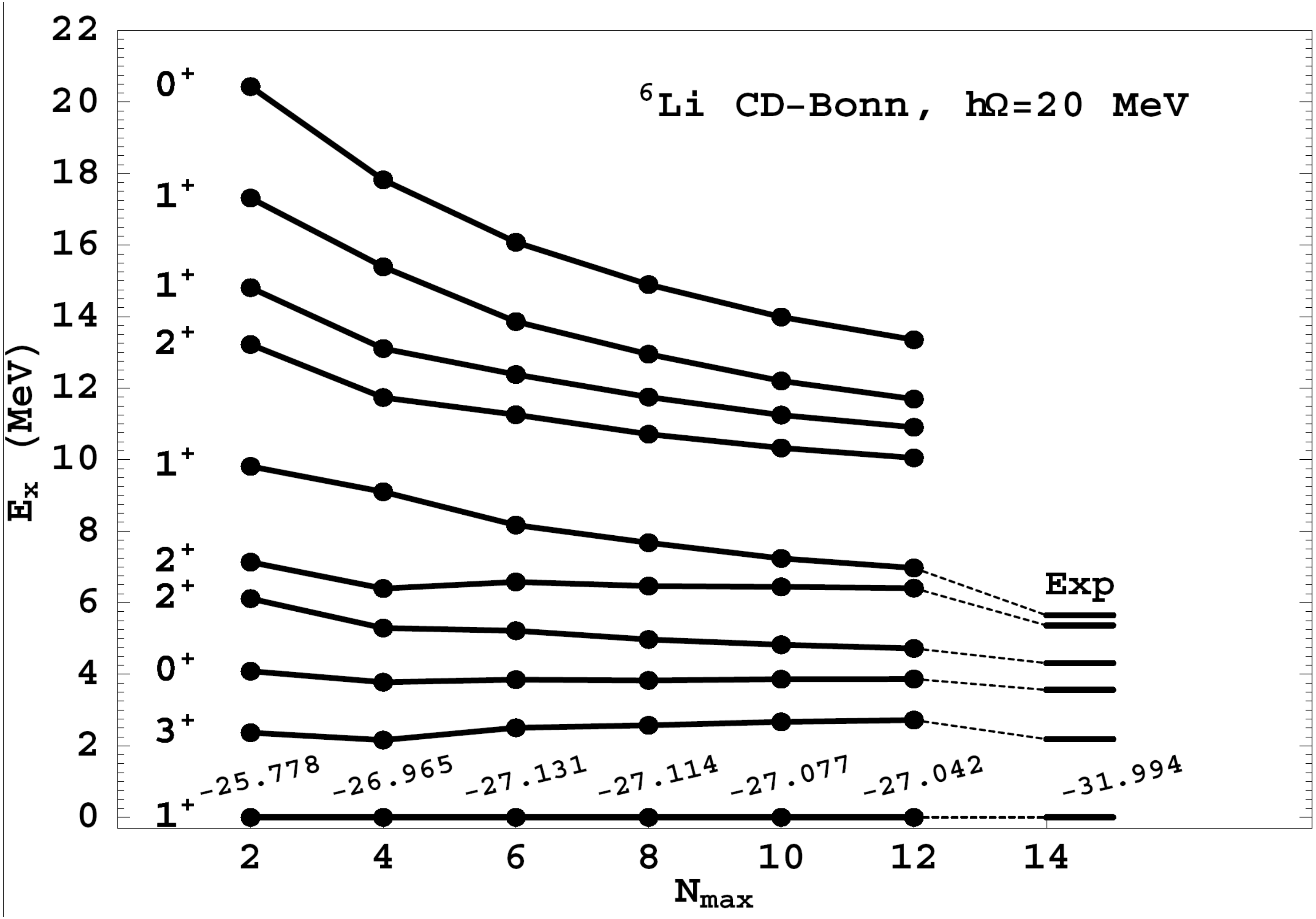
Two ways of convergence:

