Ab initio Shell Model With a Core

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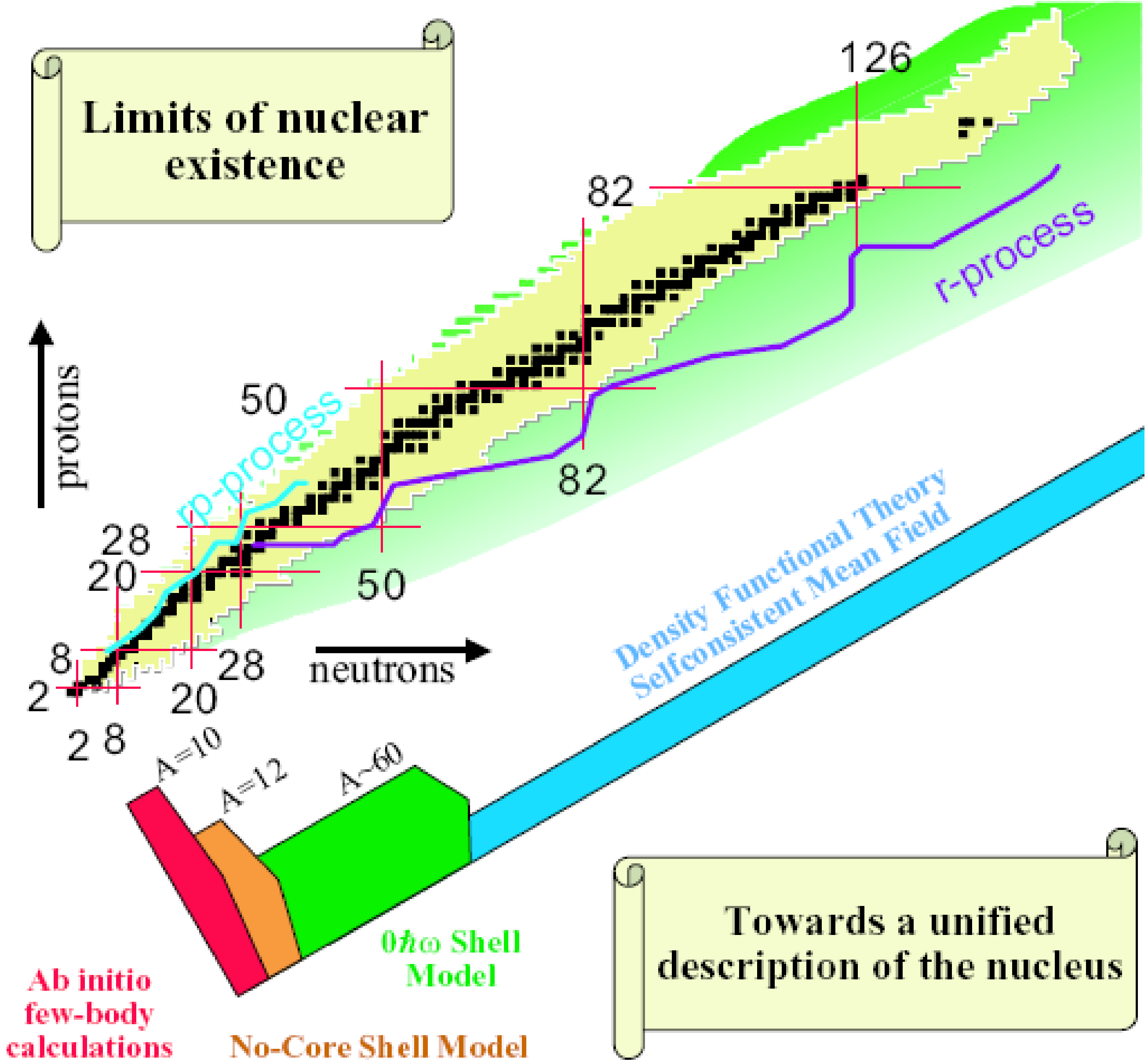
Vietri sul Mare May 22, 2010



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

Towards a unified description of the nucleus

The goal of nuclear structure theory:

exact treatment of nuclei based on NN, NNN,... interactions

⇨ need to build a bridge between:

ab initio few-body & light nuclei calculations: A $\lesssim 24$

$0\hbar\Omega$ Shell Model calculations: $16 < A < 120$

Density Functional Theory calculations: A ≥ 100

No Core Shell Model

"*Ab Initio*" approach to microscopic nuclear structure calculations, in which <u>all</u> <u>A</u> 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)

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

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

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

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

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

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

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;

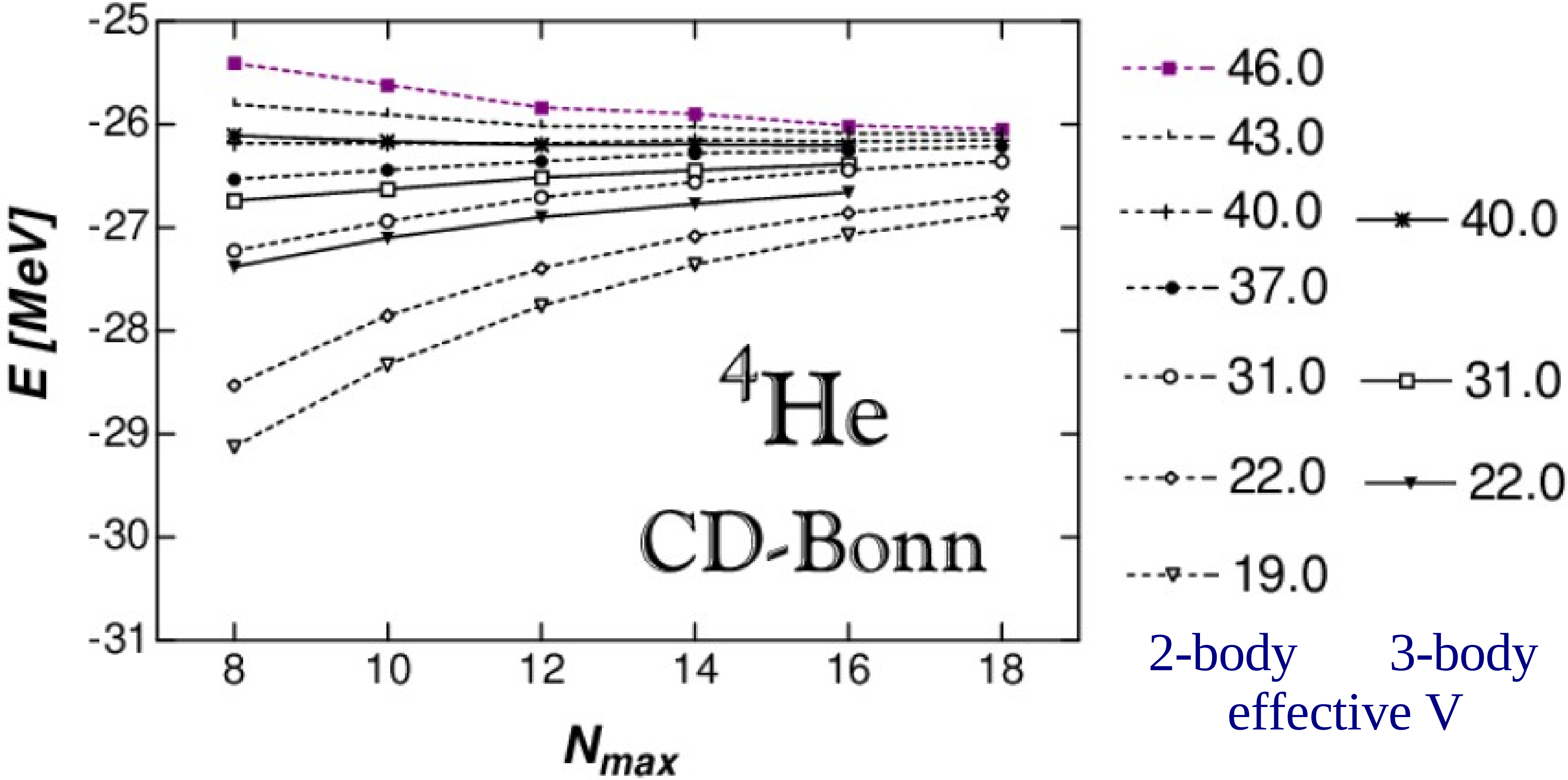
$$E^{\Omega}_{A,2} = U_2 H^{\Omega}_{A,2} U_2^{\dagger} \qquad U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} E^{\Omega}_{A,2,P} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

