Ab initio Shell Model with a Core: Importance of Three-Nucleon (Effective) Interactions

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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

↓

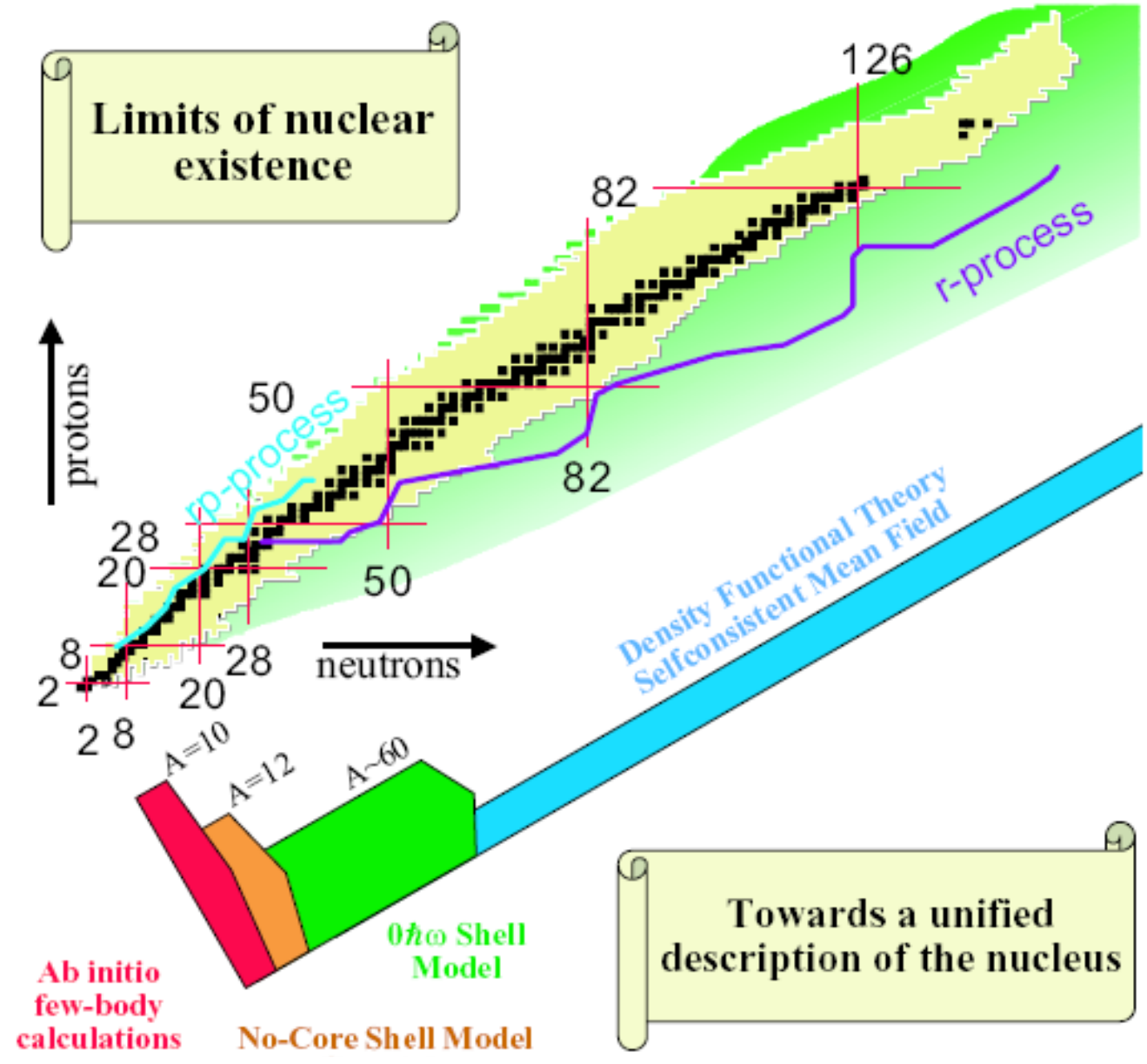
Effective interactions in cluster approximation

↓

Diagonalization of many- body Hamiltonian

↓

Many-body experimental data


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

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

Ab-initio shell model with a core

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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.

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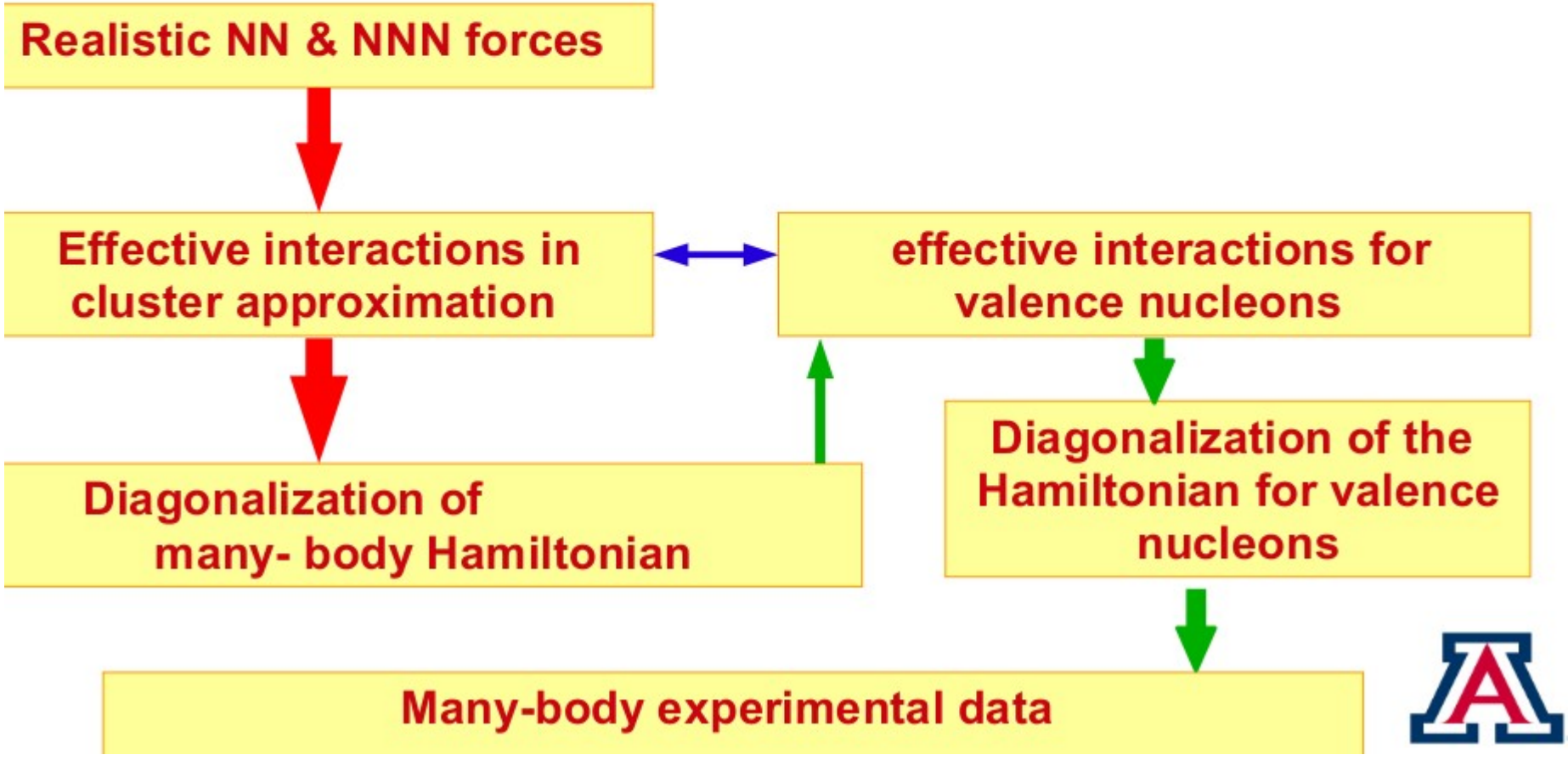
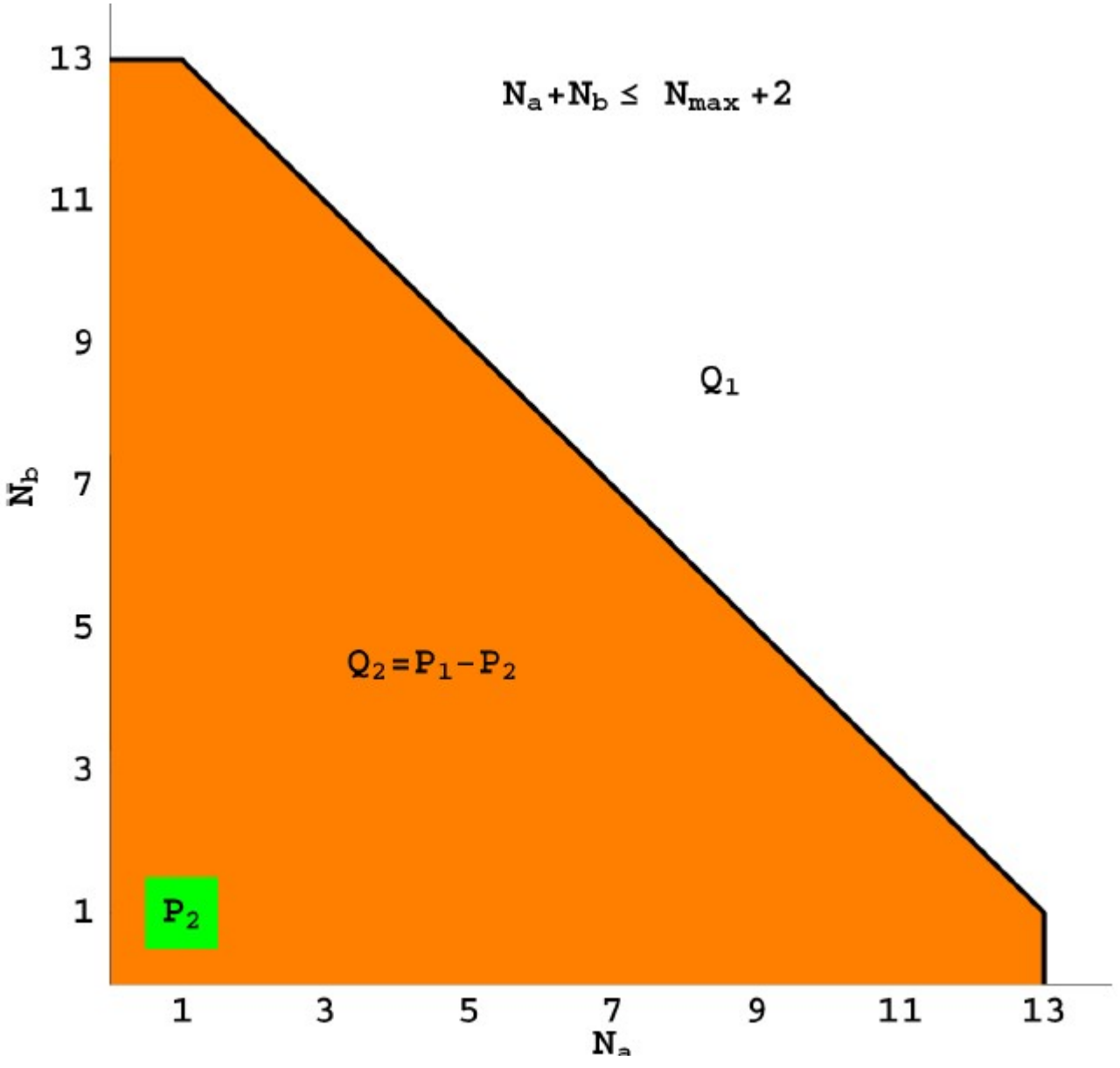
From few-body to many-body