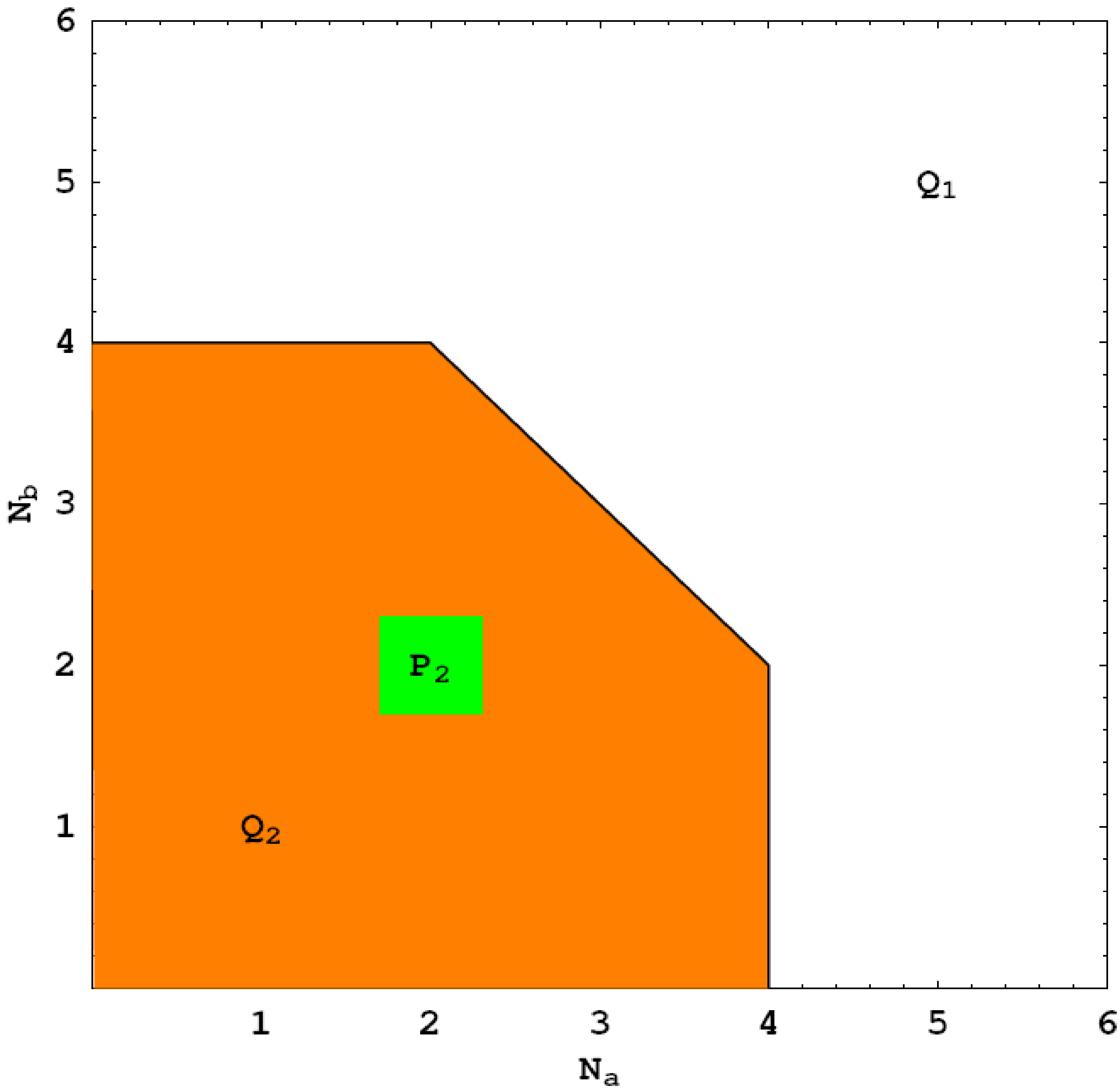
1) For P → 1 and fixed a: $H^{eff}_{A,a=2} \rightarrow H_A$

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

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





Q1
Q2
P2
Na
Nb
1
2
3
4
5
6

Effective Hamiltonian for SSM

Two ways of convergence:

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

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

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

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

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;

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

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 !!! $H^{N_{\max},\Omega,\text{eff}}_{A=6,2}$

