Investigations of the A-dependence of the Core Energies and Other Terms in the Ab Initio Shell Model Formalism

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OUTLINE

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

II. Ab Initio Shell Model with a Core Approach

III. Results: Study of A-dependence
- a) 0p-shell nuclei
- b) sd-shell nuclei

IV. Summary

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

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)
BRB, P. Navratil, J.P. Vary, Prog.Part.Nucl.Phys. 69, 131 (2013).
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

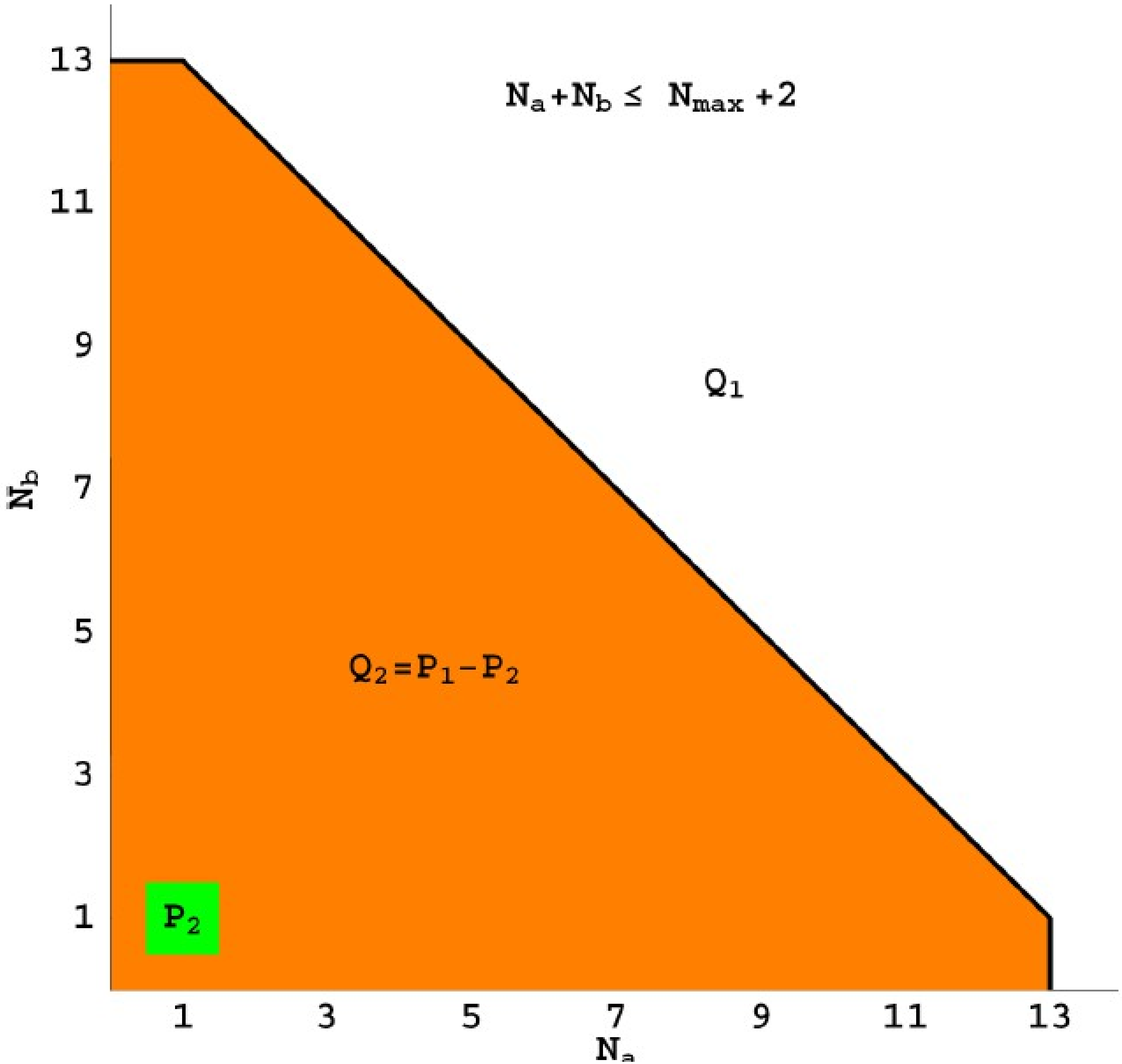
- Next, add CM harmonic-oscillator Hamiltonian

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

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}



$N_a + N_b \leq N_{max} + 2$
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

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

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

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

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;

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

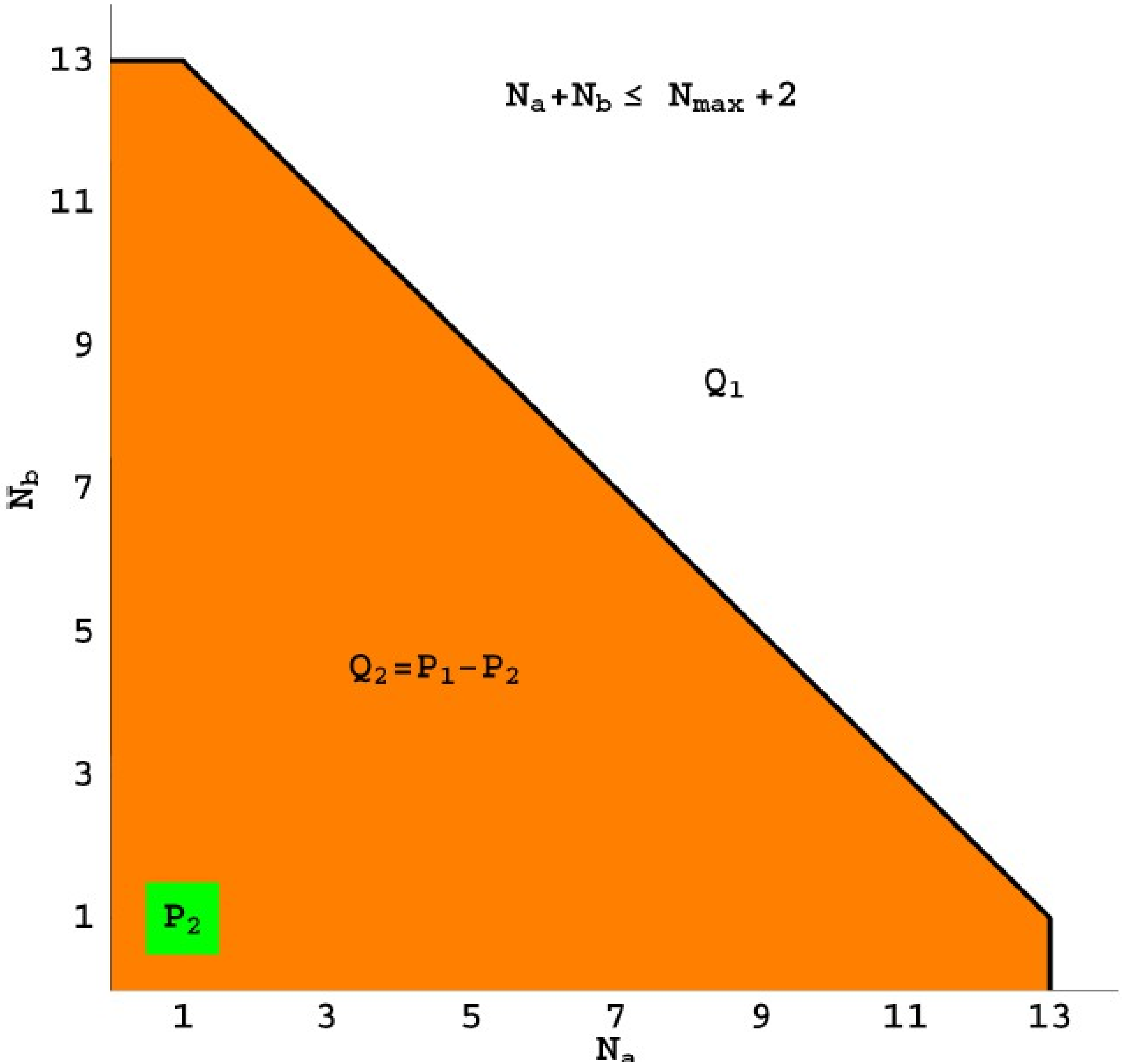
$$U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} E^{\Omega}_{A,2,P} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