Ab initio
No Core Shell Model

Core Shell Model




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

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

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

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

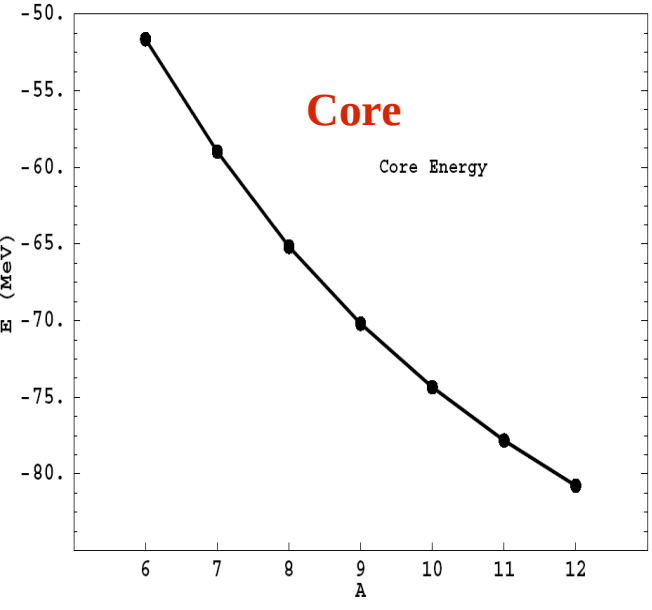
Need NCSM results in N_{max} space for

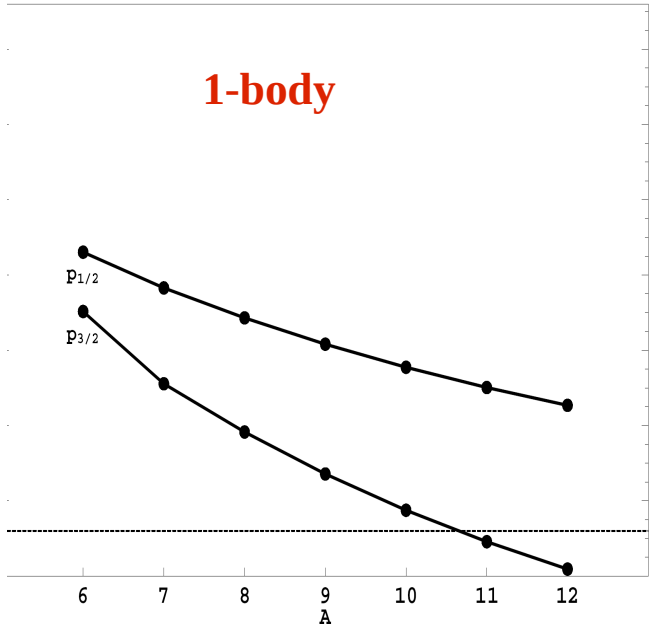
^{4}He ^{5}He ^{5}Li ^{6}He ^{6}Li ^{6}Be

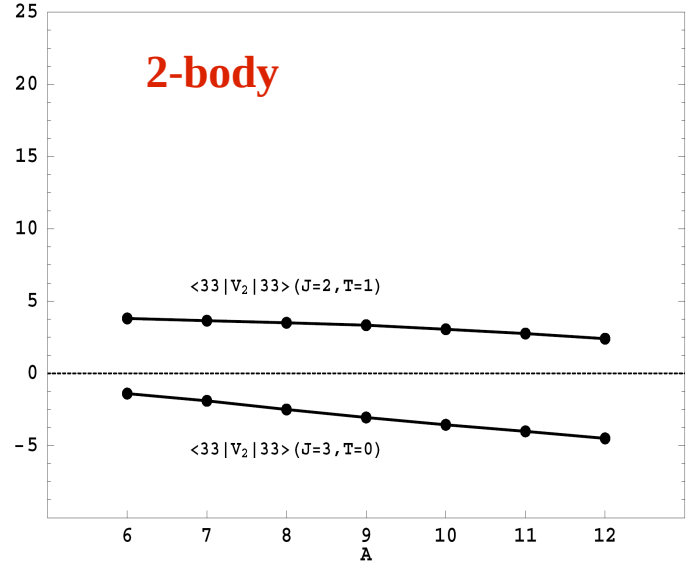
$N_{max} = 6$

With effective interaction for A !!!

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







2-body Valence Cluster approximation for A=7

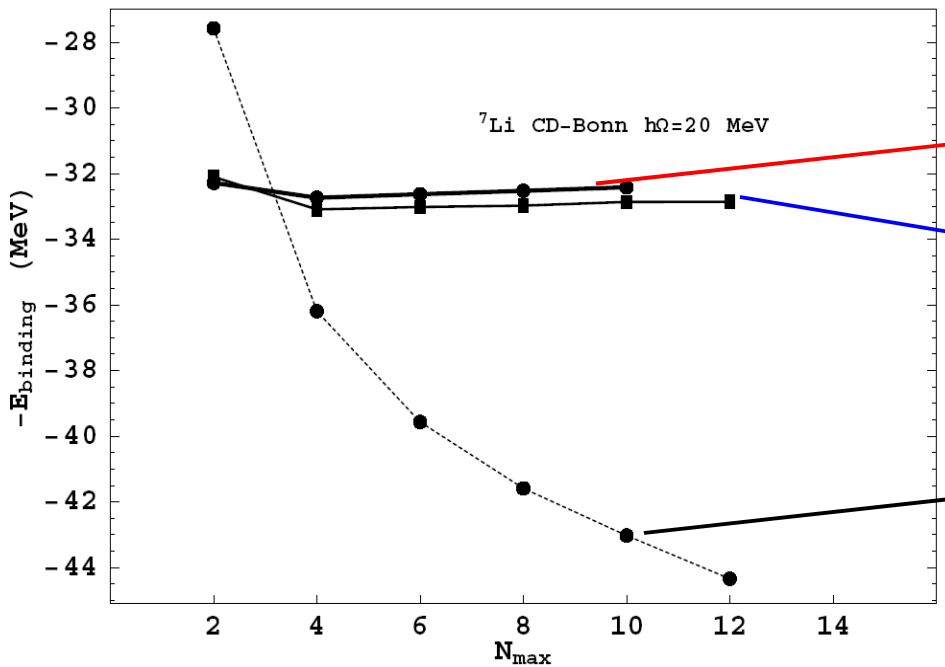
$$\mathcal{H}_A^{0,N_{\max}}{}_{,a_1=6} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6}$$

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 !!!