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

Two ways of convergence:

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

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


-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
37.0
31.0
22.0
19.0
40.0
31.0
22.0
2-body
3-body
effective V

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

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

Ab-initio shell model with a core

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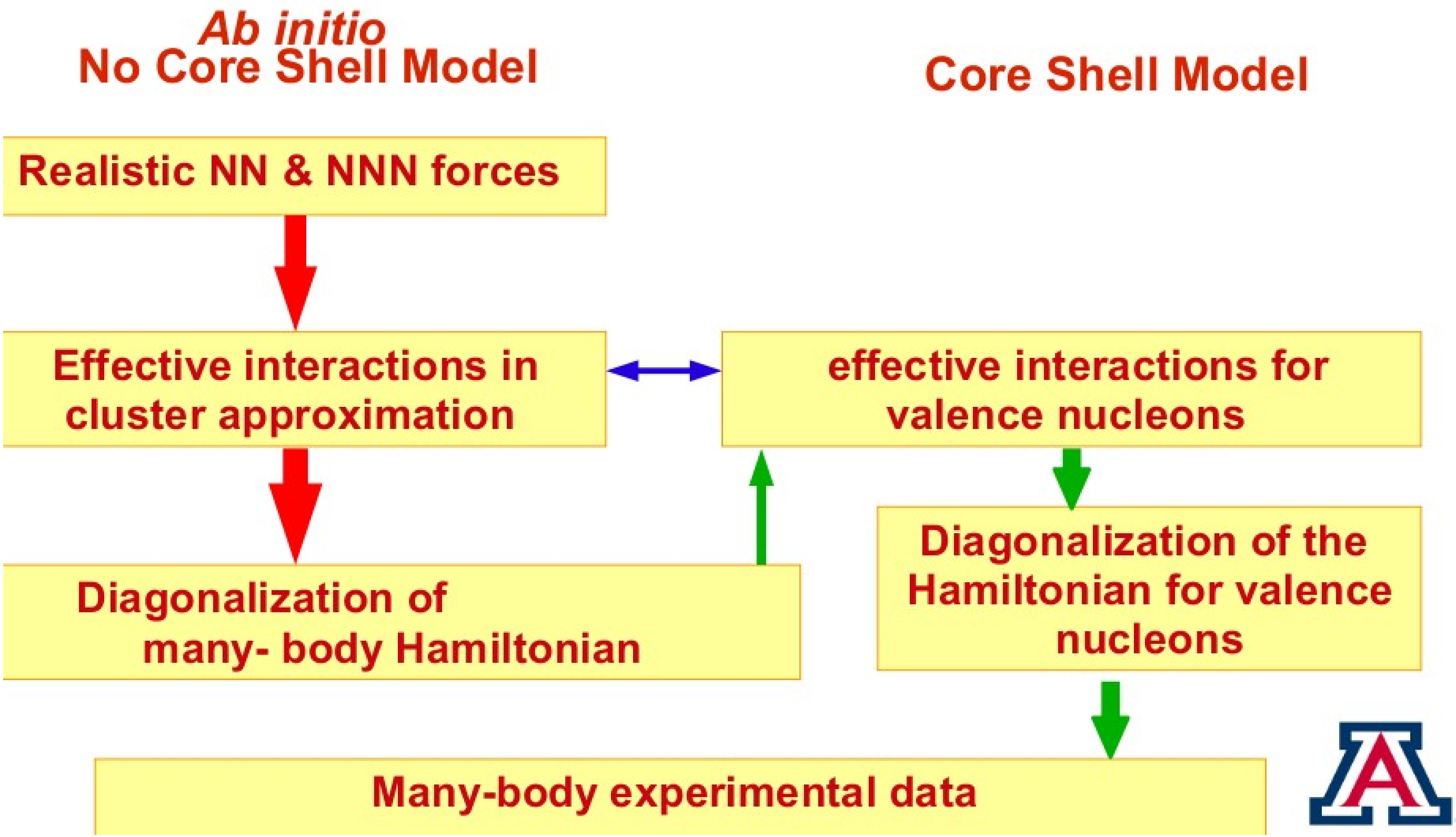
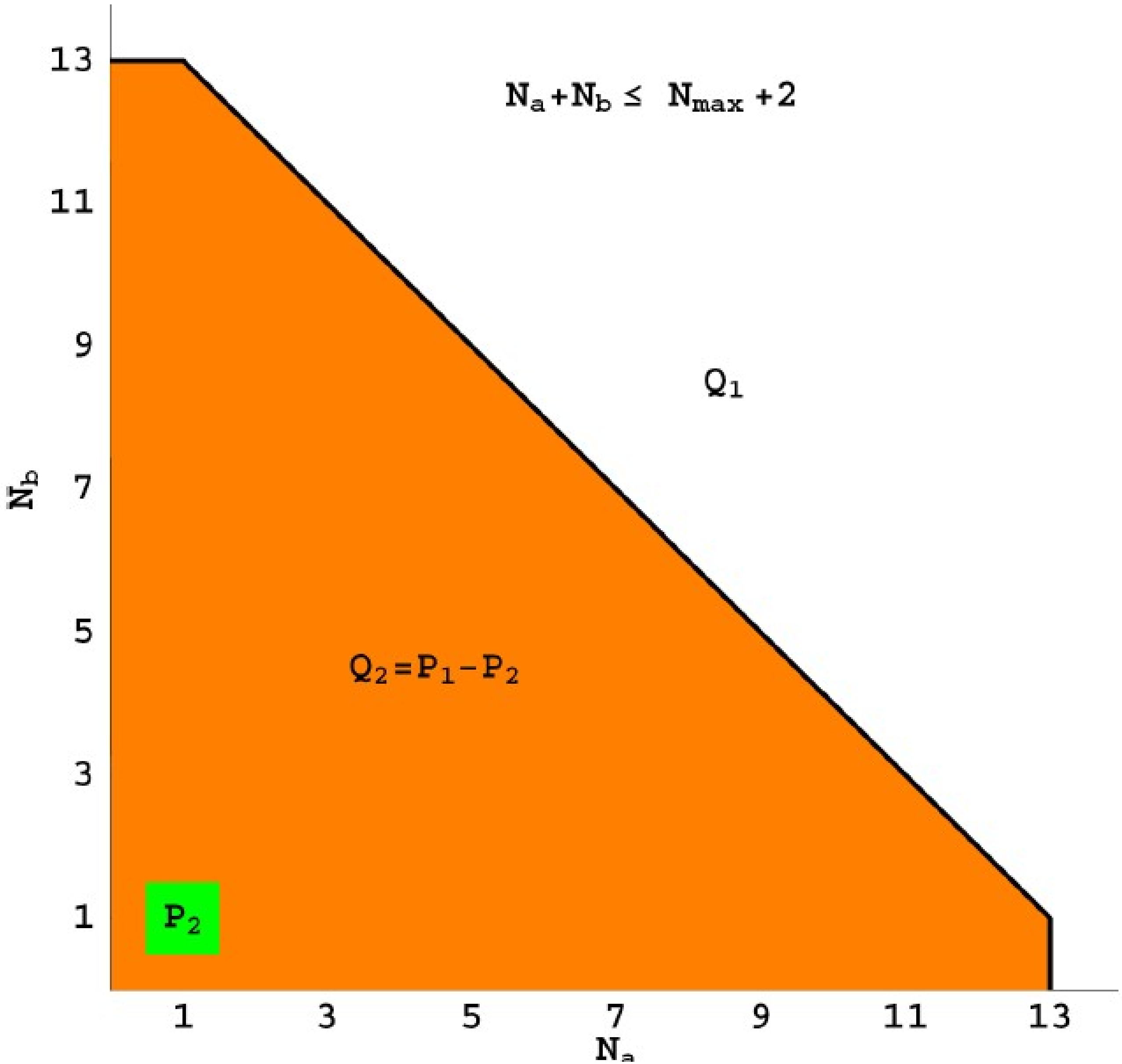
(Received 20 June 2008; published 10 October 2008)