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

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

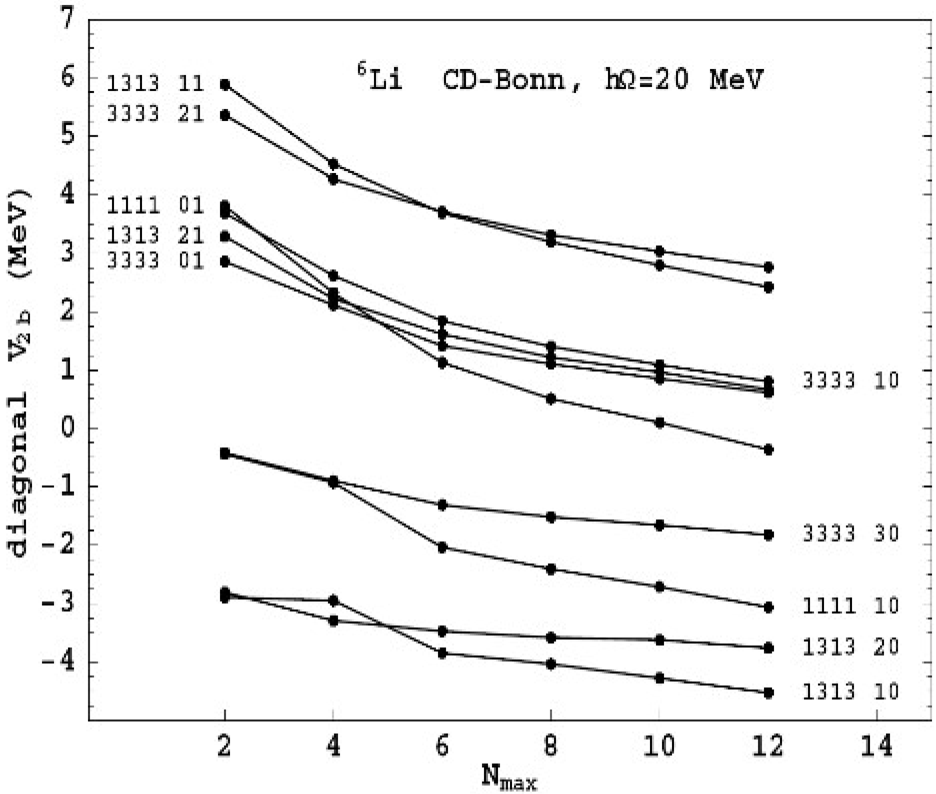
TBMEs

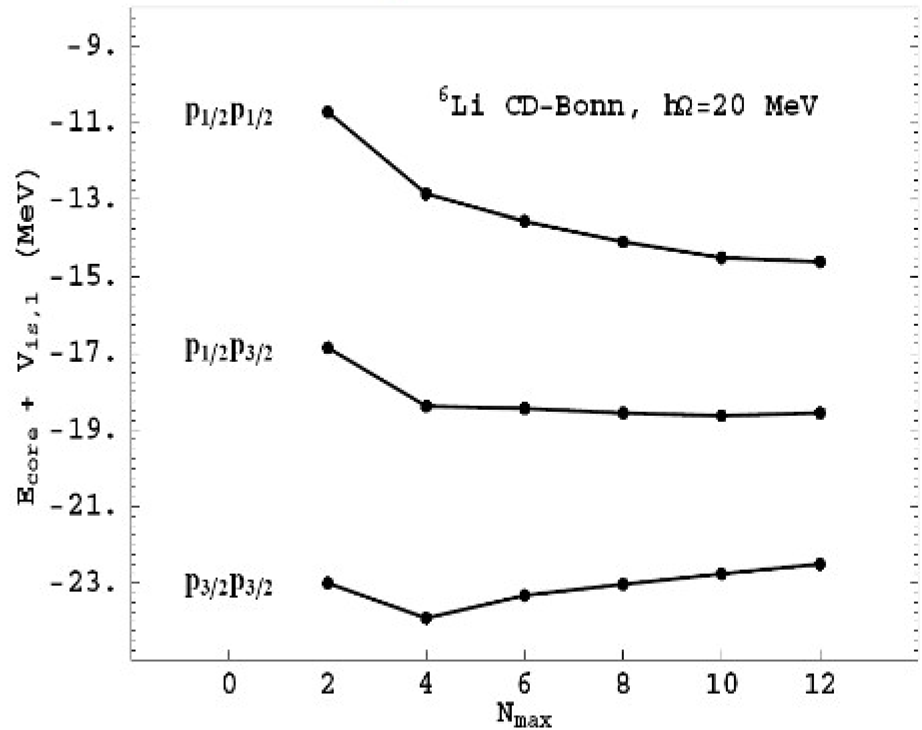
$\langle p_{3/2}p_{3/2}|V_2^{6,6}|p_{3/2}p_{3/2}\rangle_{J=3,T=0}$ = -1.825 MeV

