Ab initio Effective Interactions for sd-shell Valence Nucleons

Bruce R. Barrett
University of Arizona, Tucson

THE UNIVERSITY OF ARIZONA.
Arizona's First University.

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COLLABORATORS

Erdal Dikmen, Suleyman Demirel U., Isparta, Turkey
Michael Kruse, Lawrence Livermore National Laboratory
Alexander Lisetskiy, Mintec, Inc., Tucson
Pieter Maris, Iowa State University
Petr Navratil, TRIUMF, Vancouver, BC, Canada
A. M. Shirokov, Lomonosov Moscow State U.
Ionel Stetcu, Los Alamos National Laboratory
James P. Vary, Iowa State University

OUTLINE

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

II. Ab Initio Shell Model with a Core Approach

III. Results: sd-shell

IV. Summary/Outlook

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

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 <u>62,</u> 054311 (2000)

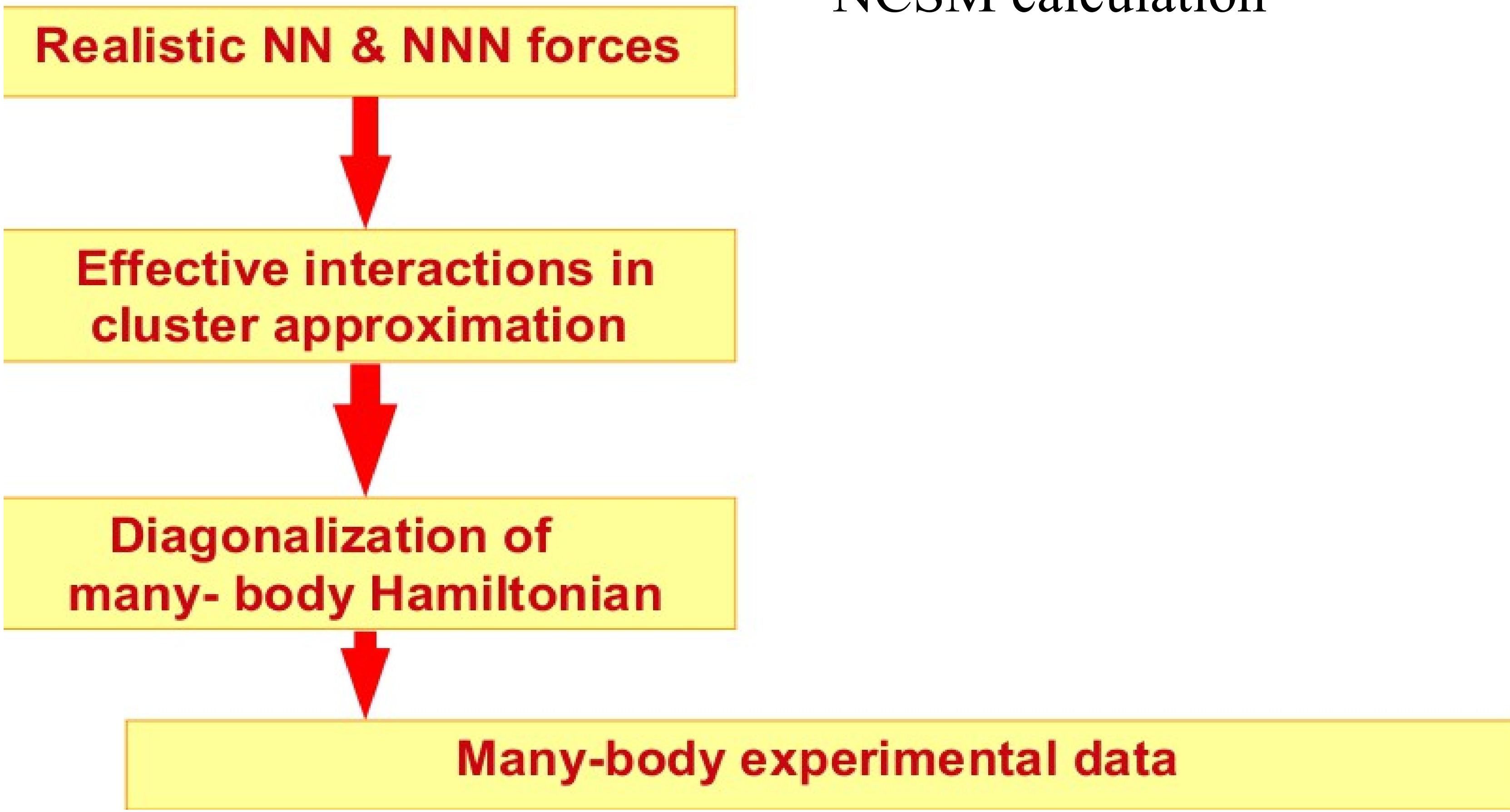
BRB, P. Navratil, J.P. Vary, Prog.Part.Nucl.Phys. 69, 131 (2013).