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





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

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

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

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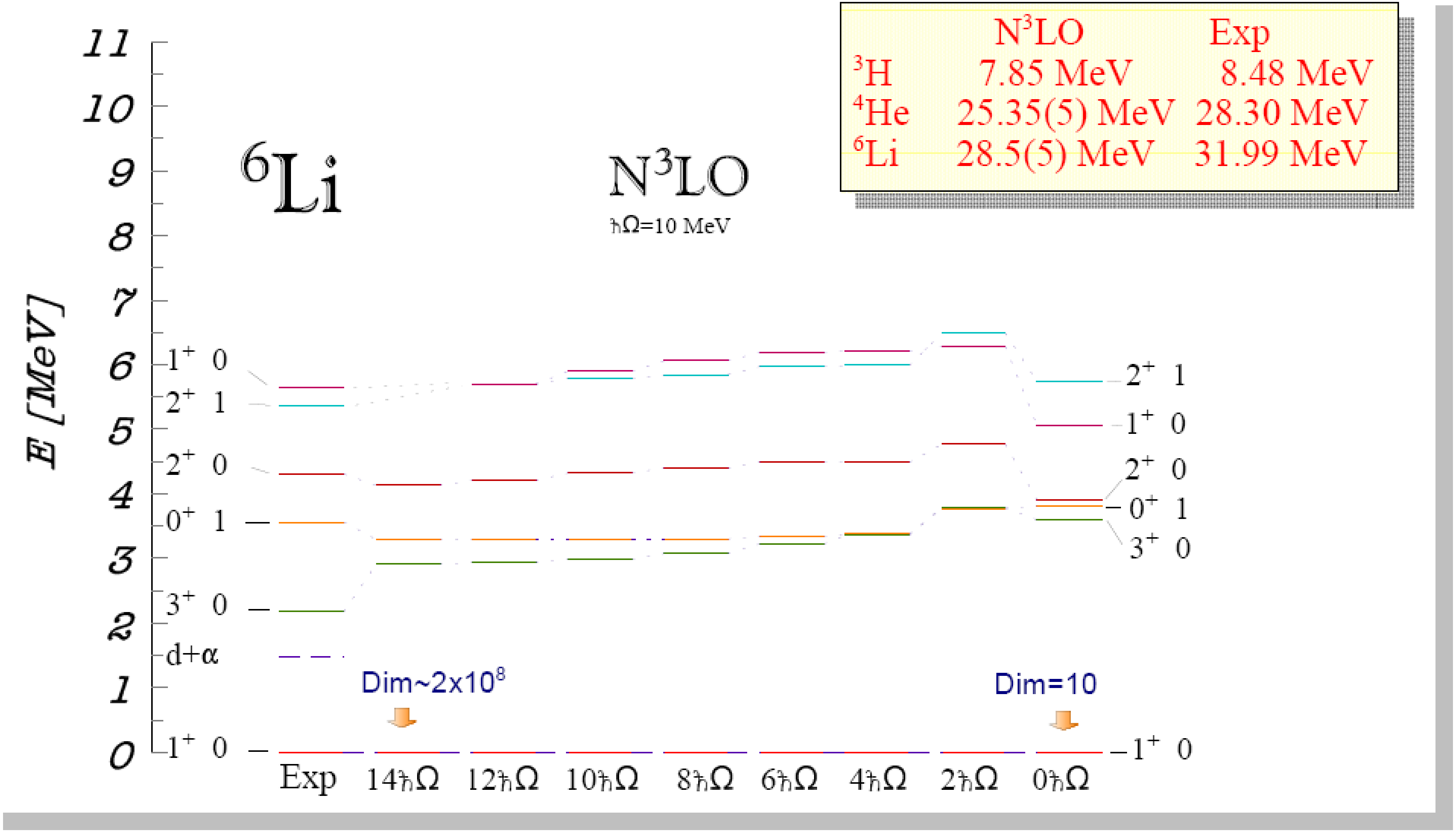
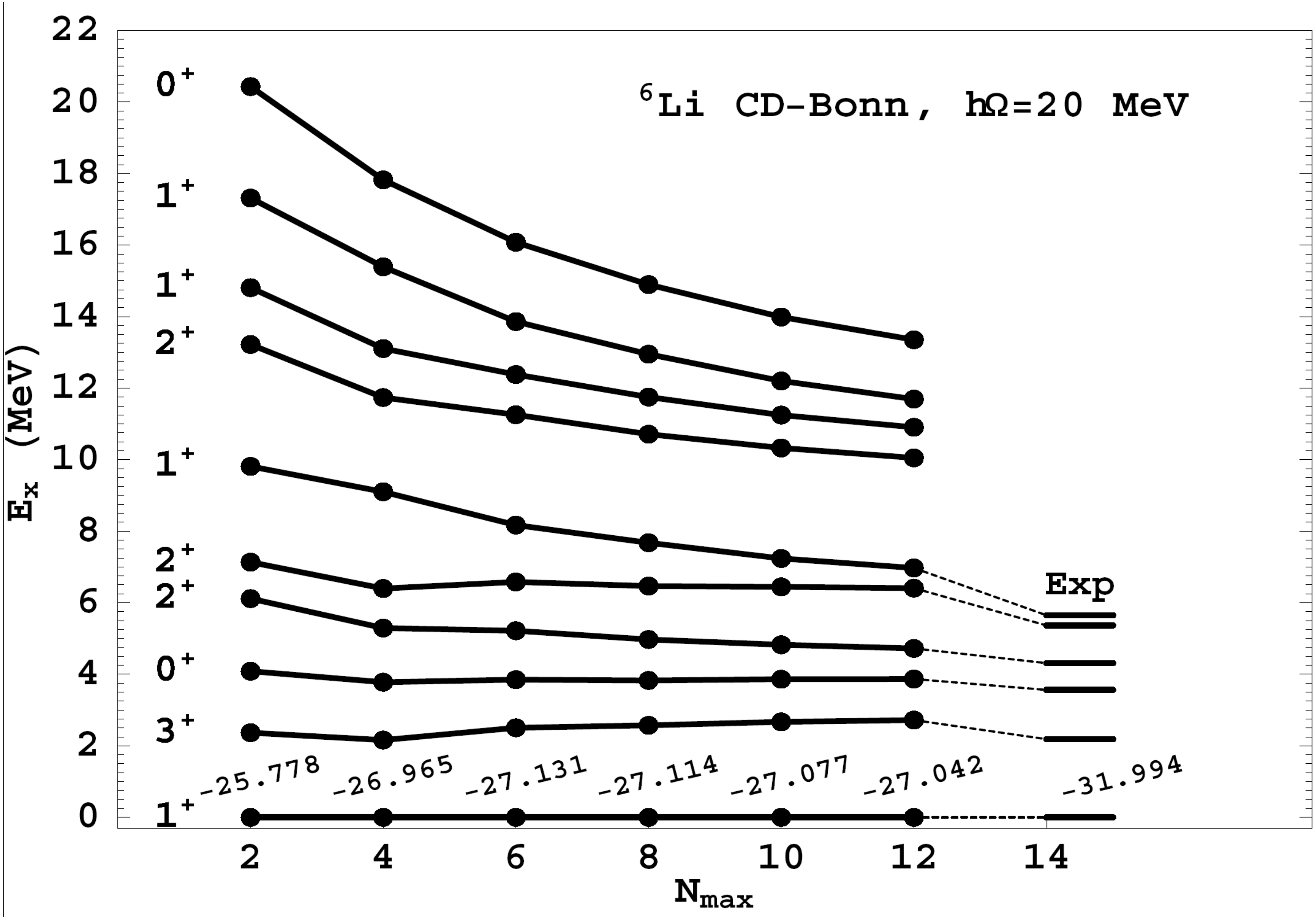
2) For a $\rightarrow$ A and fixed P: $H^{\mathrm{eff}}_{A,a} \rightarrow H_A$



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

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



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

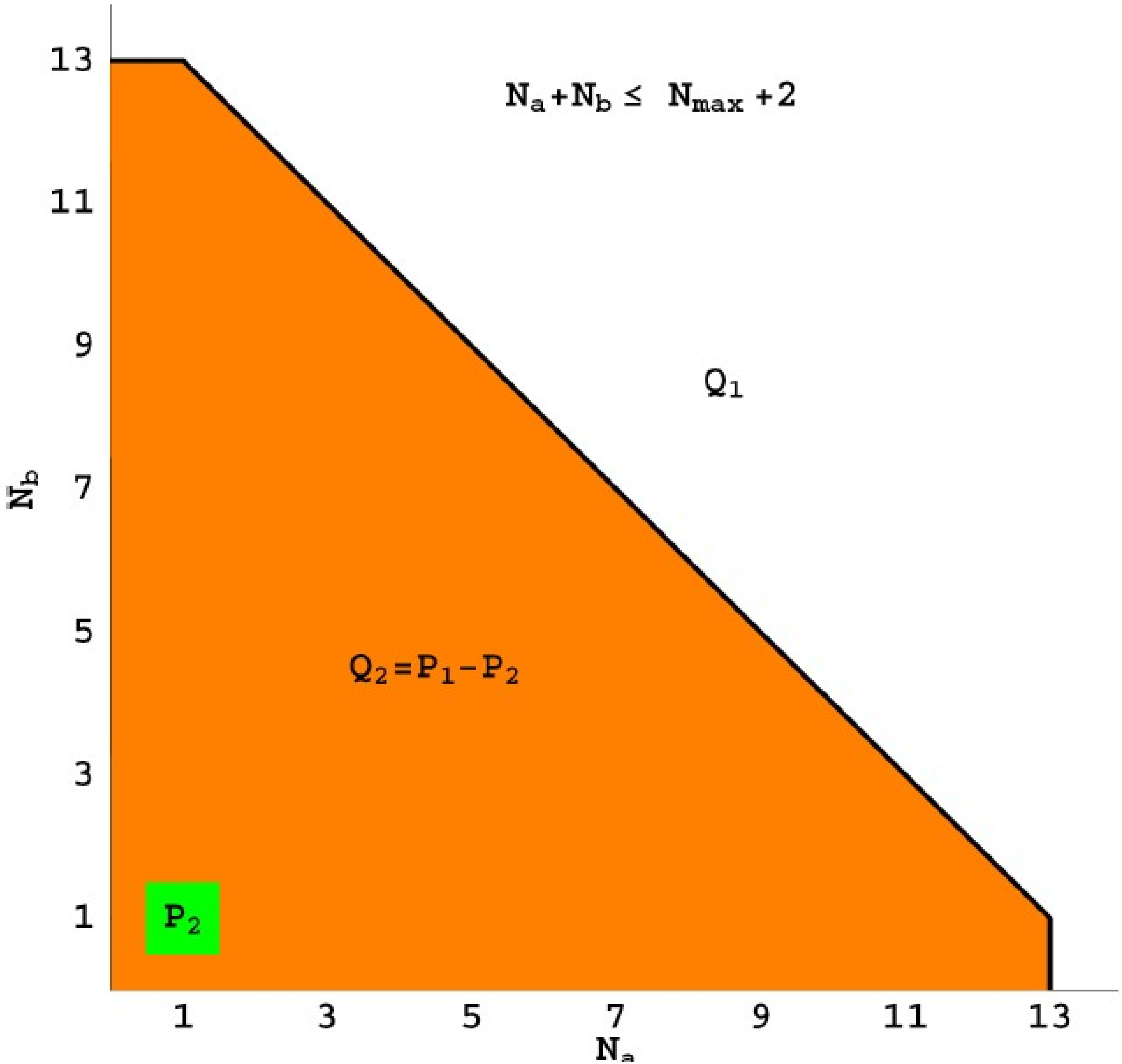
$$\mathcal{H}\Phi_\beta = E_\beta \Phi_\beta$$