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

2-body Valence Cluster approximation for A>6

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





2-body Valence Cluster approximation for A=6

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

Need NCSM results in N_{max} space for

^{4}He

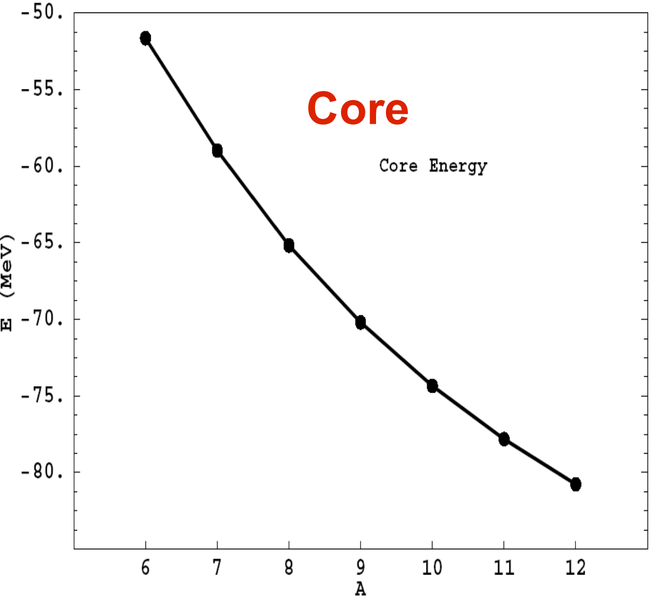
^{5}He ^{5}Li

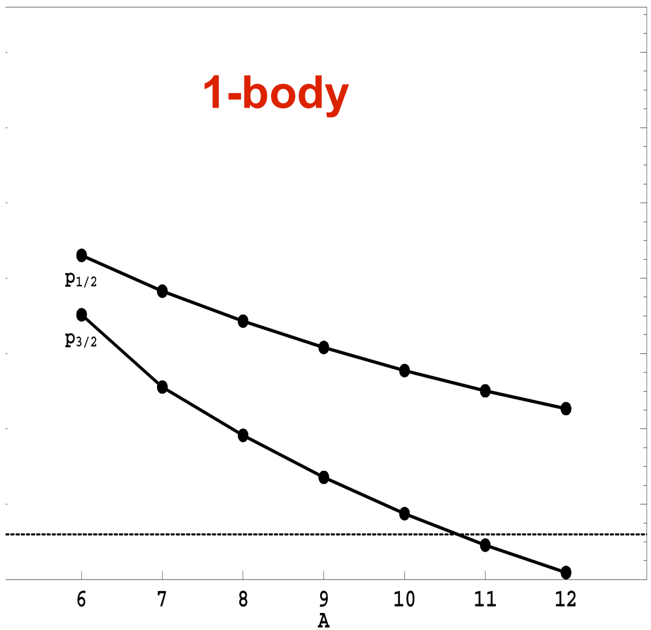
^{6}He ^{6}Li ^{6}Be

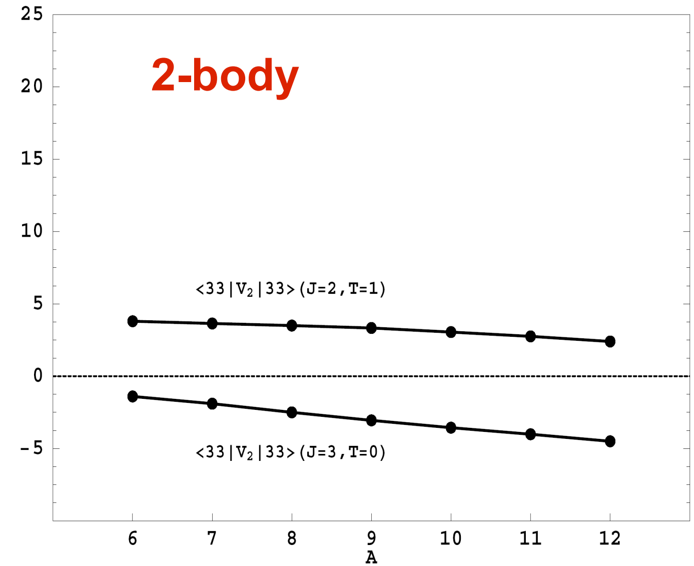
$N_{max} = 6$

With effective interaction for A !!!