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

Flow chart for a standard NCSM calculation



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

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

$$a < A$$

Effective interaction in a projected model space

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

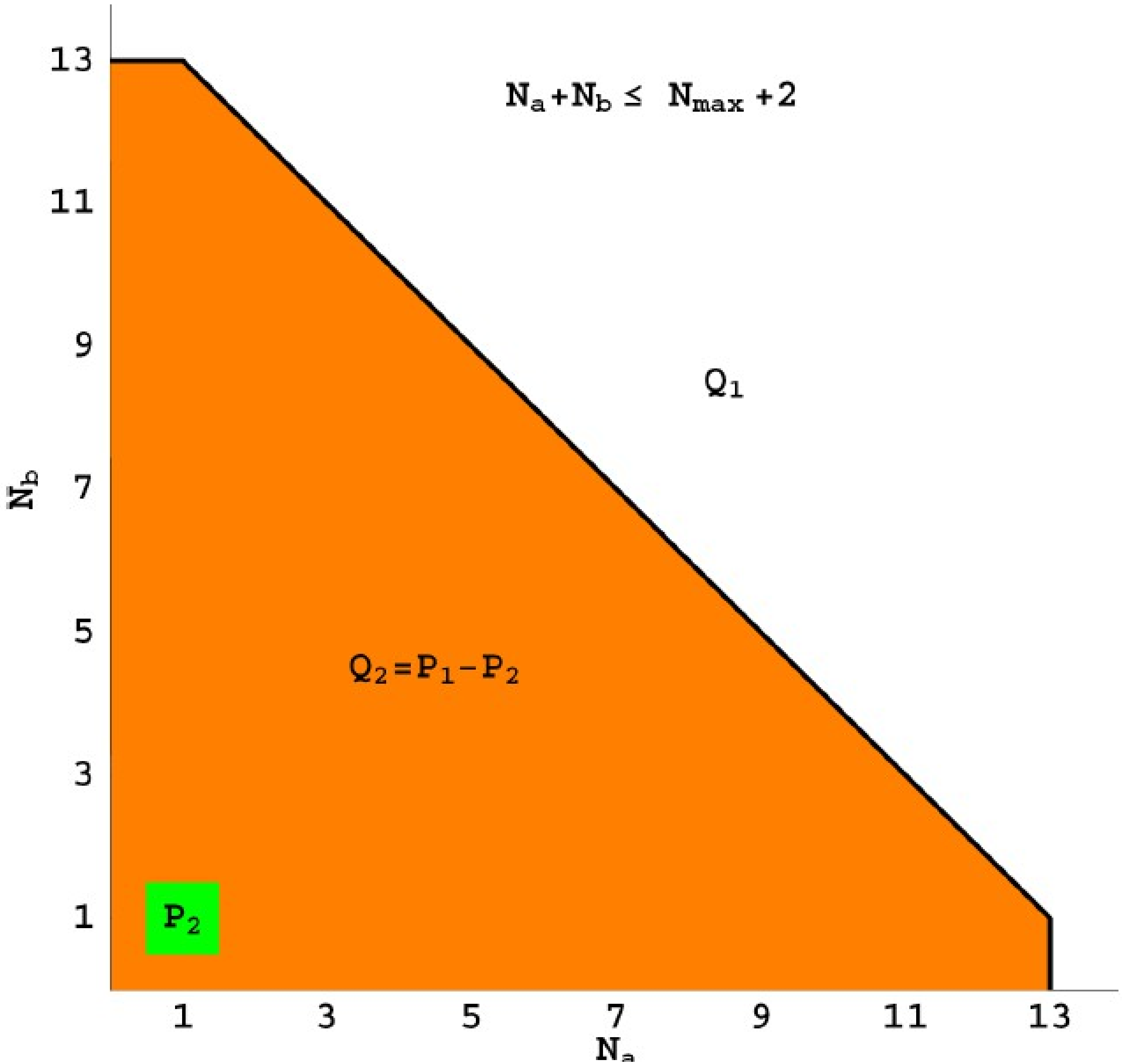
$$\mathcal{H}\Phi_\beta = E_\beta \Phi_\beta$$