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

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

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

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



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;

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

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;

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

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

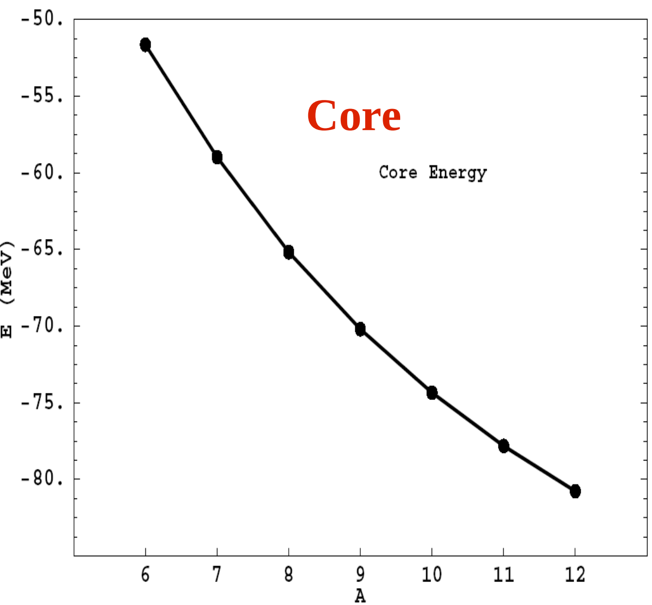
$$\mathcal{H}_{A,a_1=6}^{0,N_{\max}} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$

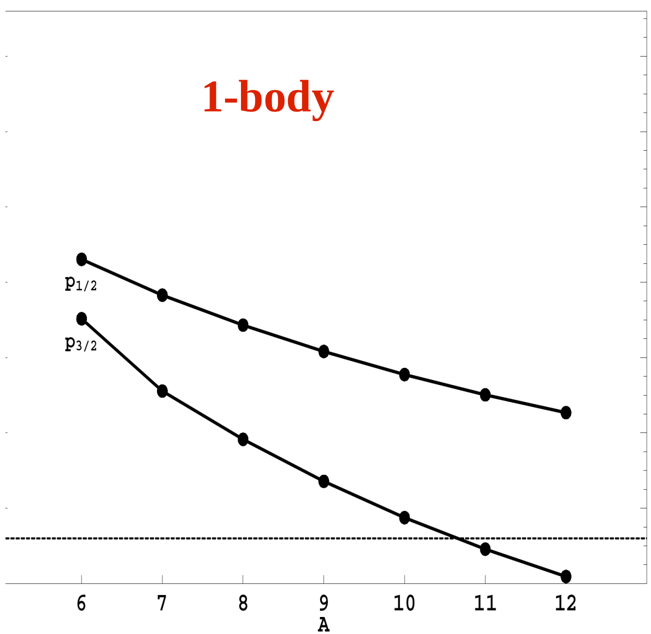
Need NCSM results in N_{max} space for **^{4}He** | **^{5}He ^{5}Li** | **^{6}He ^{6}Li ^{6}Be**

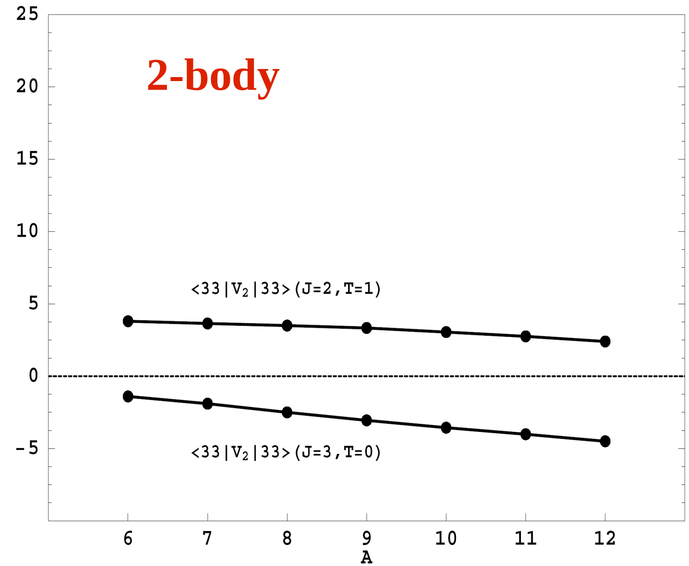
$N_{max} = 6$

With effective interaction for A !!!