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







2-body Valence Cluster approximation for A=7

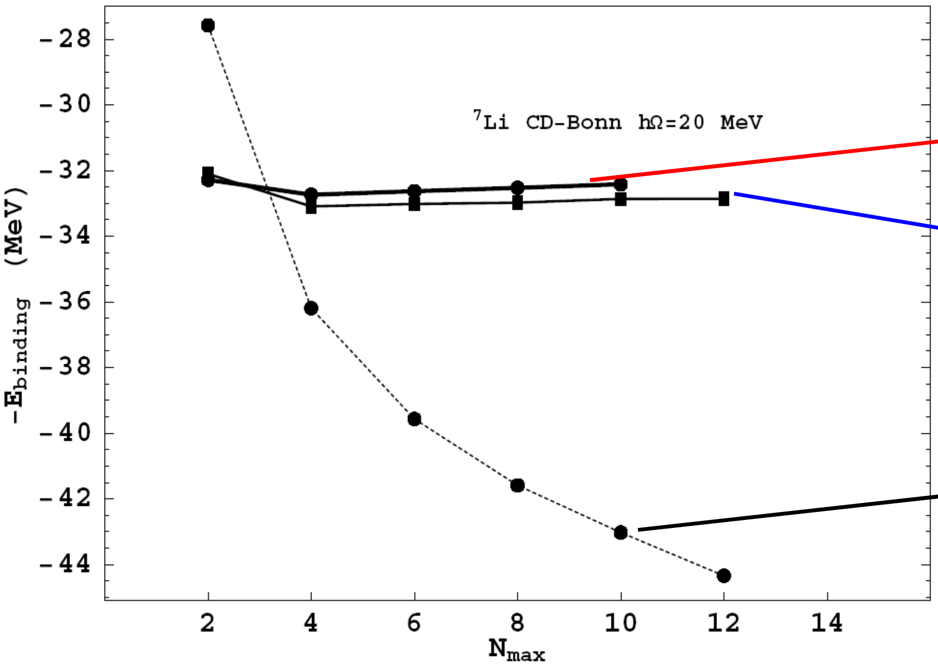
$$\mathcal{H}_{A,a_1=6}^{0,N_{\max}} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$

Need NCSM results in N_{max} space for

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

With effective interaction for A=7 !!!