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

Two ways of convergence:

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

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



$N_a + N_b \leq N_{max} + 2$
Q_1
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N_b
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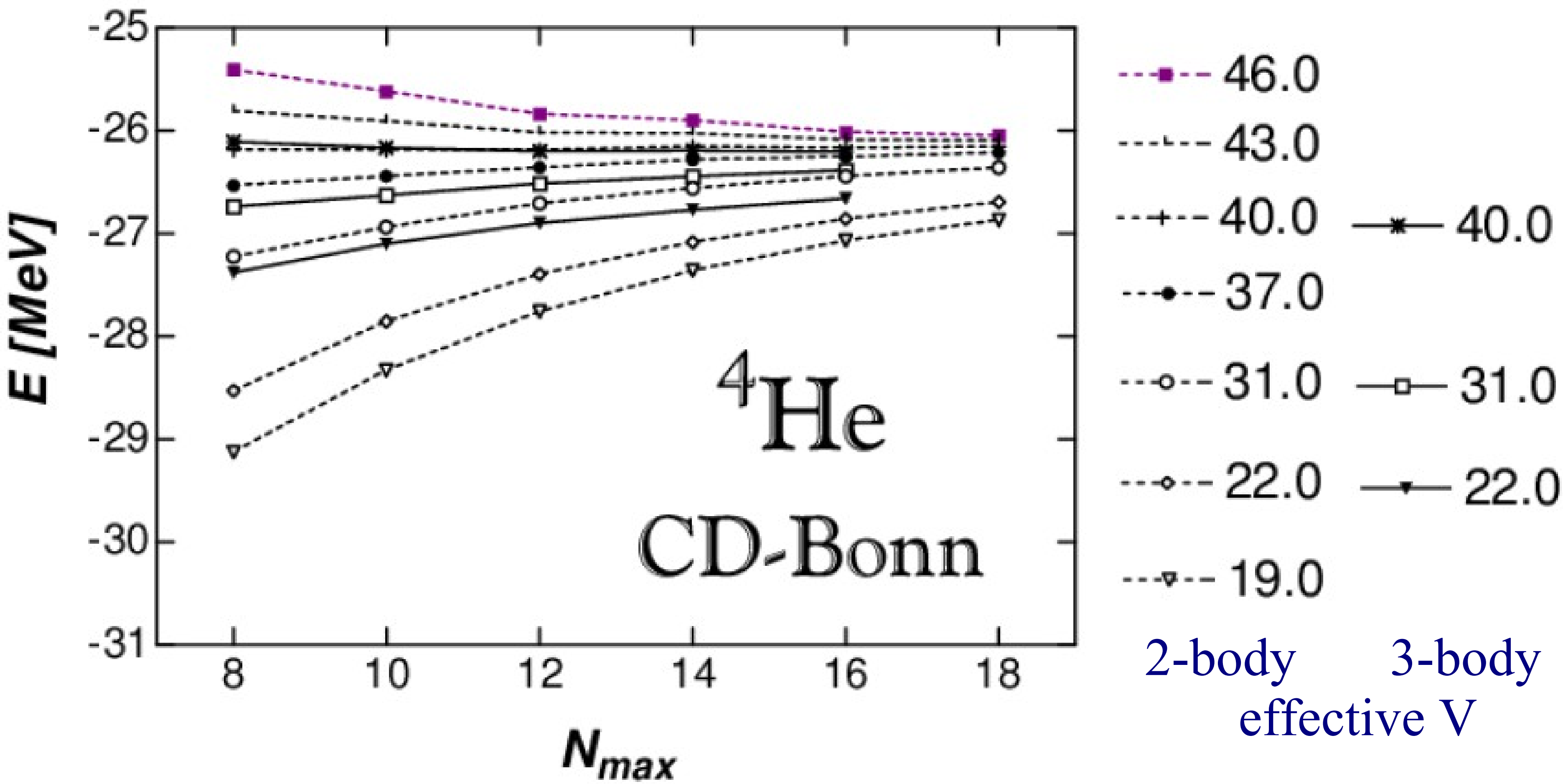
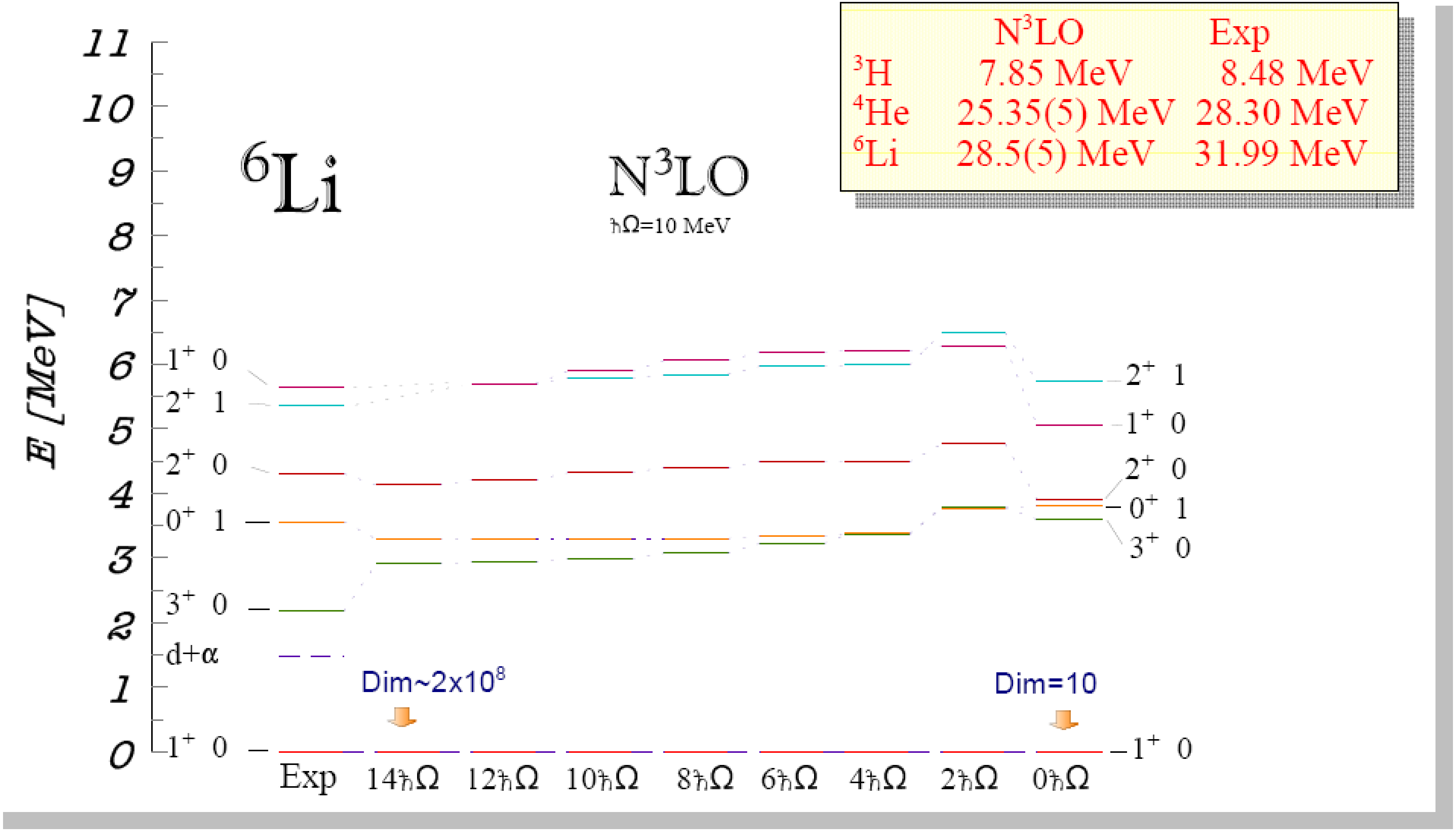
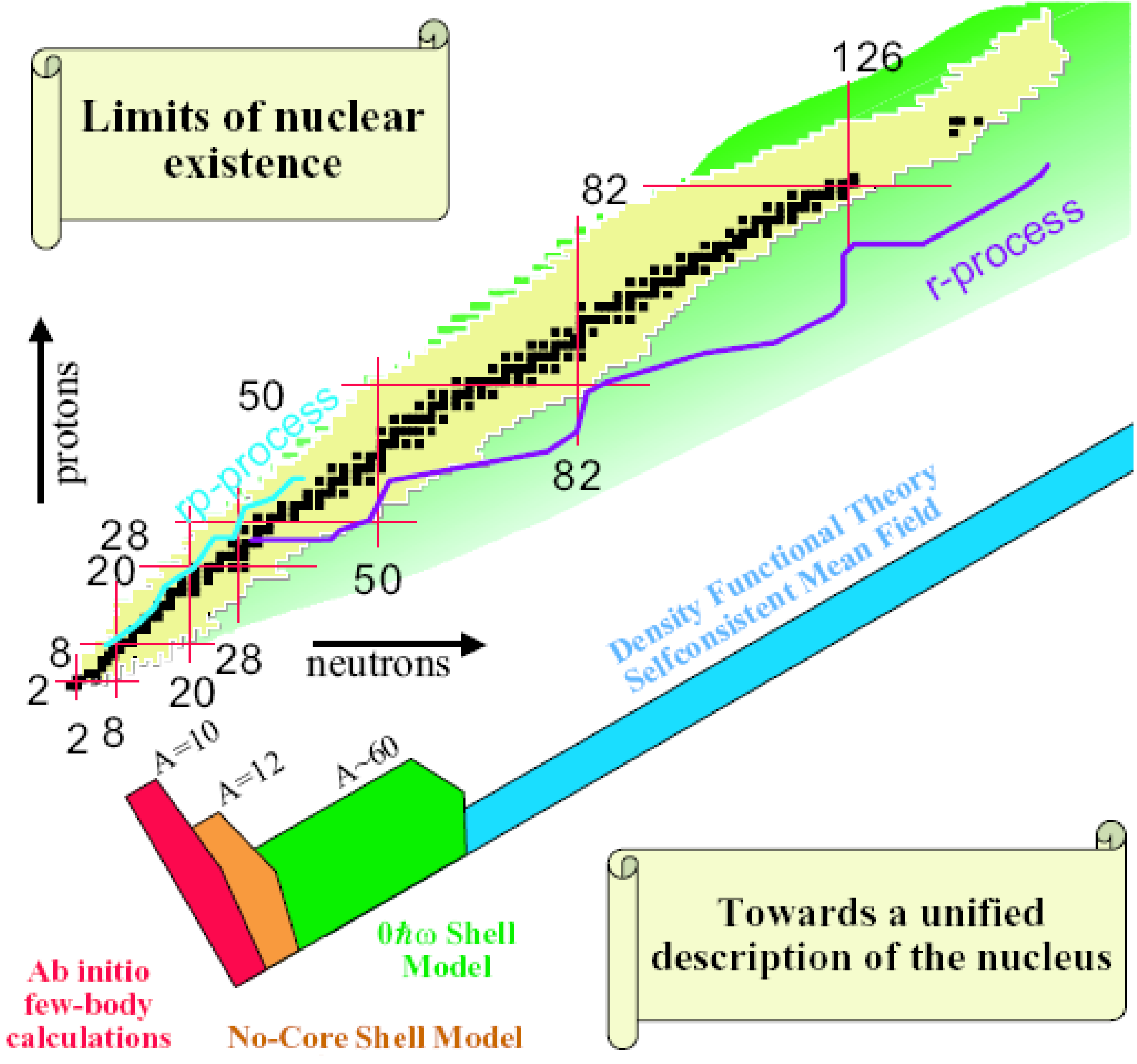


-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N_{max}
^{4}He
CD-Bonn
46.0
43.0
40.0
40.0
37.0
31.0
31.0
22.0
22.0
19.0
2-body
3-body
effective V