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







2-body Valence Cluster approximation for A=7

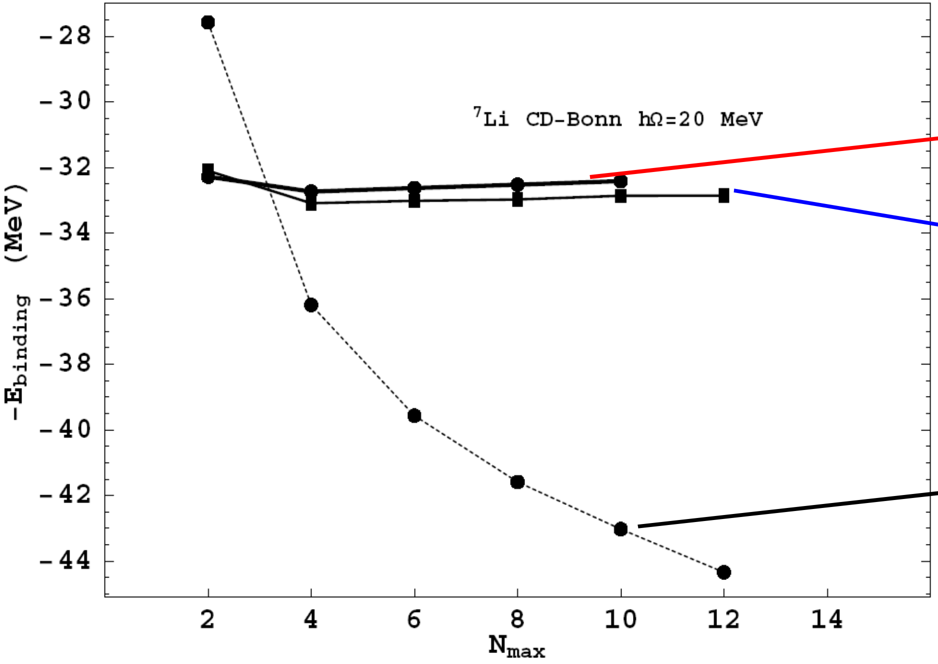
$$\mathcal{H}^{0,N_{max}}_{A,a_1=6} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$

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 !!!