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



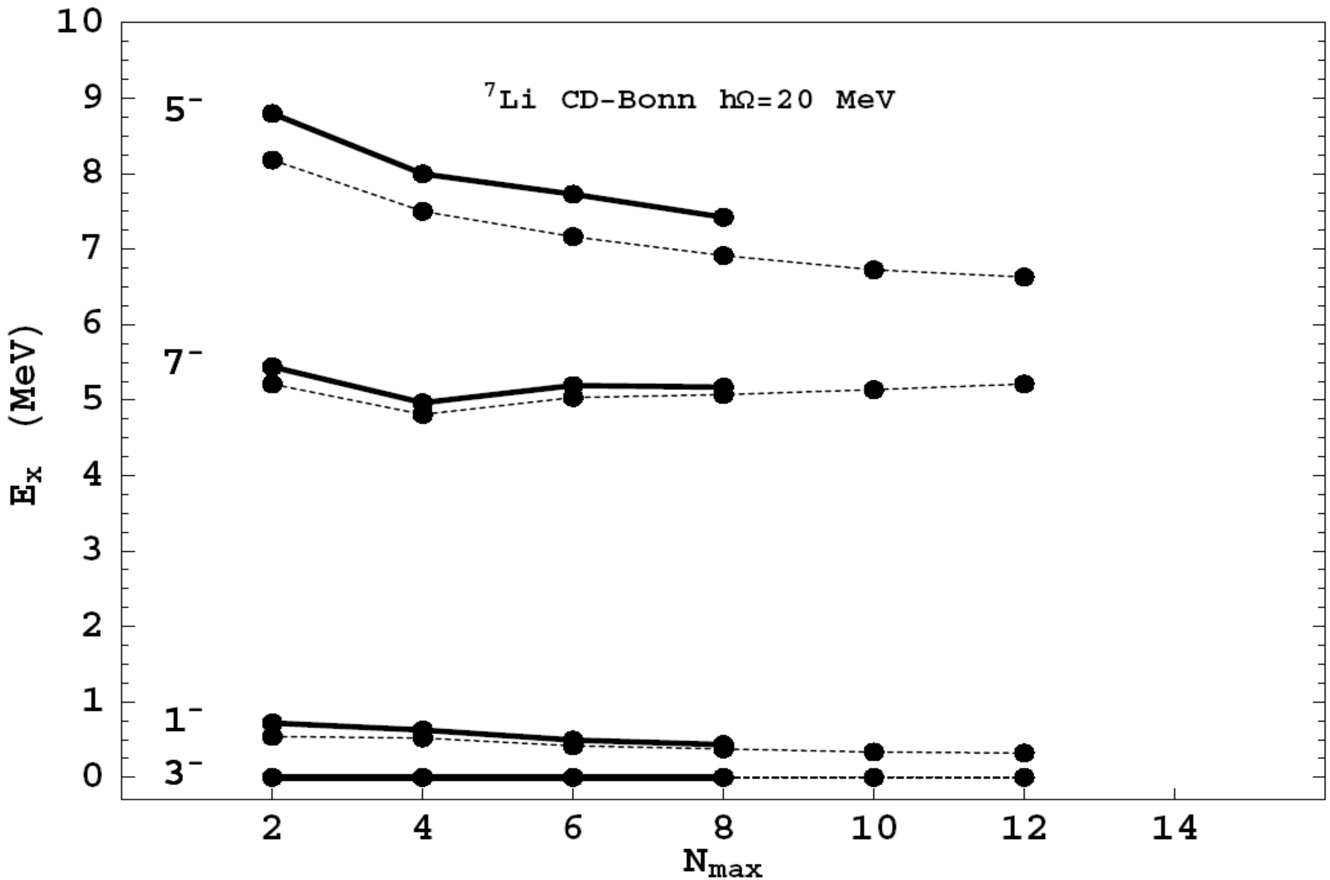
Exact NCSM

SSM with A-dependent core

SSM with inert core

2-body Valence Cluster approximation for A=7

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



3-body Valence Cluster approximation for A>6

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

Need NCSM results in N_{max} space for

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

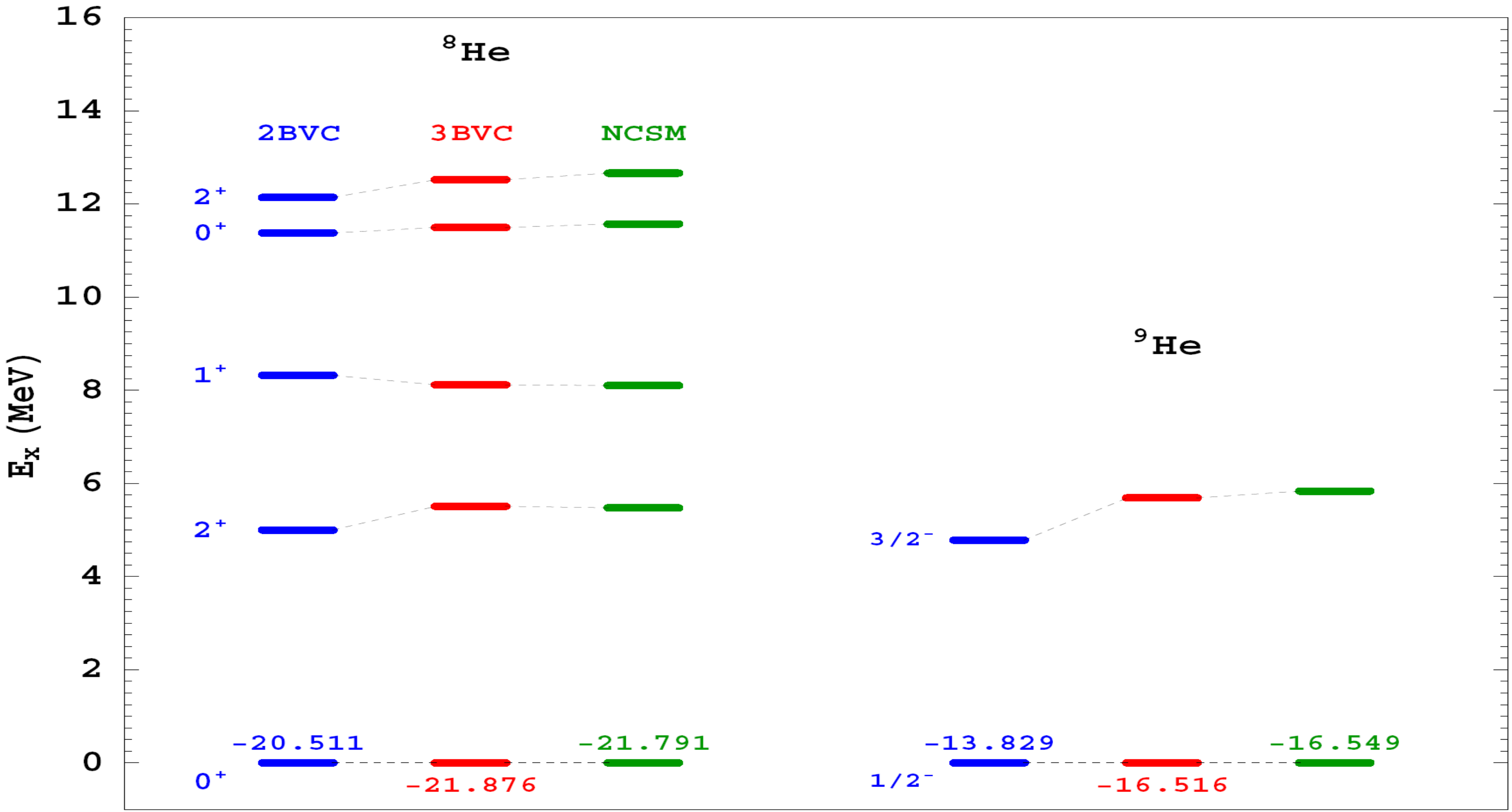
With effective interaction for A !!!