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



Limits of nuclear existence
protons
neutrons
rp-process
r-process
126
82
50
28
20
8
2
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

II. Ab Initio Shell Model with a Core Approach

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

Ab-initio shell model with a core

A. F. Lisetskiy,[1,*] B. R. Barrett,[1] M. K. G. Kruse,[1] P. Navratil,[2] I. Stetcu,[3] and J. P. Vary[4]
[1]*Department of Physics, University of Arizona, Tucson, Arizona 85721, USA*
[2]*Lawrence Livermore National Laboratory, Livermore, California 94551, USA*
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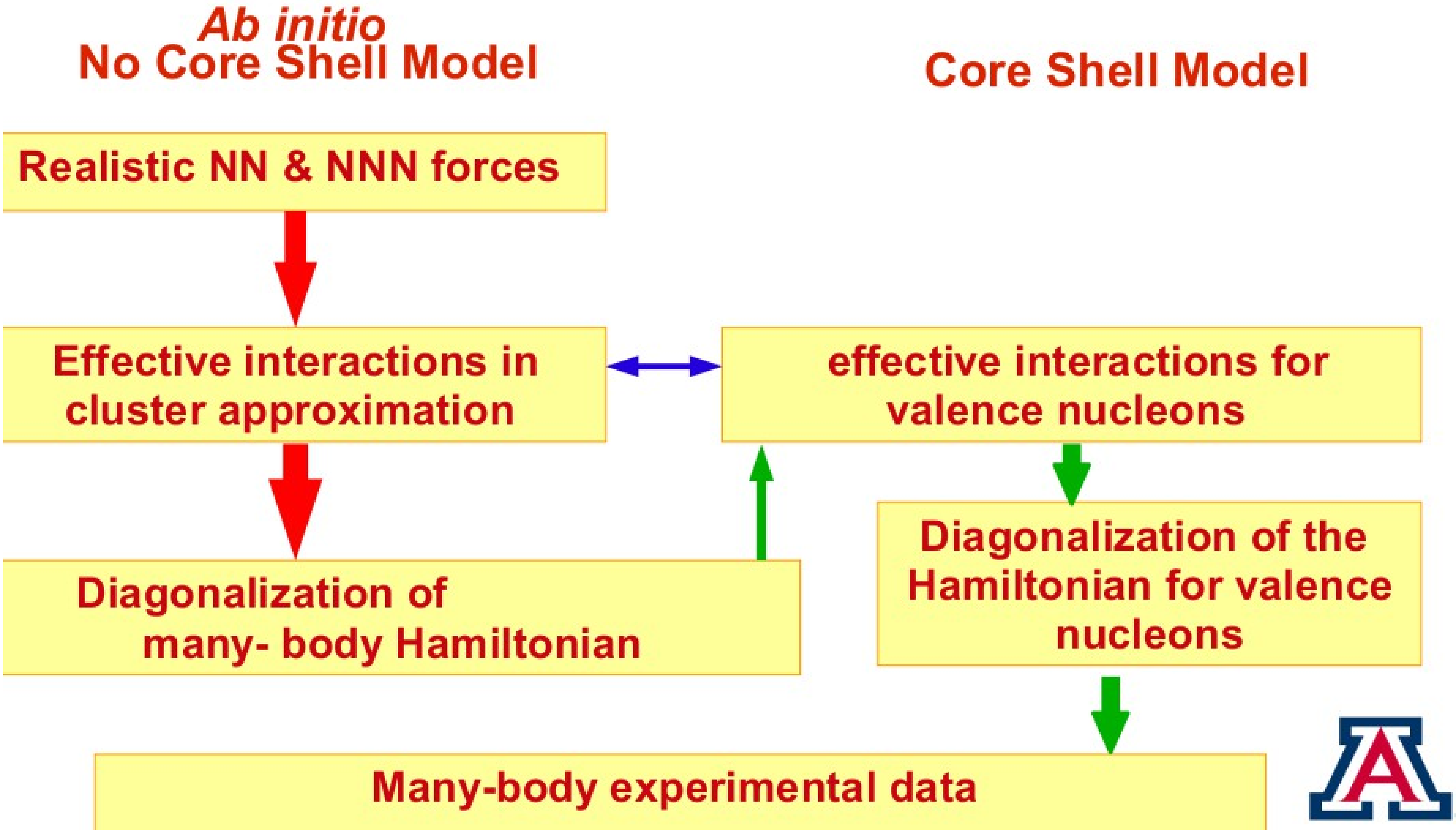
[4]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
(Received 20 June 2008; published 10 October 2008)

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.

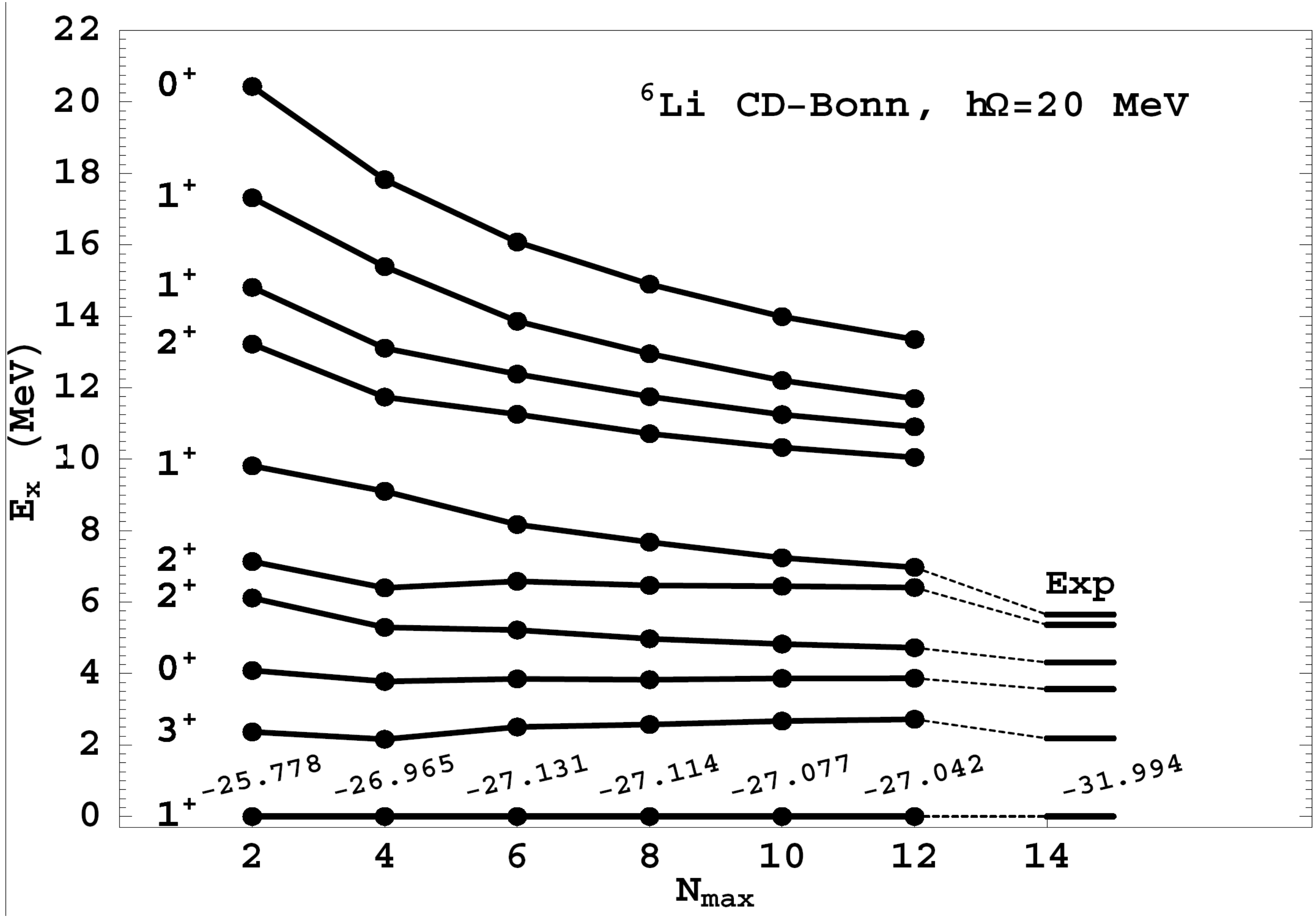
DOI: 10.1103/PhysRevC.78.044302 PACS number(s): 21.10.Hw, 21.60.Cs, 23.20.Lv, 27.20.+n