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



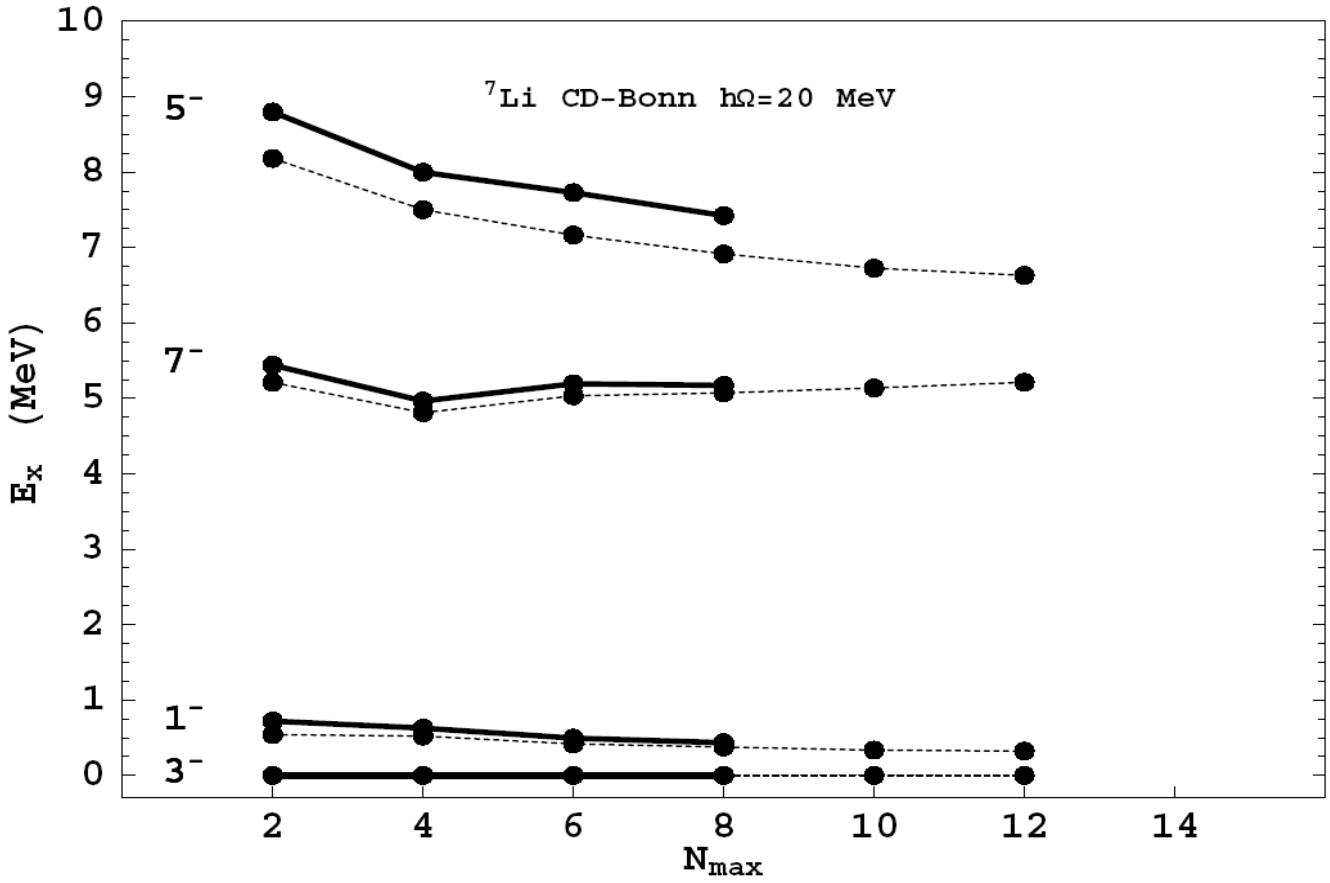
Exact NCSM

SSM with A-dependent core

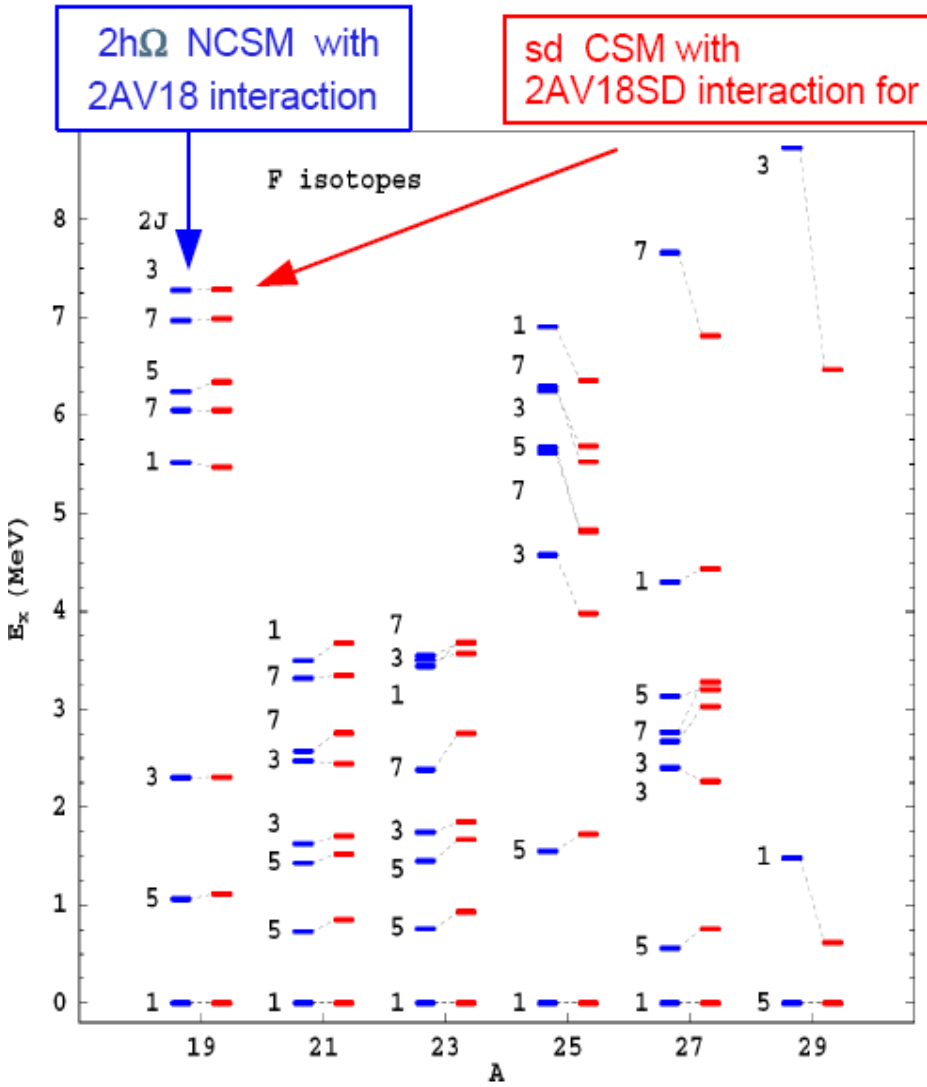
SSM with inert core

2-body Valence Cluster approximation for A=7

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



Testing effective interactions for the F isotopes in 2hΩ space



Maximum dimension

^{23}F

sd-space: 1 469

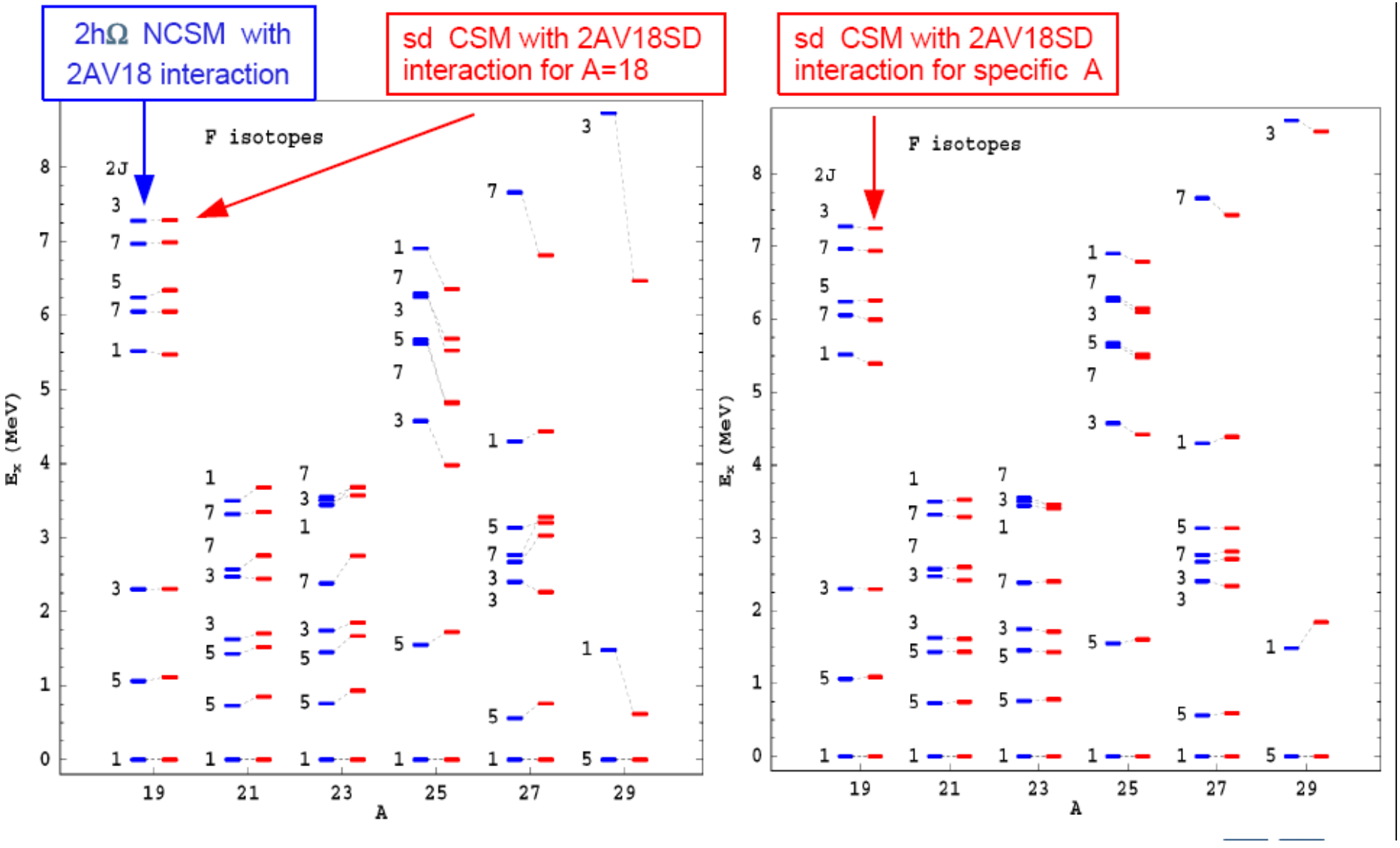
2hΩ-space: 1 725 000

Sources of difference:
a) many-body correlations
b) mass dependence

NCSM 2AV18 is A-dependent
CSM 2AV18SD is for A=18

Source b) can be eliminated by deriving 2AV18SD interaction for specific mass A

Testing effective interaction for F isotopes in 2hΩ space (+mass dependence)



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

$V_0^{A,4}$: ^{4}He

$V_1^{A,5}$: ^{5}He ^{5}Li

$V_2^{A,6}$: ^{6}He ^{6}Li ^{6}Be

$V_3^{A,7}$: ^{7}He ^{7}Li ^{7}B ^{7}Be

With effective interaction for A !!!