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

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

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

3-body Valence Cluster approximation for A>6



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

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:

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

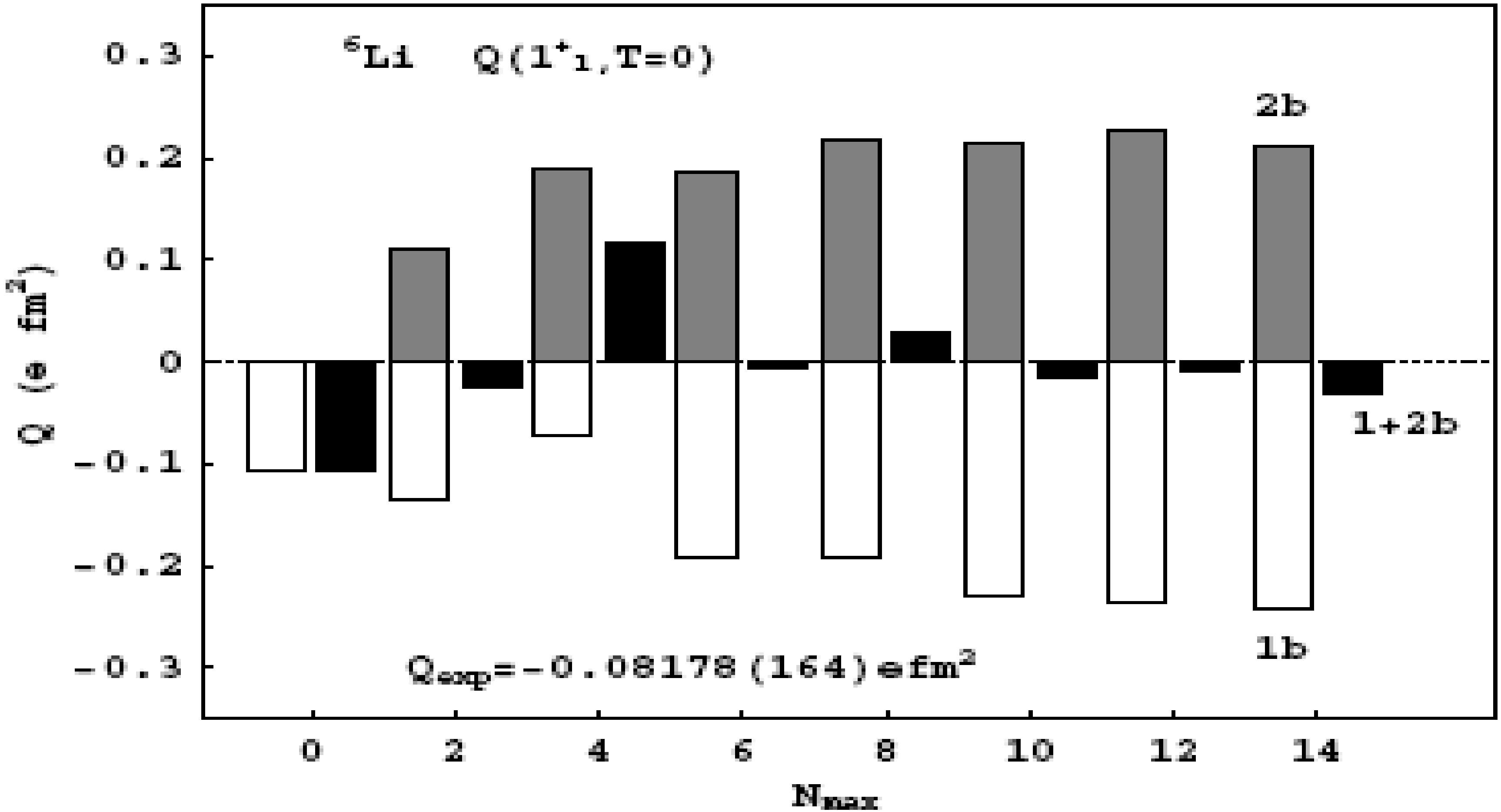


FIG. 6: The quadrupole moment of the ground state for ^{6}Li ($1^+(T = 0)$) is shown in terms of one- and two-body contributions as a function of increasing model space size.