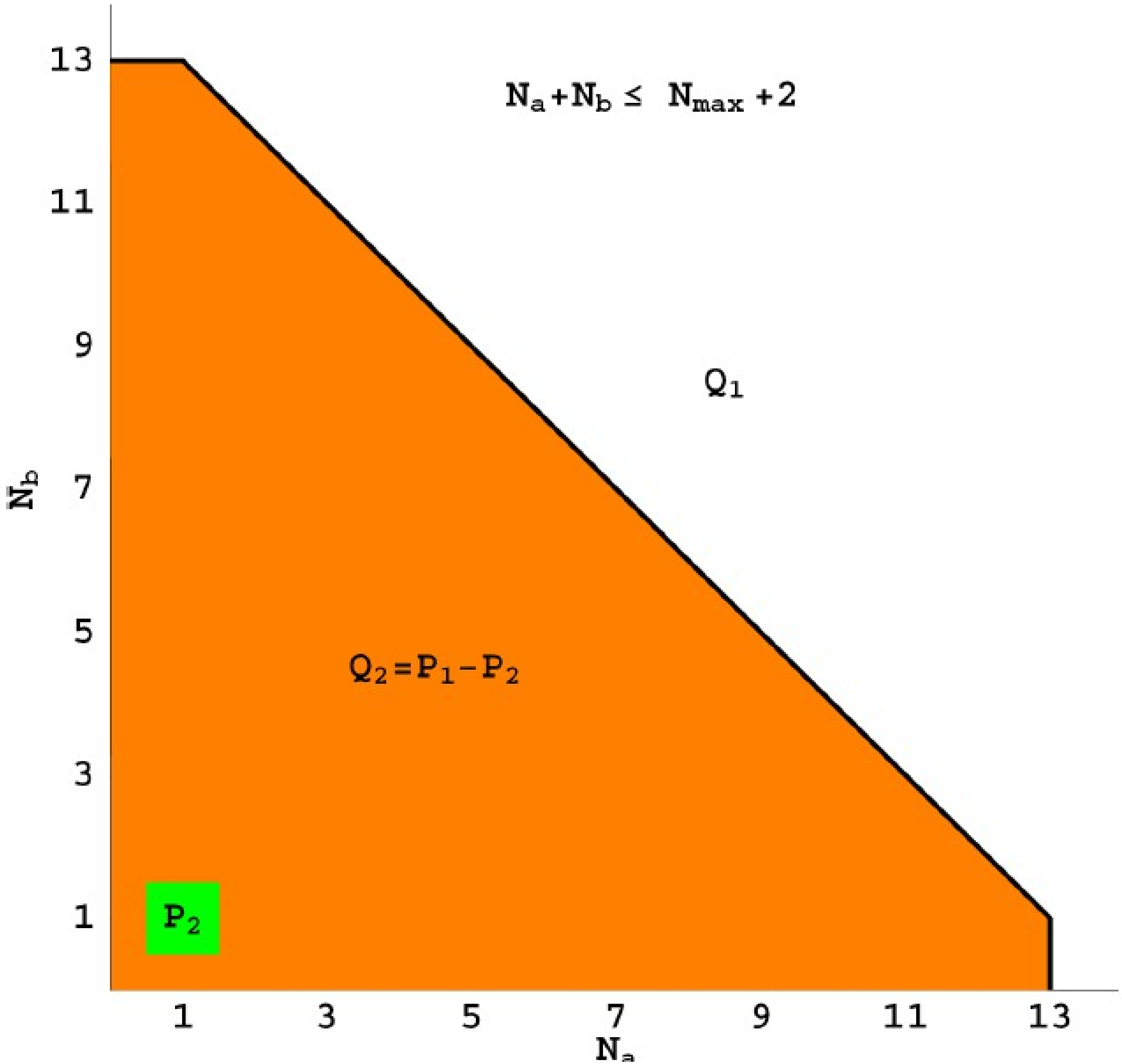
From few-body to many-body



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





13
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N_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 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;