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



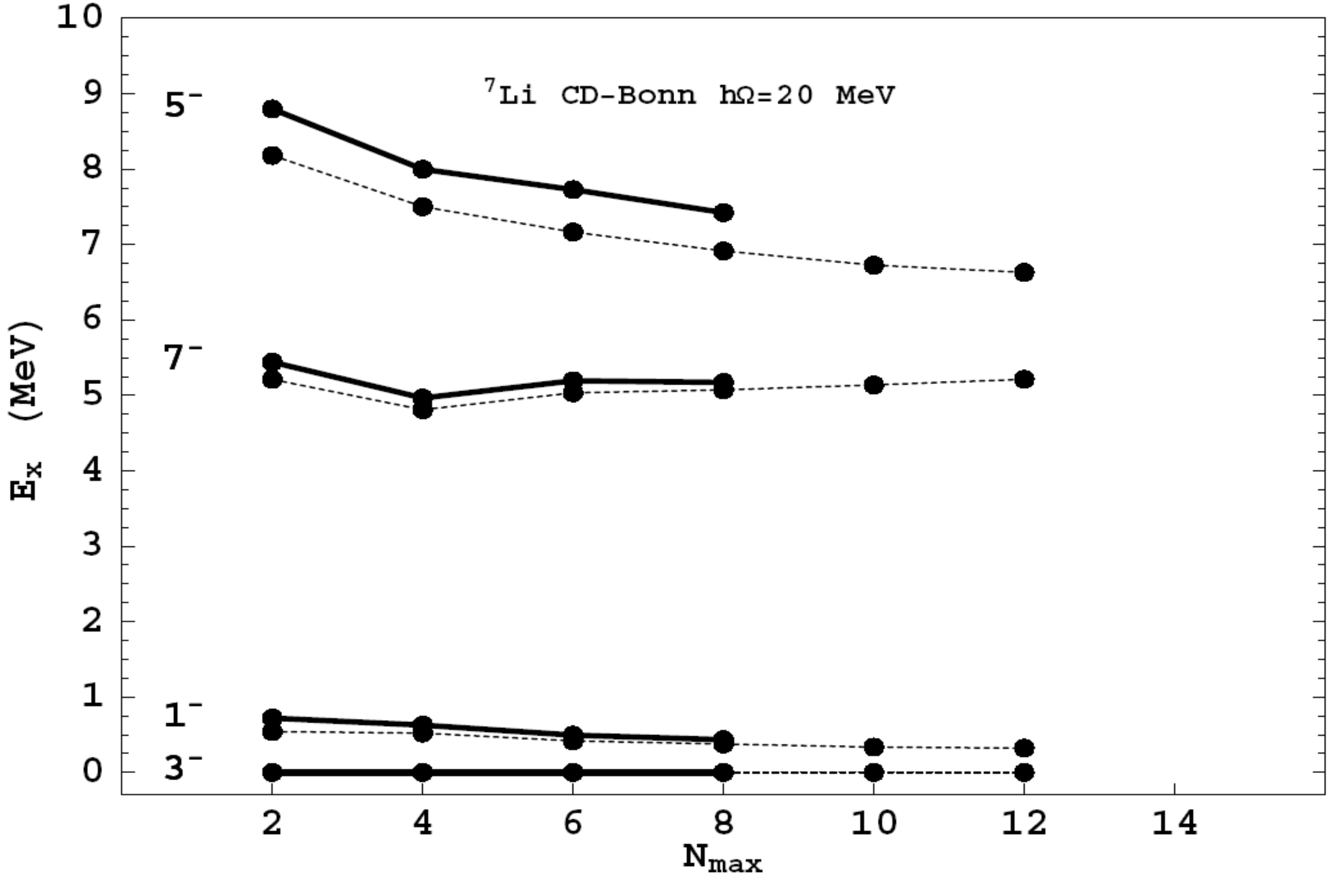
Exact NCSM

SSM with A-dependent core

SSM with inert core

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

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