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

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

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

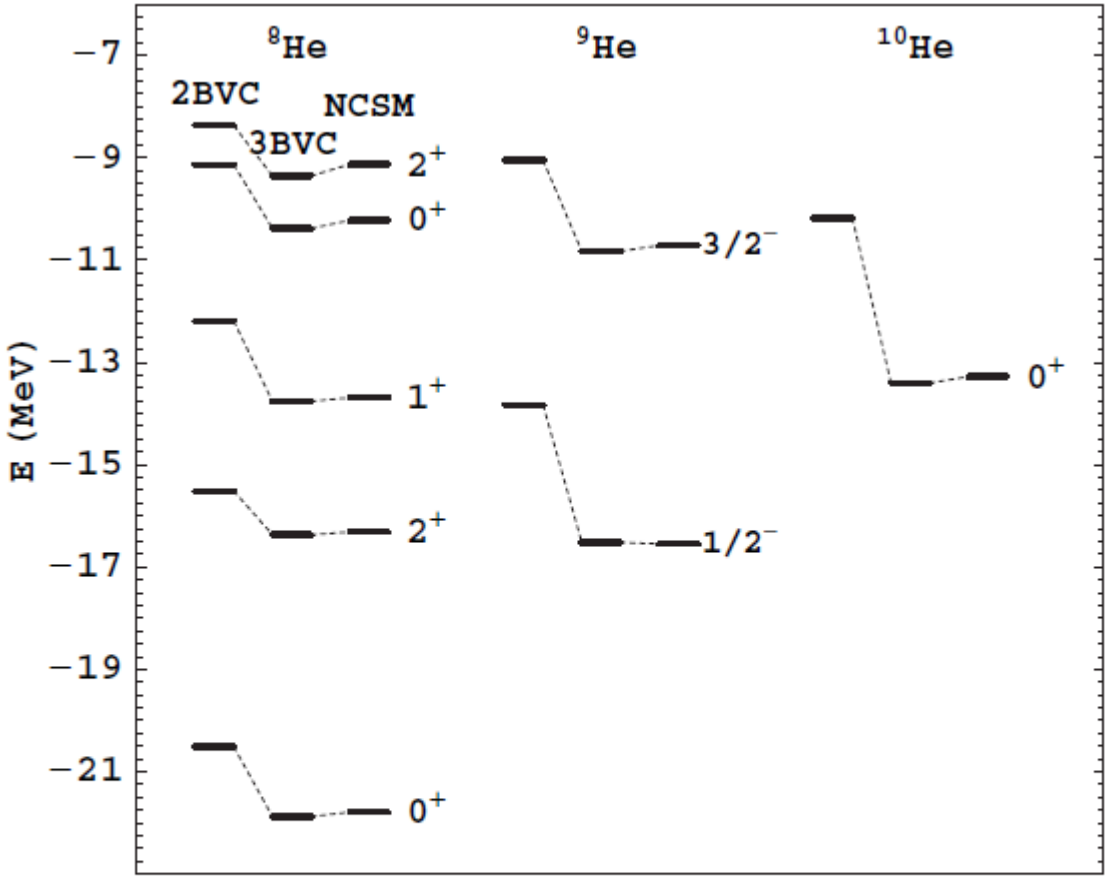


FIG. 9. Comparison of spectra for ^{8}He, ^{9}He, and ^{10}He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$ and $\hbar\Omega = 20$ MeV using the CD-Bonn interaction.

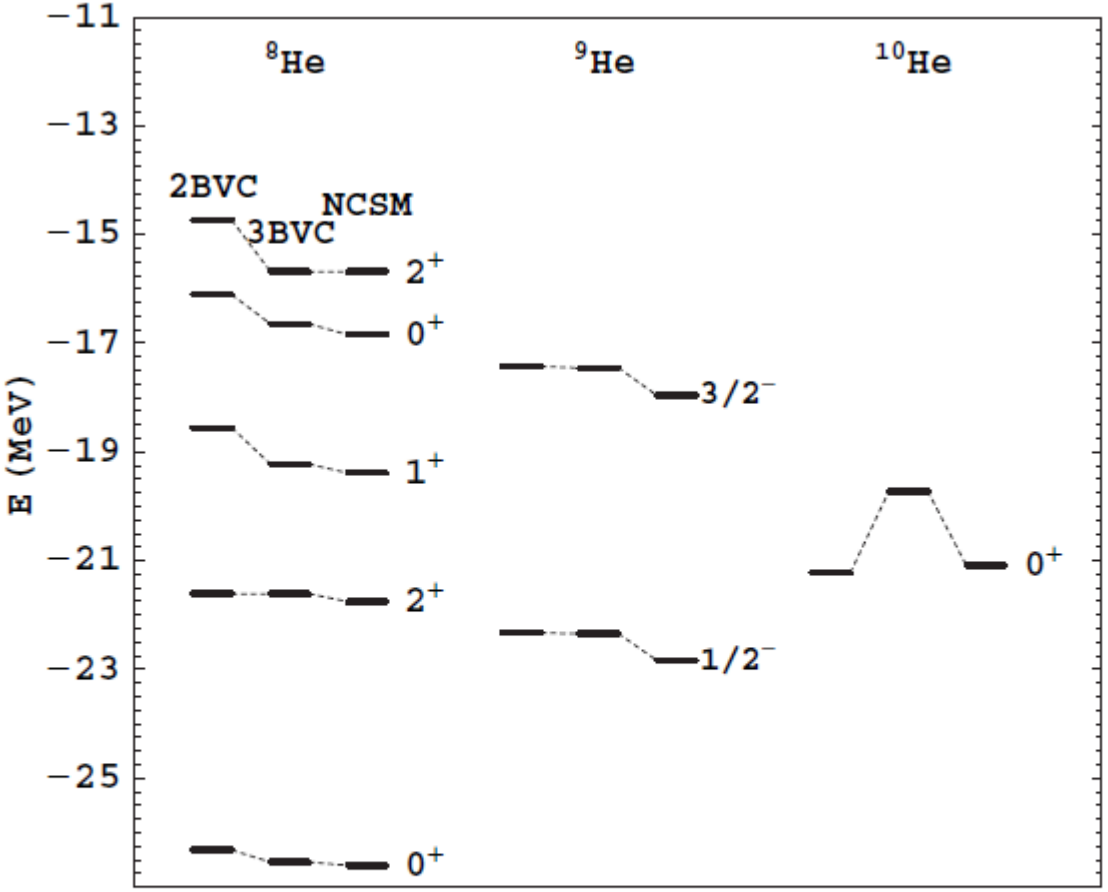
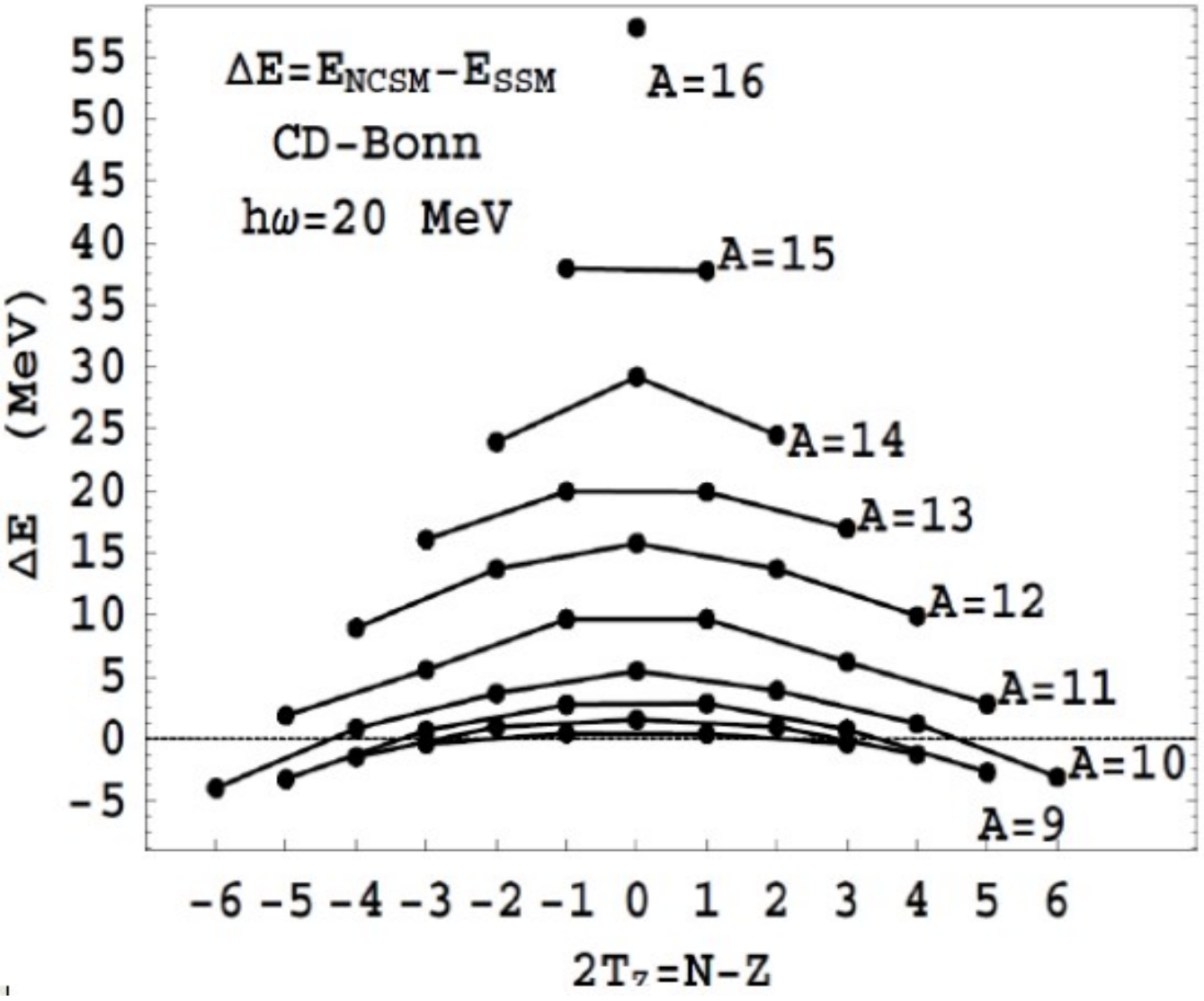