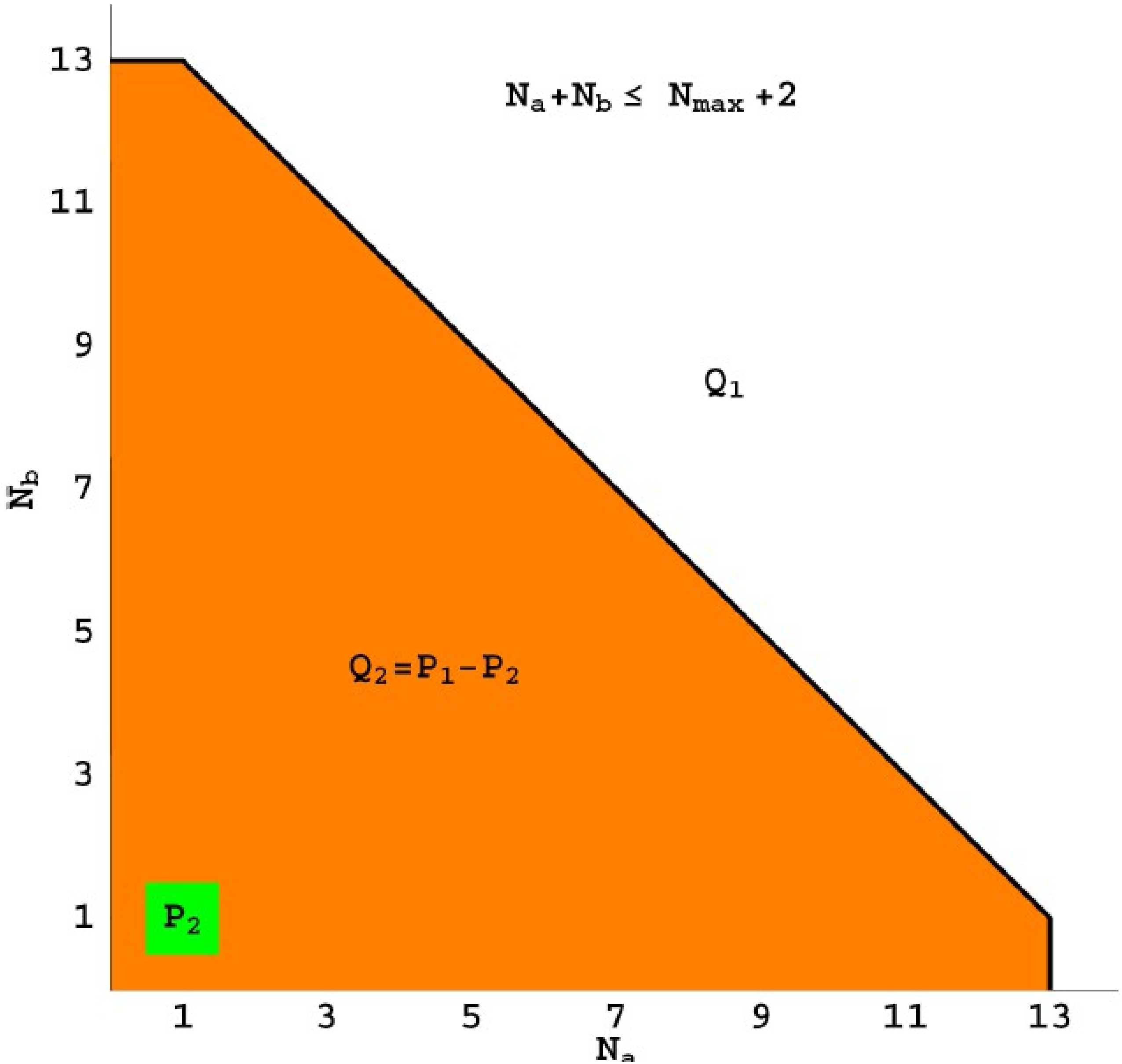
$$\mathcal{H}_{A,a_1}^{N_{1,\max},N_{\max}} = \frac{U^{A,\dagger}_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1} U^{A}_{a_1,P_1}}} E^{N_{\max},\Omega}_{A,a_1,P_1} \frac{U^{A}_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1} U^{A}_{a_1,P_1}}}$$

<u>Valence Cluster Expansion</u>

$N_{1,max} = 0$ 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;

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


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

Effective Hamiltonian for SSM

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Valence Cluster Expansion

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A_C - number of nucleons in core; a_V - order of valence cluster;

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

III. Results: Study of A-dependence

a) 0p-shell nuclei

b) sd-shell nuclei

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

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

CD-Bonn potential

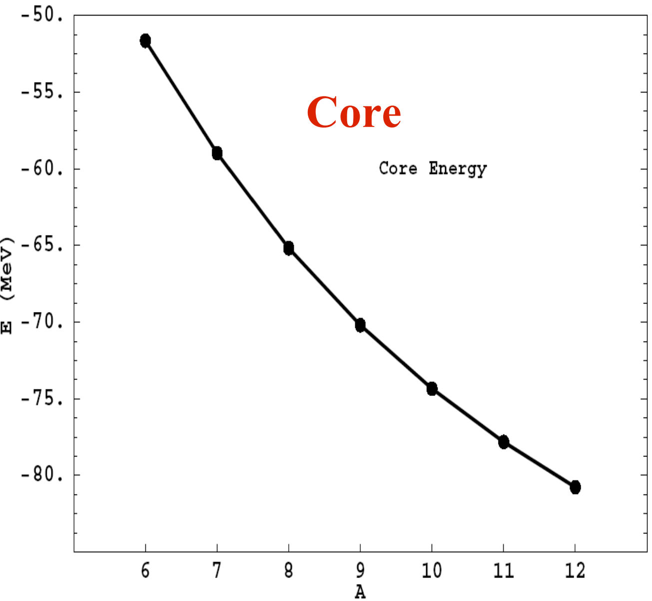
Need NCSM results in N_{max} space for

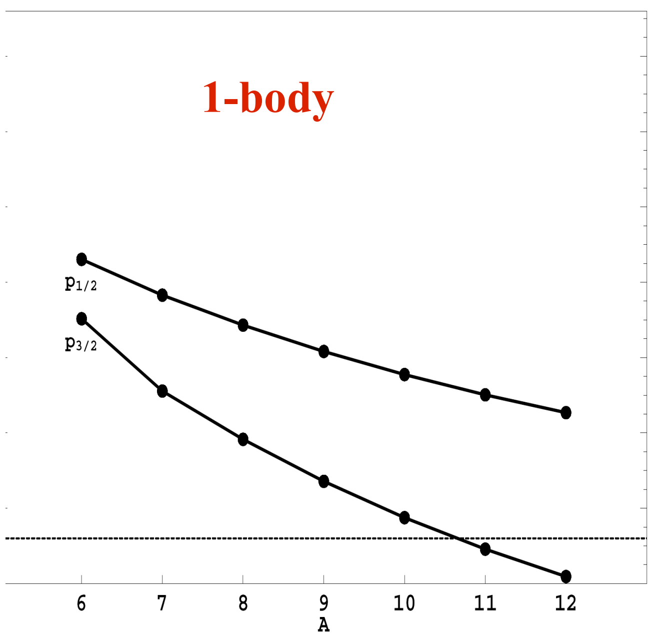
^{4}He | ^{5}He ^{5}Li | ^{6}He ^{6}Li ^{6}Be