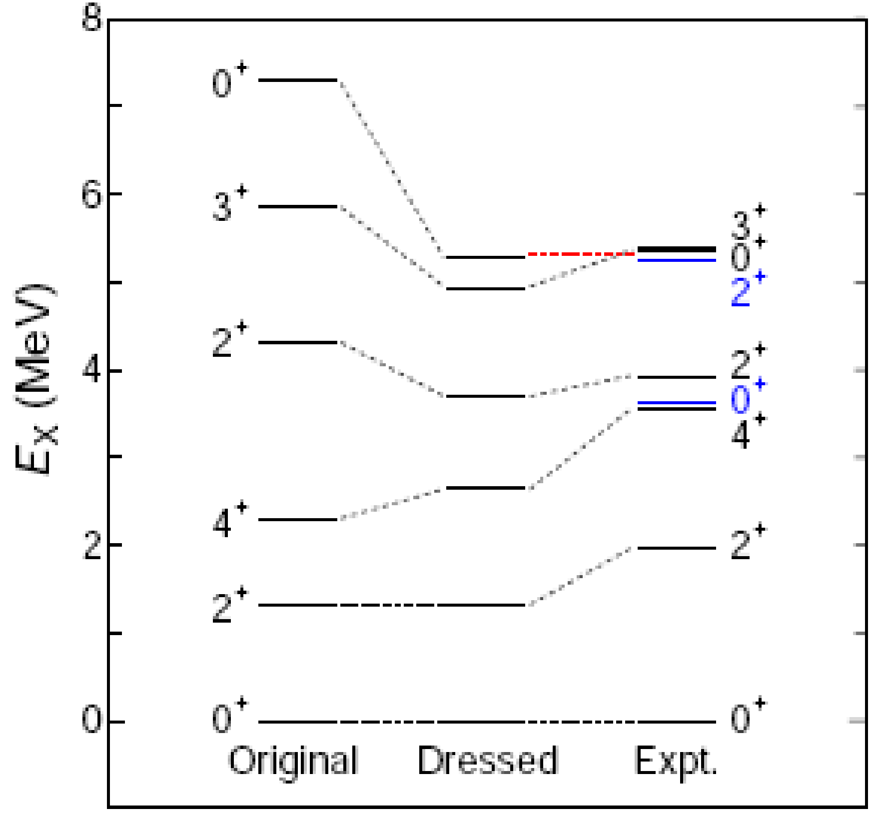


FIG. 2: Low-lying energy levels of the positive-parity states in ^{18}O.

S. Fujii and B.R.B. Nucl-th arXiv: 0902.216

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

COLLABORATORS

Alexander Lisetskiy, U. of Arizona
Michael Kruse, U. of Arizona
Ionel Stetcu, LANL
Petr Navratil, LLNL
James Vary, Iowa State U.

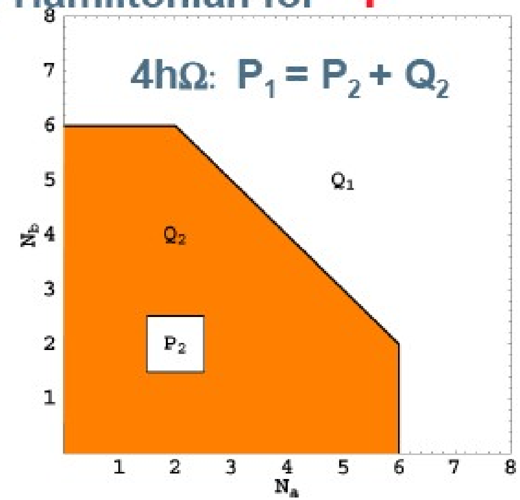
From 4hΩ NCSM to sd CSM for ^{18}F

Petr Navrátil, Michael Thoresen, and Bruce R. Barrett, Phys. Rev. C 55, R573 (1997)

Step 2: Projection of 18-body 4hΩ Hamiltonian onto 0hΩ 2-body Hamiltonian for ^{18}F

$H_{eff}([sd]^2) = \Sigma_k\ |k,N_{max}=4,A=18 > E_k\ (A=18) < \overline{k,N_{max}=4,A=18)|}$

$|k,N_{max}=4,A=18 > = U_{k,kp2}|k_{p2}[0h\Omega,18]> + U_{k,kq2}|k_{q2}[2+4h\Omega,18]>$



dim(P_1) = 6 706 870 dim(P_2)=28 dim(Q_2) = 6 706 842

$$H_{\rm diag} = U H U^\dagger$$

$$U = \begin{pmatrix} U_{PP} & U_{PQ} \\ U_{QP} & U_{QQ} \end{pmatrix}$$

E_k(A=18) H(N_{max}=4,A=18)

$$H_{\rm eff} = \frac{U_p^\dagger}{\sqrt{U_p^\dagger U_p}} H^p_{\rm diag} \frac{U_p}{\sqrt{U_p^\dagger U_p}}.$$

$H_{eff} = H_{eff}(1b) + H_{eff}(2b) + H_{eff}(3b) + H_{eff}(4b) + \ldots$