Need NCSM results in N_{max} space for

^4He

^5He ^5Li

^6He ^6Li ^6Be

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

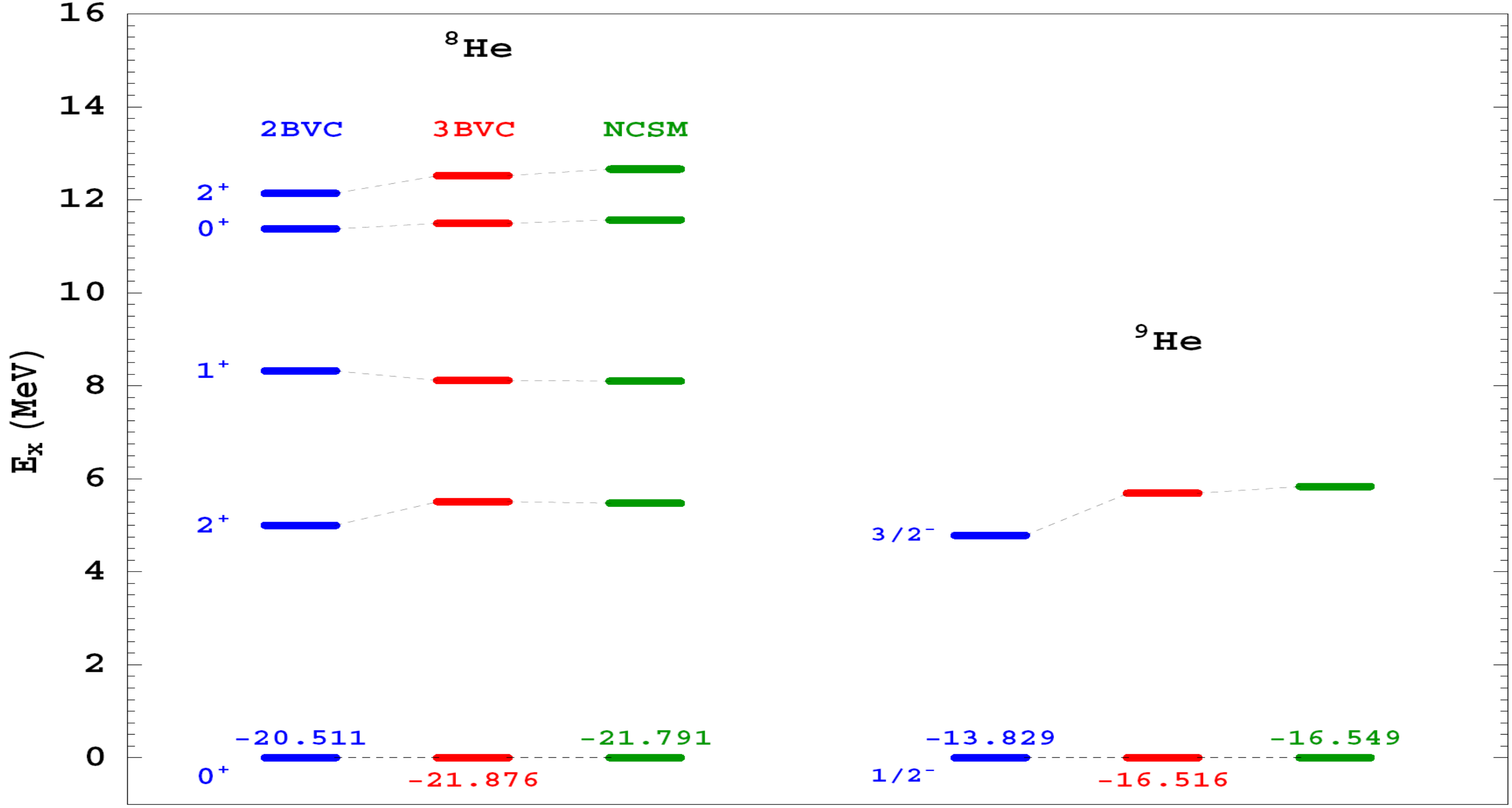
With effective interaction for A !!!

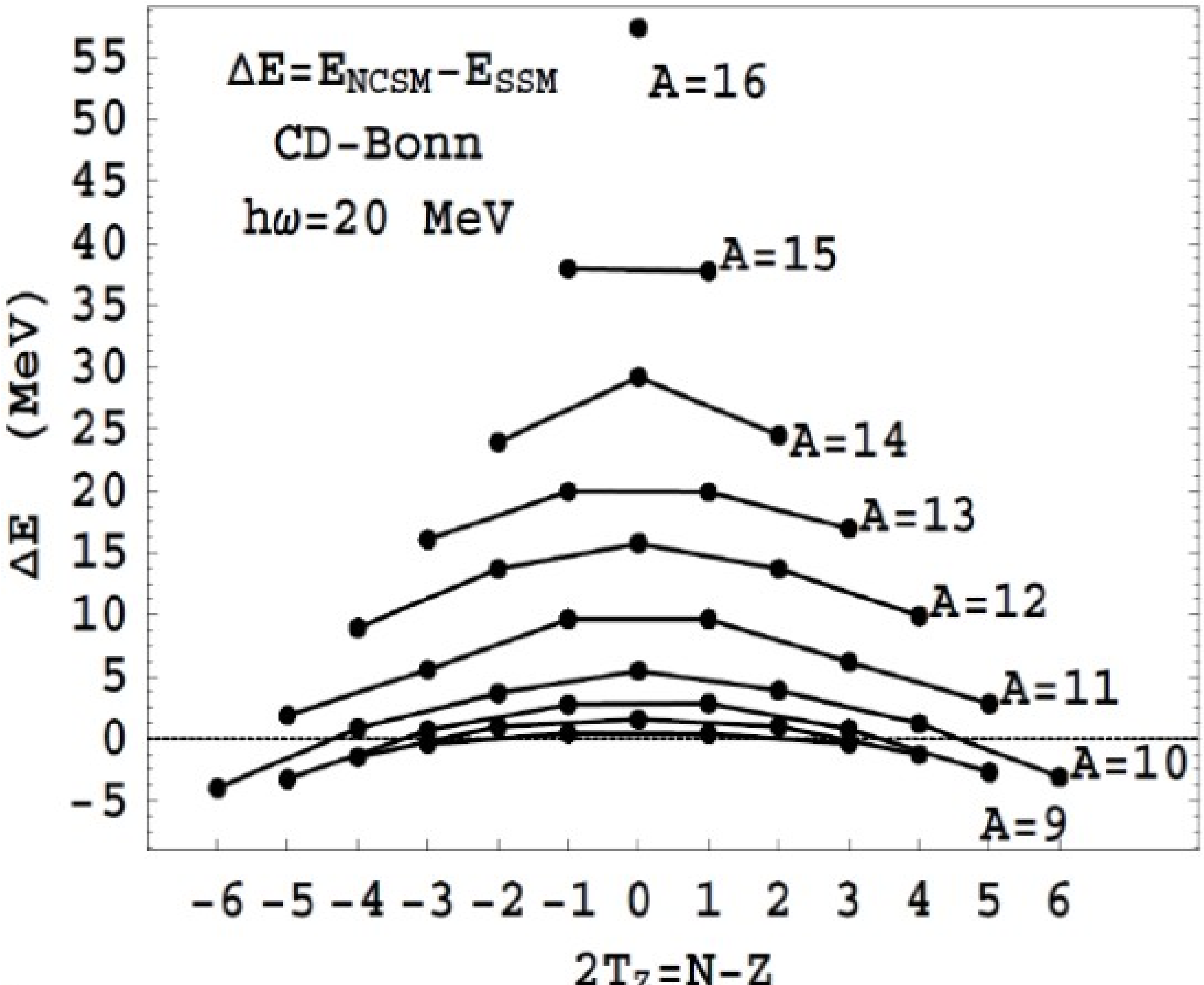
$$H_{A,2}^{N_{\max},\Omega,\mathrm{eff}}$$