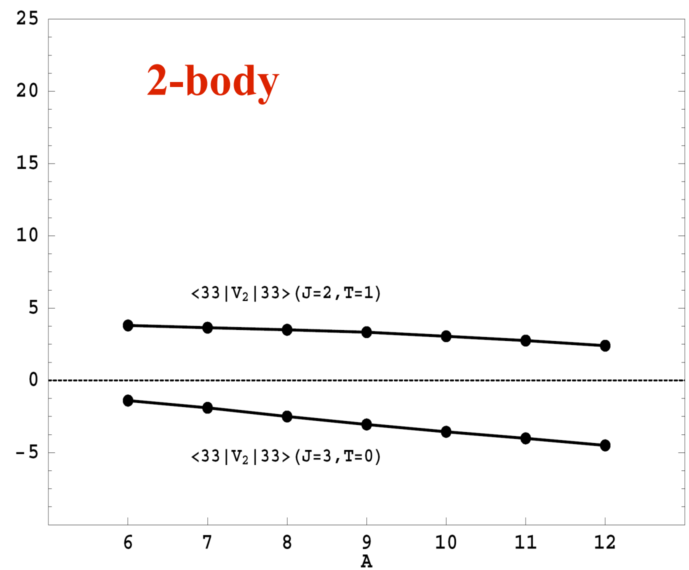
$$H_{A,2}^{N_{\max},\Omega,\mathrm{eff}}$$

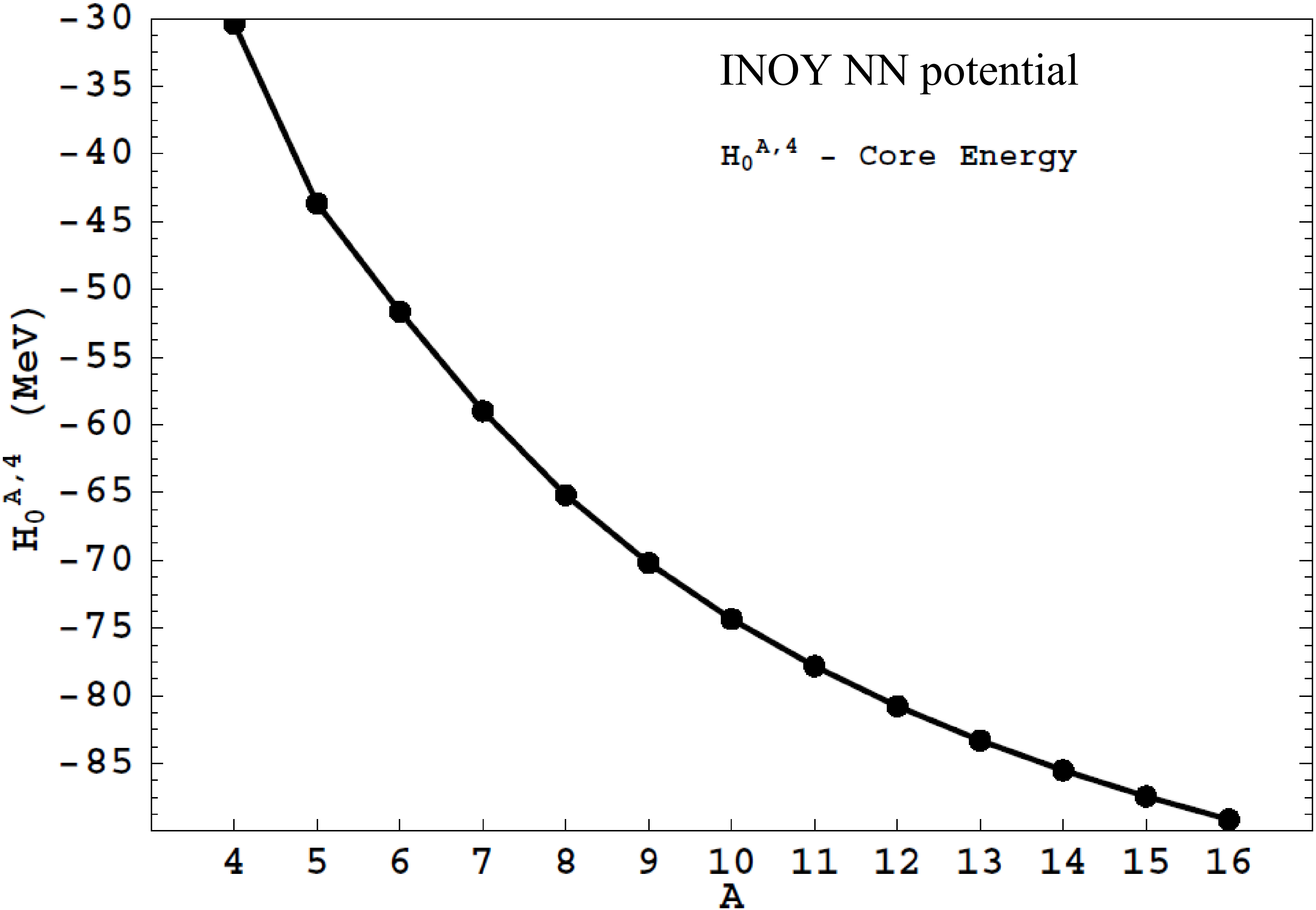
$N_{max} = 6$

With effective interaction for A !!!









INOY NN potential
$H_0^{A,4}$ - Core Energy
$H_0^{A,4}$ (MeV)
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
4
5
6
7
8
9
10
11
12
13
14
15
16
A

Manuscript in preparation for submission for publication

Ab initio effective interactions for *sd*-shell valence nucleons

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[2]*Department of Physics, University of Arizona, Tucson,AZ 85721*
[3]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011*
[4]*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119234, Russia*
[5]*Pacific National University, 136 Tikhookeanskaya st., Khabarovsk 680035, Russia*

We perform *ab initio* no core shell model calculations for $A = 18$ and 19 nuclei in a $4\hbar\Omega$ model space using JISP16 and CD-Bonn nucleon-nucleon potentials and project the many-body Hamiltonians onto the $0\hbar\Omega$ model space to construct the effective A-body Hamiltonians in the *sd*-shell. We separate the effective A-body Hamiltonians with $A = 18$ and $A = 19$ into inert core, one- and two-body components. Then, these core, one- and two-body components are used to perform standard shell model calculations for the $A = 18$ and $A = 19$ systems with valence nucleons in the *sd*-shell. Finally, we compare the standard shell model results with the exact no core shell model results in the $4\hbar\Omega$ model space for the $A = 18$ and $A = 19$ systems.

PACS numbers: 21.10.Hw,21.60.Cs,23.20.En,23.20.Lv,23.20.-g,27.40.+z
Keywords: NCSM, ab initio, effective interactions

TABLE II: Proton and neutron single particle energies for JISP16 interactions with the mass of $A = 18$ and $A = 19$.

	$A = 18$ ($E_{core} = -115.529$)			$A = 19$ ($E_{core} = -115.319$)		
a	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$
ϵ_a^p	0.603	9.748	1.398	0.627	9.774	1.419
ϵ_a^n	-3.068	6.262	-2.270	-3.044	6.289	-2.248

TABLE III: Proton and neutron single particle energies for CD-Bonn interactions with the mass of $A = 18$ and $A = 19$.