FIG. 8. Comparison of spectra for ^{8}He, ^{9}He, and ^{10}He from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$ and $\hbar\Omega = 14$ MeV using the INOY interaction.


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

3-body Valence Cluster approximation for p-shell

Step 1: Determine three-body matrix elements employing three-body

valence cluster approximation

Step 2: Calculate monopole part of the three-body effective Hamiltonian

$$\mathcal{H}_{3,\mathrm{mon}}(n,T) = \sum_{r\leq s\leq u=1}^{n} \left[D^{rsu}_{1/2}(n,T)\cdot W^{rsu}_{1/2} + D^{rsu}_{3/2}(n,T)\cdot W^{rsu}_{3/2} \right]$$

$$W^{rsu}_{T_3} = \frac{\sum (2J_{rsu}+1)\langle rsu; J_{rsu}T_3 | V_3 | rsu; J_{rsu}T_3\rangle}{g_{rsu}(T_3)}$$

$$g_{rsu}(T_3) = \sum_{J_{rsu}} (2J_{rsu}+1)$$

Three-body valence cluster approximation

Step 3: Calculate average three-body monopole, diagonal terms only

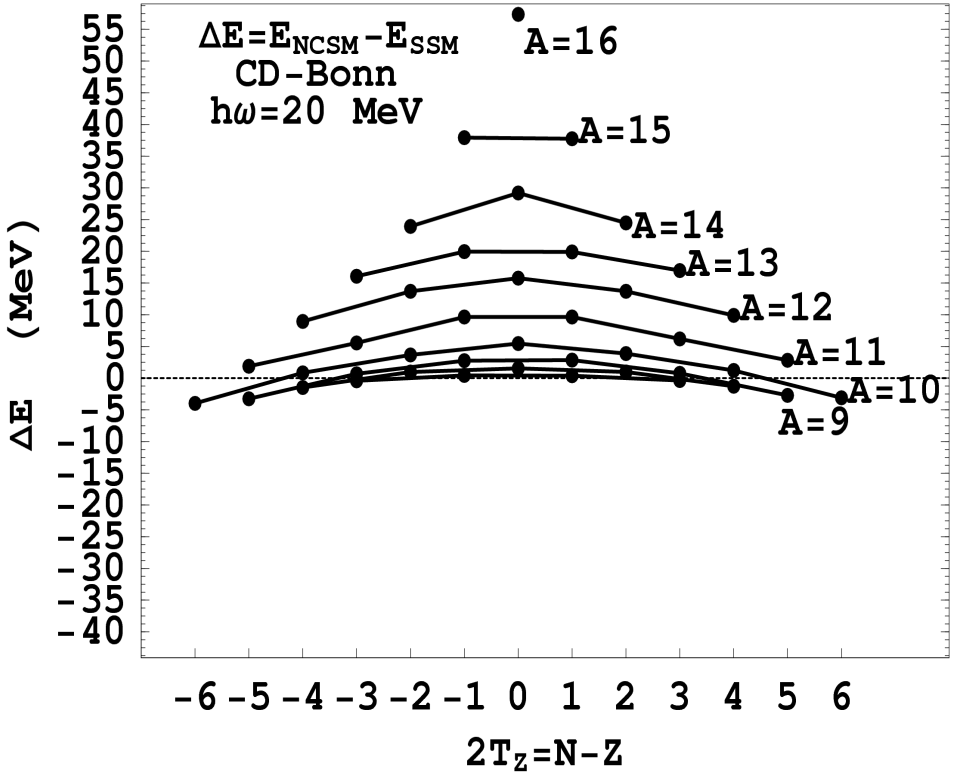
$$W_{T_3} = \frac{1}{\sum_{rsu=1}^{3} g_{rsu}(T_3)} \sum_{rsu=1}^{3} g_{rsu}(T_3) W_{T_3}^{rsu}$$

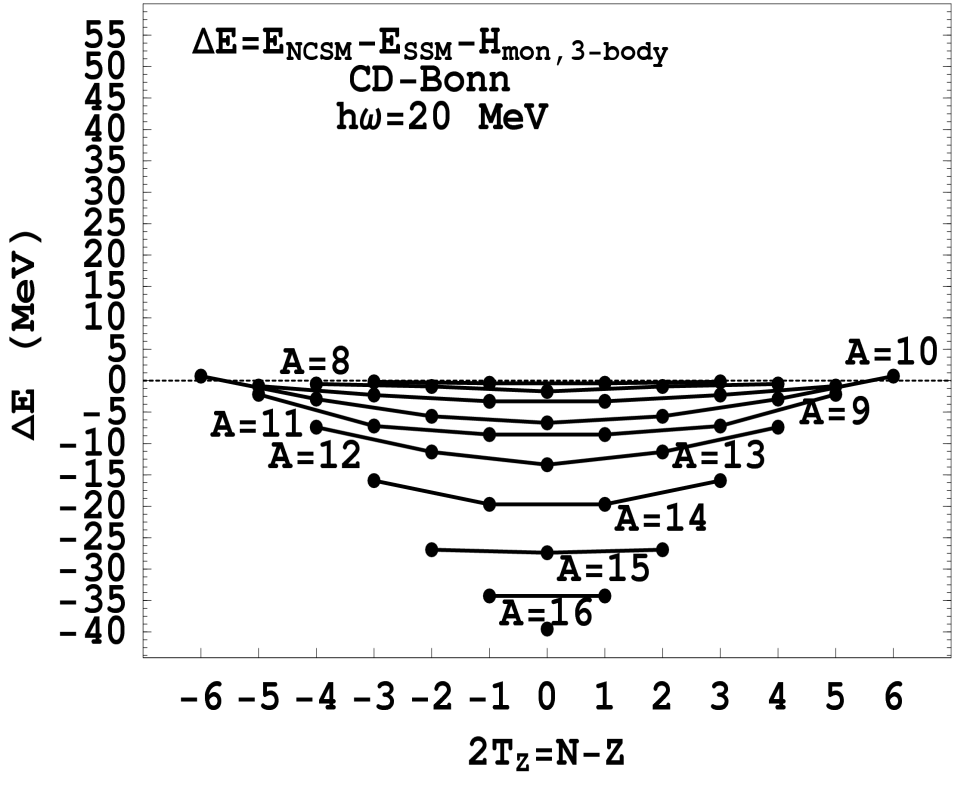
A=7: $W_{1/2}$ = 0.814 MeV $W_{3/2}$ = - 0.213 MeV

$$\mathcal{H}_{3,\mathrm{mon}}(n,T) = \frac{n-2}{3}\left[D_1(n,T)\cdot W_{3/2} + D_0(n,T)\cdot W_{1/2}\right]$$

$$D_1(n,T) = \frac{3n(n-2)}{8} + \frac{1}{2}T(T+1), \qquad D_0(n,T) = \frac{n(n+2)}{8} - \frac{1}{2}T(T+1)$$