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

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

3-body Valence Cluster approximation for A>6





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

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Effective operators from exact many-body renormalization

A. F. Lisetskiy,[1,2,*] M. K. G. Kruse,[1] B. R. Barrett,[1] P. Navratil,[3] I. Stetcu,[4] and J. P. Vary[5]

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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:

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

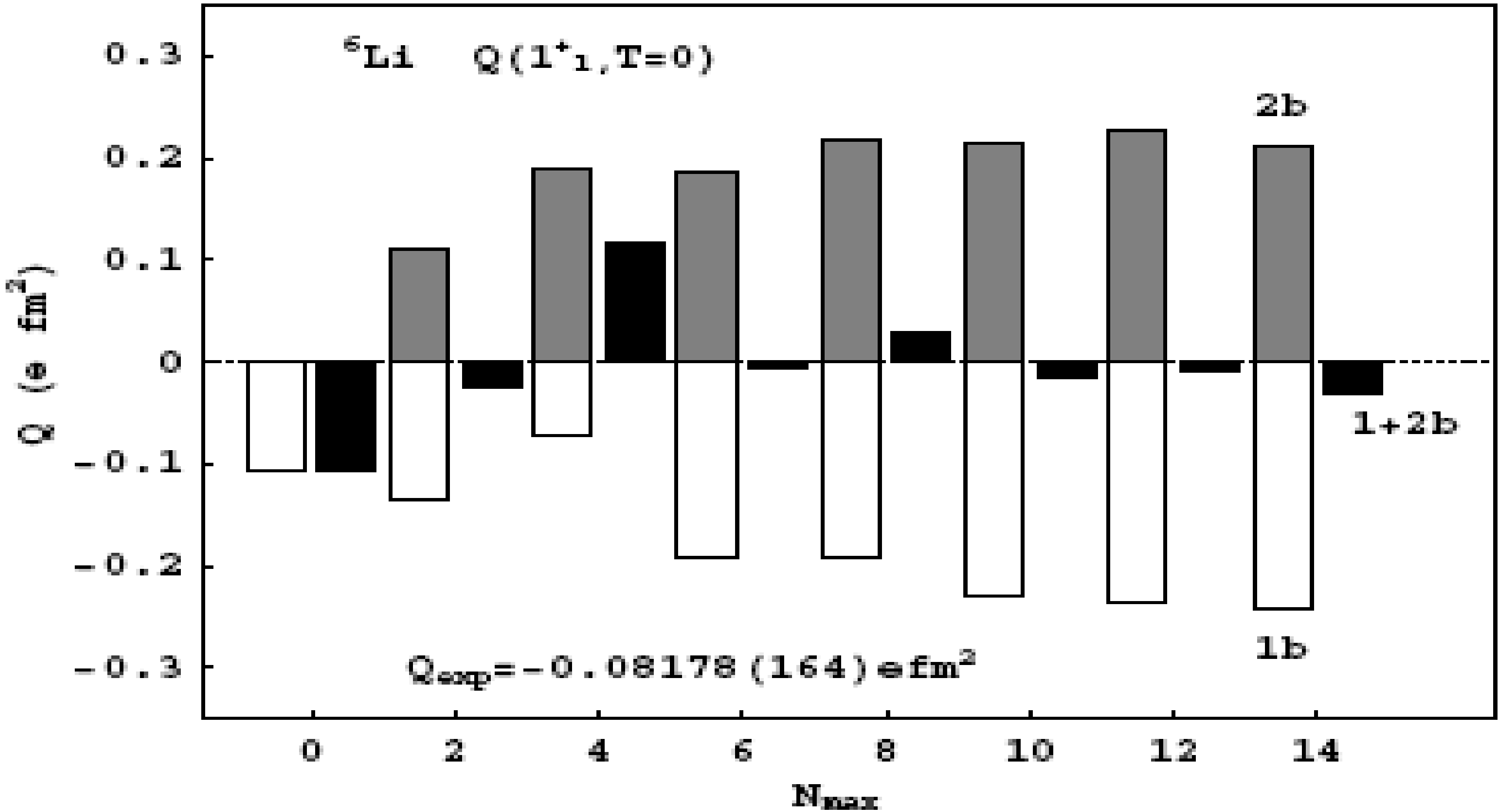

FIG. 6: The quadrupole moment of the ground state for ^{6}Li $(1^+(T = 0))$ is shown in terms of one- and two-body contributions as a function of increasing model space size.

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

COLLABORATORS

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PROCEEDINGS
OF THE
INTERNATIONAL CONFERENCE
ON
NUCLEAR STRUCTURE

KINGSTON, CANADA

AUGUST 29 - SEPTEMBER 3

1960

EDITED BY

D.A. BROMLEY

E.W. VOGT

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1960

how matter came about, and they add a great deal of significance and importance to nuclear physics and to certain experiments in nuclear physics which would have only little importance to the problems we have discussed here. Perhaps in the next conference we should have a session where we discuss these things; it is not enough just to go to Mr. Cameron or Mr. Fowler and ask him what shall we measure, we ought to know why we do it.

The second and last point I would like to raise is this. To round up the conference I come back to the first remark of Peierls, when he opened up the conference and asked the question, why are we interested in nuclear structure. May I add my own little verse to this. I have heard many people say that Nuclear Structure is not a fundamental problem, the real thing is high energy physics; the object of nuclear structure is after all nothing else but solving a Schroedinger equation for A particles. I strongly disagree with this point of view. The discovery and the understanding of phenomena hidden in a many-body problem can be a task of fundamental importance, if the object itself is of central interest.

Physics inquires into the nature of things. The nucleus, our nucleus, is an essential part of nature, it is the centre of the atom. It is not just a little phenomenon, it is the most prominent constituent of matter. The understanding of the phenomena occurring in this nucleus is therefore of paramount importance. Hence Nuclear Physics is an essential part of physics. I found out that some theorists, both in the east and in the west, consider the only thing worth doing is elementary particle physics. Experimentalists usually don't say so because they work with real matter and hence they know that the nucleus is an important thing. These theorists, however, worship the theory of elementary particles, a theory which in fact doesn't even exist. They knock their heads daily against a wall of dispersion-relations, Mandelstam representations and the like. Let them do it. After all the proton and the meson are also an important part of nature. In fact we should give them all the moral support they need. They are a brave lot who fight a very difficult fight and some day they will find the theory. But don't let yourself be talked into believing that the nucleus is not interesting. It is so small and it has so few parts and still it shows a tremendous variety of phenomena. Its investigation requires the whole arsenal of presently available experimental techniques and its understanding makes use of almost all branches of theoretical physics. What a marvellous invention! It is worth devoting a lifetime to it.