	$A = 18$ ($E_{core} = -148.268$)			$A = 19$ ($E_{core} = -162.418$)		
a	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$
ϵ_a^p	15.812	23.463	16.349	13.927	21.671	14.343
ϵ_a^n	12.069	19.863	12.565	10.154	18.043	10.534

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}

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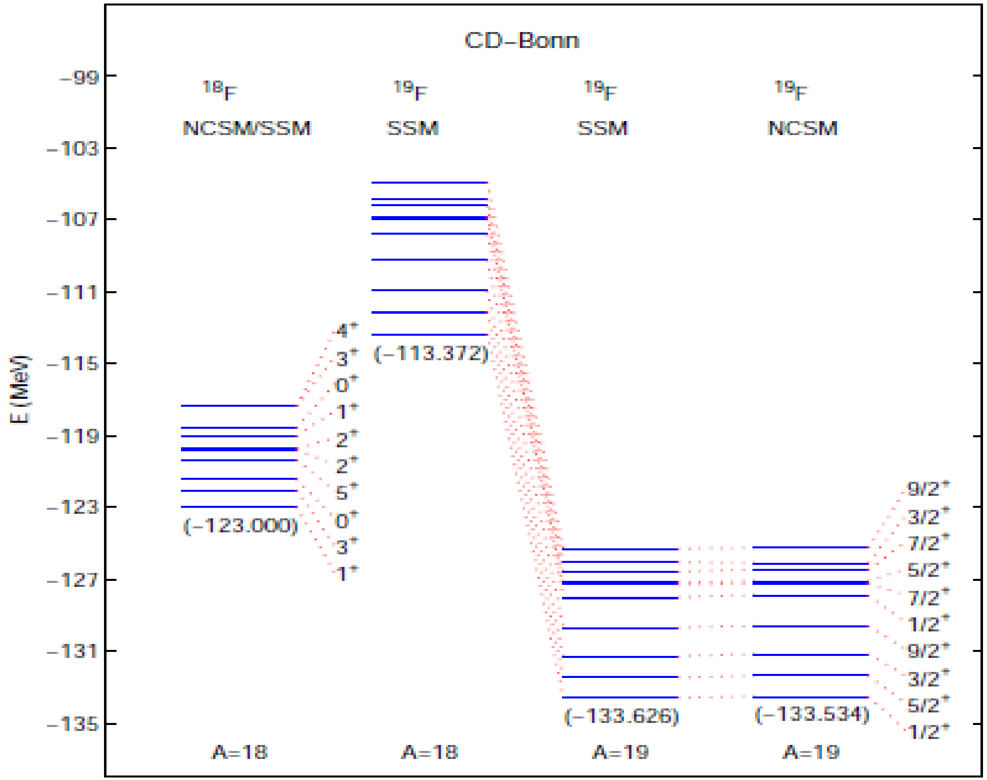

FIG. 2: The ground and low-lying excited states energies of ^{18}F and ^{19}F obtained by the SSM and NCSM calculations using the effective CD-Bonn interaction with the mass of $A = 18$ and $A = 19$. The tags $A = 18$ and $A = 19$ at the bottom of each column refer to the effective CD-Bonn interaction obtained by using the mass of $A = 18$ and $A = 19$.

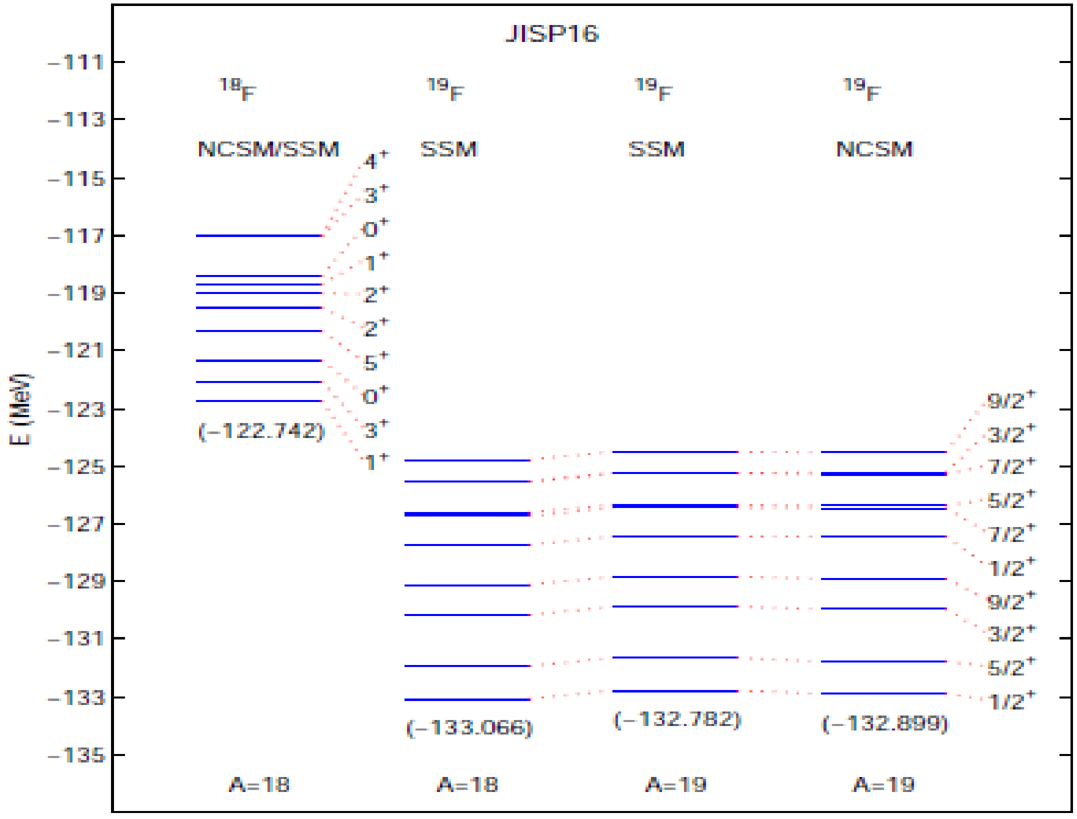

FIG. 1: The ground and low-lying excited states energies of ^{18}F and ^{19}F obtained by the SSM and NCSM calculations using the effective JISP16 interaction with the mass of $A = 18$ and $A = 19$. The tags $A = 18$ and $A = 19$ at the bottom of each column refer to the effective JISP16 interaction obtained by using the mass of $A = 18$ and $A = 19$.

IV. Summary

The separation of the doubly truncated 2-body matrix elements into a core energy, s.p. energies, and residual 2-body effective interactions is not unique.

A new procedure for performing this separation yields results that are closer to the usual input for Standard Shell Model calculations and have a much weaker A-dependence.

Additional calculations are being performed to further investigate this new procedure, especially for sd-shell nuclei.