3-body monopole, diagonal terms only





Three-body valence cluster approximation

Step 3: Calculate average three-body monopole, exact for A=7

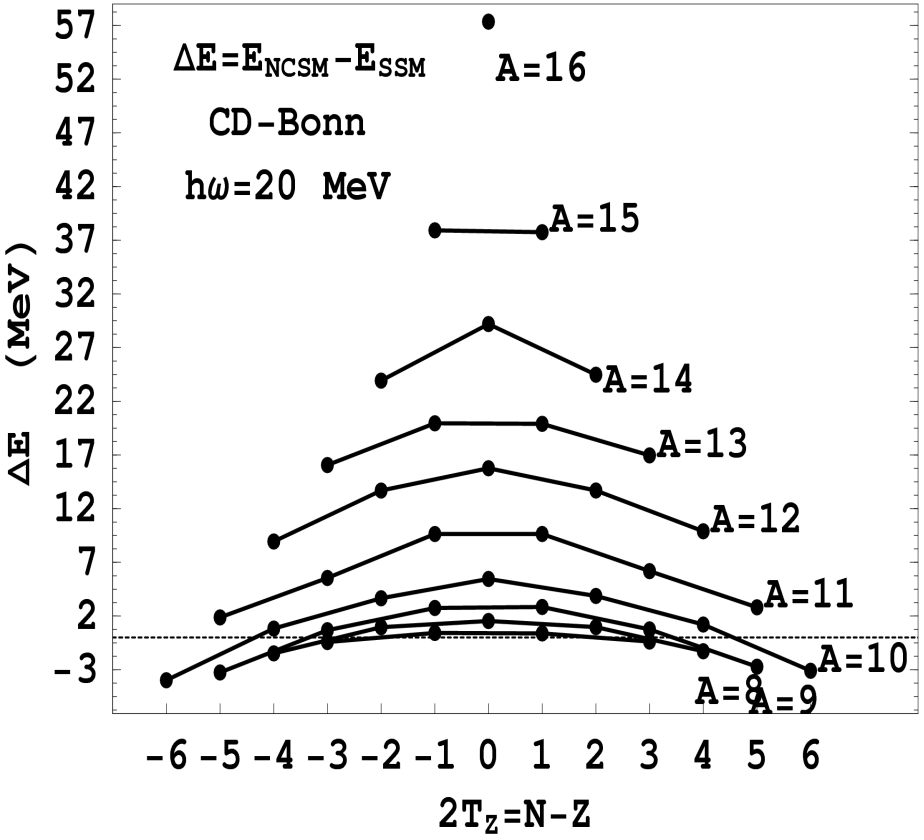
$$W_{T_3} = \frac{1}{\sum_{rsu=1}^{3} g_{rsu}(T_3)} \sum_{rsu=1}^{3} g_{rsu}(T_3) W_{T_3}^{rsu}$$

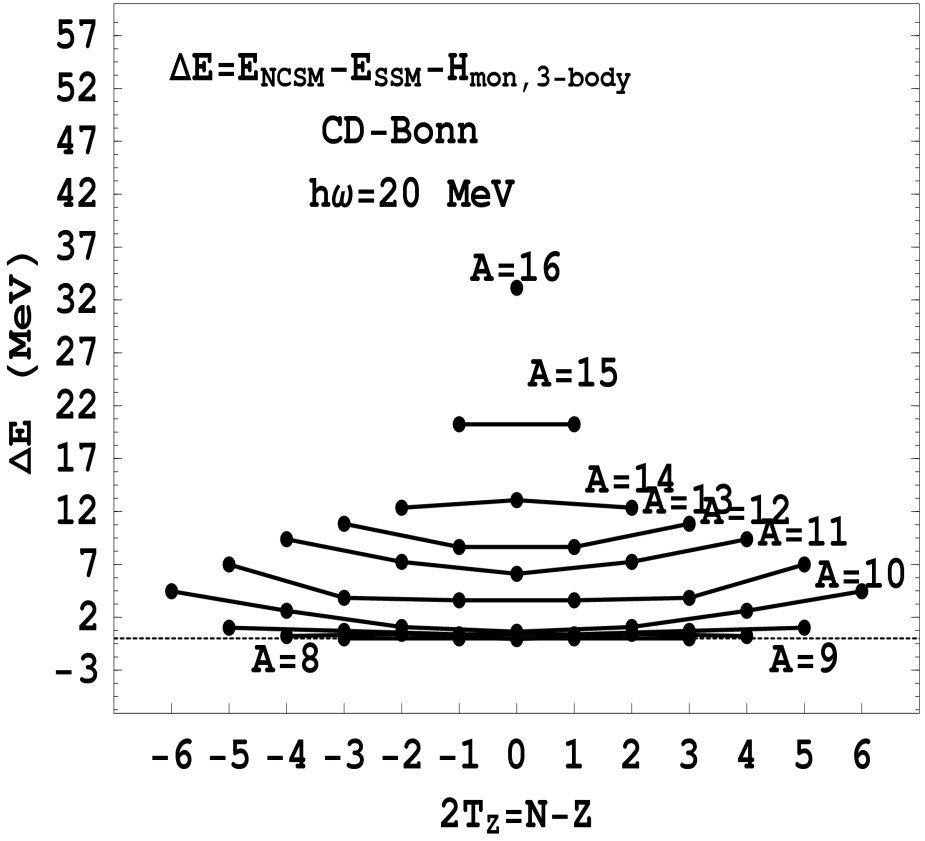
A=7: $W_{1/2}$ = 0.402 MeV $W_{3/2}$ = - 0.400 MeV

$$\mathcal{H}_{3,\mathrm{mon}}(n,T) = \frac{n-2}{3}\left[D_1(n,T)\cdot W_{3/2} + D_0(n,T)\cdot W_{1/2}\right]$$

$$D_1(n,T) = \frac{3n(n-2)}{8} + \frac{1}{2}T(T+1), \qquad D_0(n,T) = \frac{n(n+2)}{8} - \frac{1}{2}T(T+1)$$

Global three-body monopole, exact for A=7





Three-Body Forces and the Limit of Oxygen Isotopes

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The limit of neutron-rich nuclei, the neutron drip line, evolves regularly from light to medium-mass nuclei except for a striking anomaly in the oxygen isotopes. This anomaly is not reproduced in shell-model calculations derived from microscopic two-nucleon forces. Here, we present the first microscopic explanation of the oxygen anomaly based on three-nucleon forces that have been established in few-body systems. This leads to repulsive contributions to the interactions among excess neutrons that change the location of the neutron drip line from ^{28}O to the experimentally observed ^{24}O. Since the mechanism is robust and general, our findings impact the prediction of the most neutron-rich nuclei and the synthesis of heavy elements in neutron-rich environments.

DOI: 10.1103/PhysRevLett.105.032501 PACS numbers: 21.10.−k, 21.30.−x, 21.60.Cs, 27.30.+t

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

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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.

PACS numbers: 21.30.Fe, 21.60.Cs, 23.40.-s

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, its A-dependence is important

3) negligible role of 4-body and higher-order interactions for identical nucleons (for CD Bonn).

4) need to do SSM calculations with full 3-body effective interactions

5) It is always best to include the full 3-body effective/"real" interaction whenever possible!

COLLABORATORS

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Petr Navratil, Lawrence Livermore National Laboratory
Ionel Stetcu, University of Washington
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3BME with T=3/2 & 2BME with T=1

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

$$V_3^A(333;\frac{3}{2}) = \frac{1}{2}V_{2,3}^A(33;0) + \frac{5}{2}V_{2,3}^A(33;2)$$

$$V_3^A(331;\frac{1}{2}) = \frac{3}{4}V_{2,3}^A(13;1) + \frac{5}{4}V_{2,3}^A(13;2) + V_{2,3}^A(33;0)$$

$$V_3^A(331;\frac{3}{2}) = \frac{6}{4}V_{2,3}^A(13;1) + \frac{2}{4}V_{2,3}^A(13;2) + V_{2,3}^A(33;2)$$

$$V_3^A(331;\frac{5}{2}) = \frac{1}{4}V_{2,3}^A(13;1) + \frac{7}{4}V_{2,3}^A(13;2) + V_{2,3}^A(33;2)$$

$$V_3^A(311;\frac{3}{2}) = \frac{3}{4}V_{2,3}^A(13;1) + \frac{5}{4}V_{2,3}^A(13;2) + V_{2,3}^A(11;0)$$

on-diagonal 3BME with T=3/2 & 2BME with T=1

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

$$\langle 333|V_3^{A,7}|331\rangle_{3/2} = -\sqrt{\frac{5}{4}}\langle 33|V_{2,3}^{A,7}|31\rangle_2,$$

$$\langle 331|V_3^{A,7}|311\rangle_{3/2} = -\sqrt{\frac{5}{4}}\langle 33|V_{2,3}^{A,7}|31\rangle_2,$$

$$\langle 333|V_3^{A,7}|311\rangle_{3/2} = -\sqrt{\frac{1}{2}}\langle 33|V_{2,3}^{A,7}|11\rangle_0$$

$$V_2^{A,6}(ab;J_2) \to V_2^{A,6}(ab;J_2) + \frac{A-A_c-2}{3}V_{2,3}^{A}(ab;J_2)$$

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

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

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

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

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

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

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;

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

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

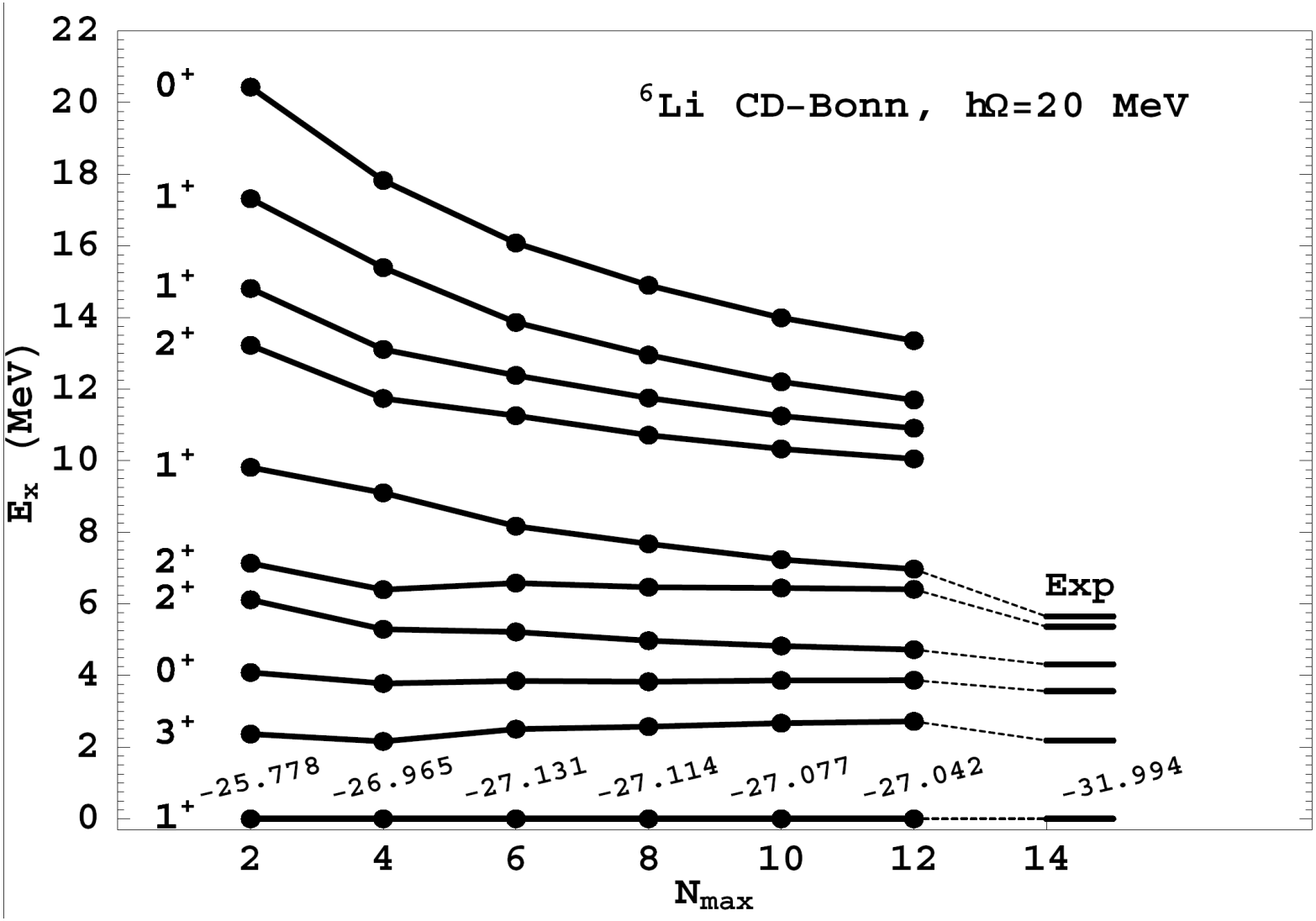
Two ways of convergence:

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

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

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



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;

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

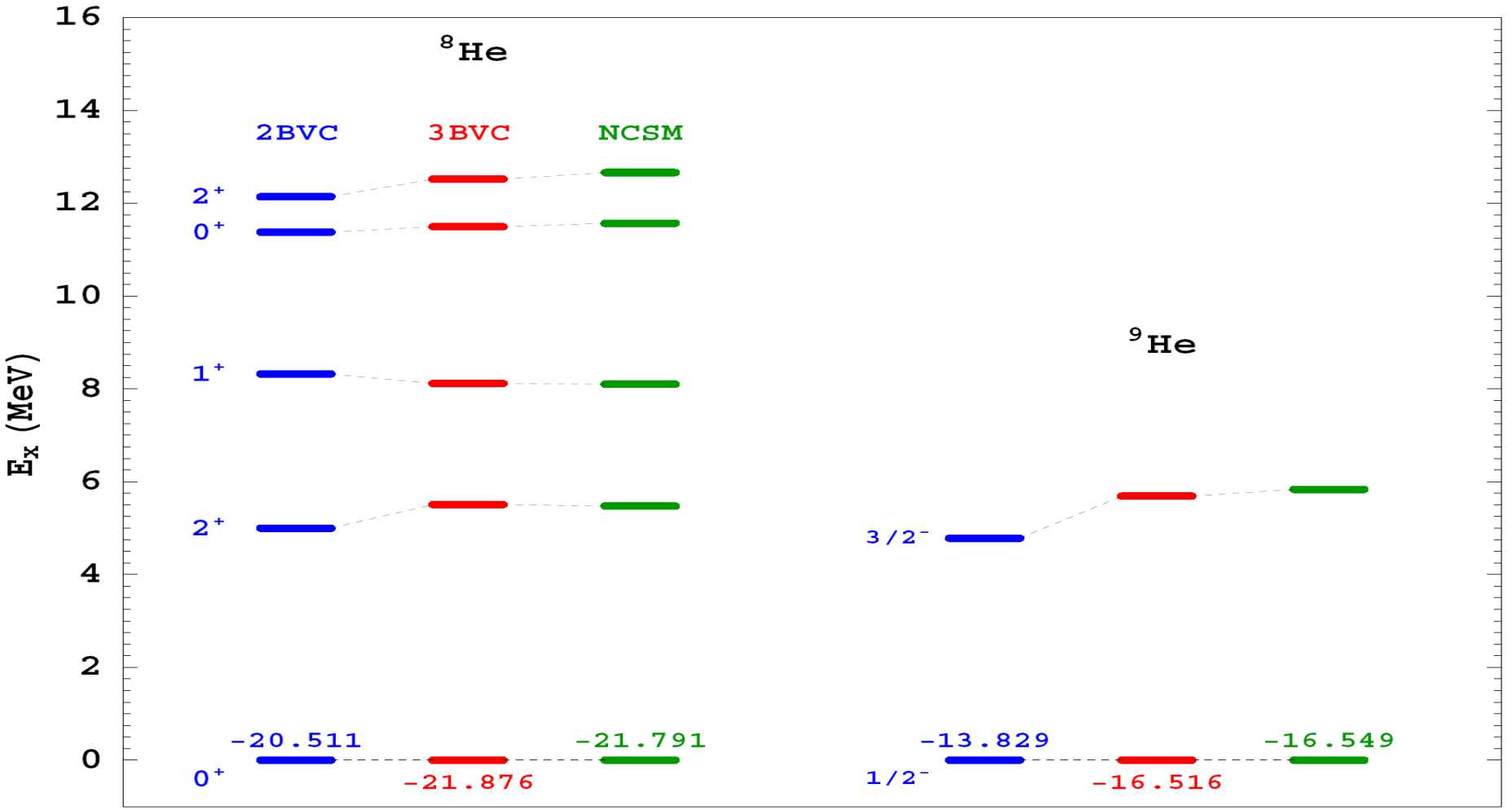
Valence Cluster Expansion

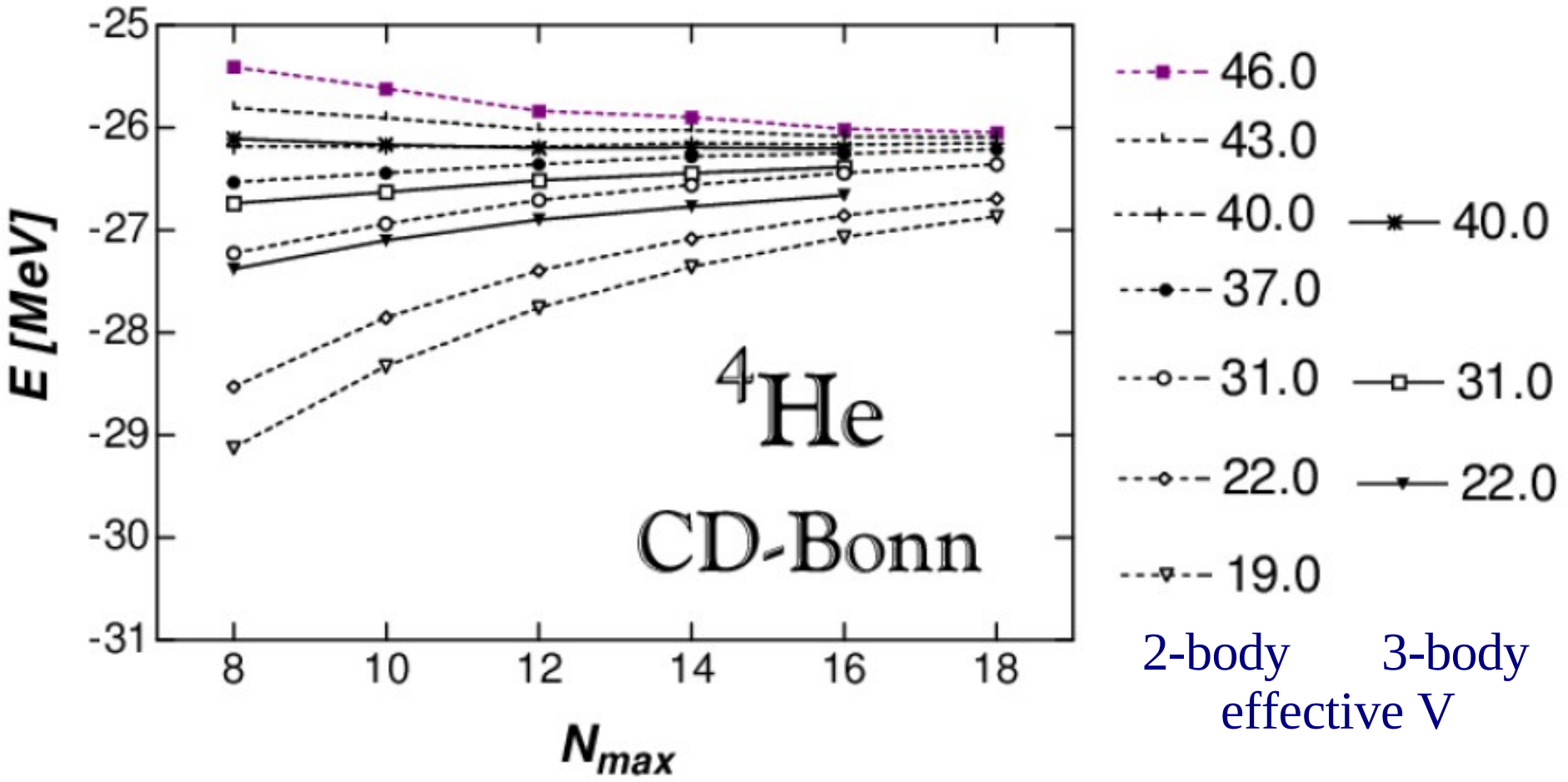
$N_{1,max} = 0$ space (p-space) ; $a_1 = A_c + a_v$; a_1 - order of cluster;

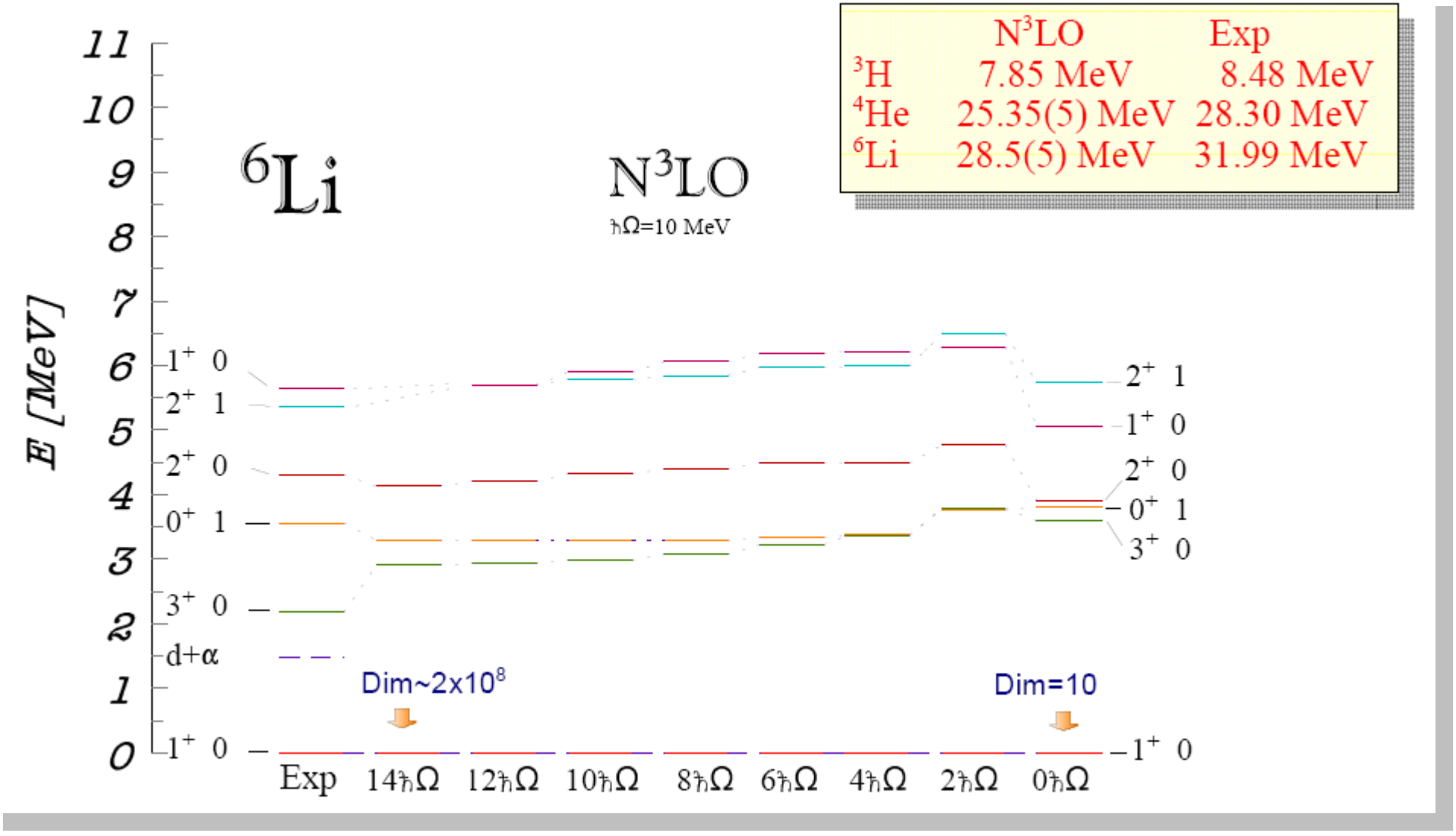
A_c - number of nucleons in core; a_v - order of valence cluster;

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

3-body Valence Cluster approximation for A>6




E [MeV]
-25
-26
-27
-28
-29
-30
-31
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



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

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

Effective operators from exact many-body renormalization

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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.

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

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:

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

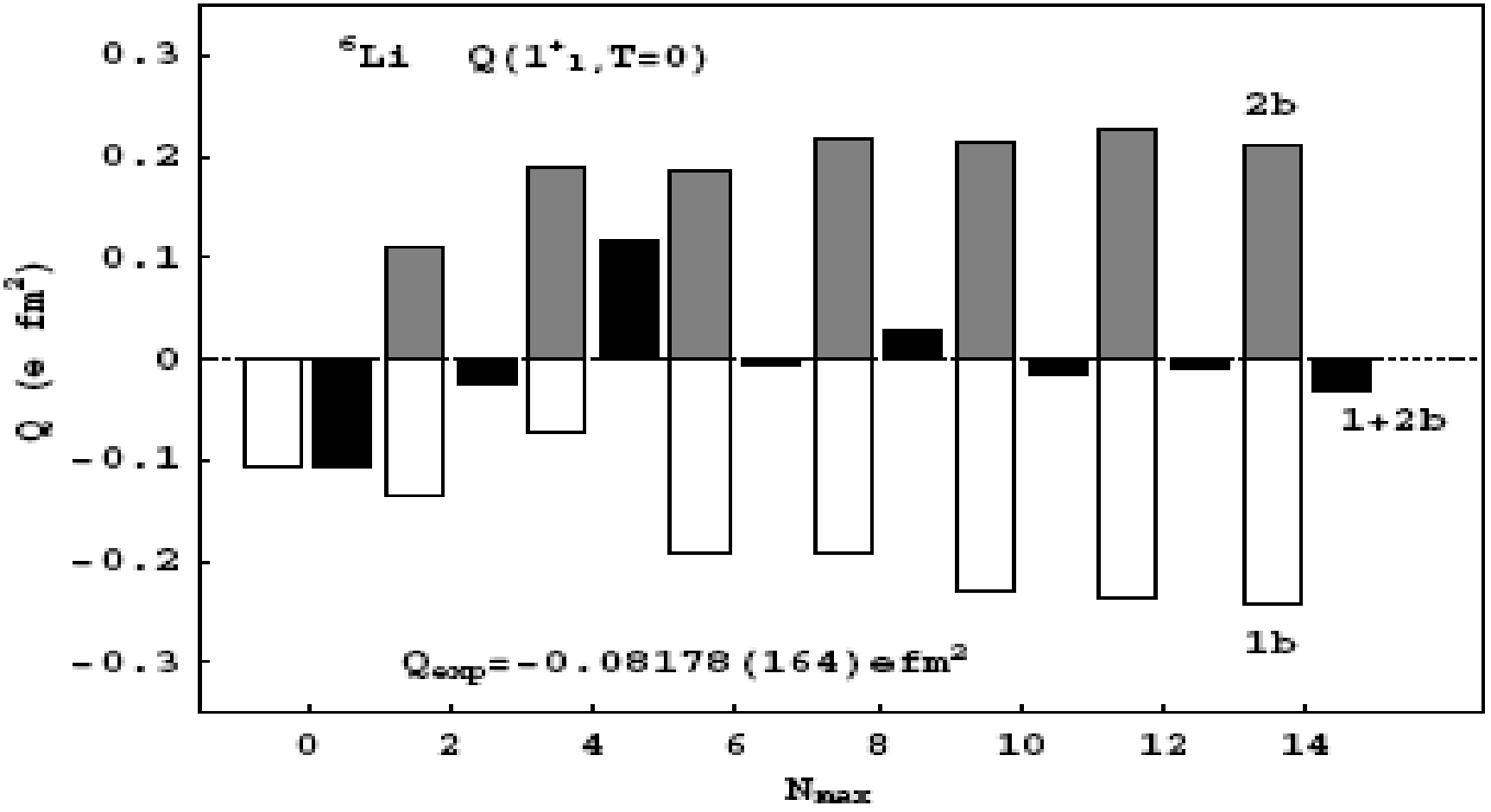

FIG. 6: The quadrupole moment of the ground state for ^{6}Li ($1^+(T = 0)$) is shown in terms of one- and two-body contributions as a function of increasing model space size.