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

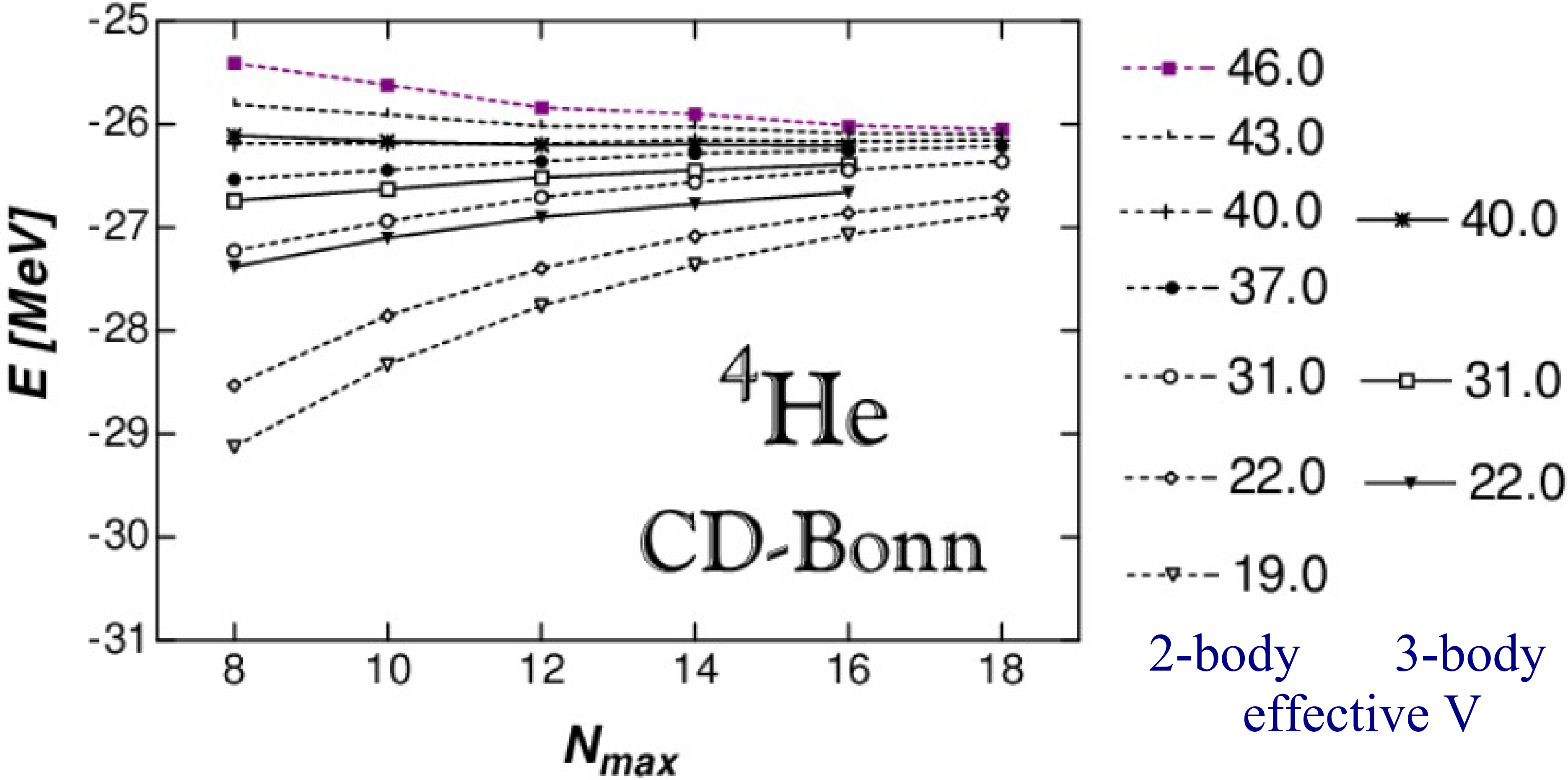
P is a projection operator from S into $\mathcal{S}$

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

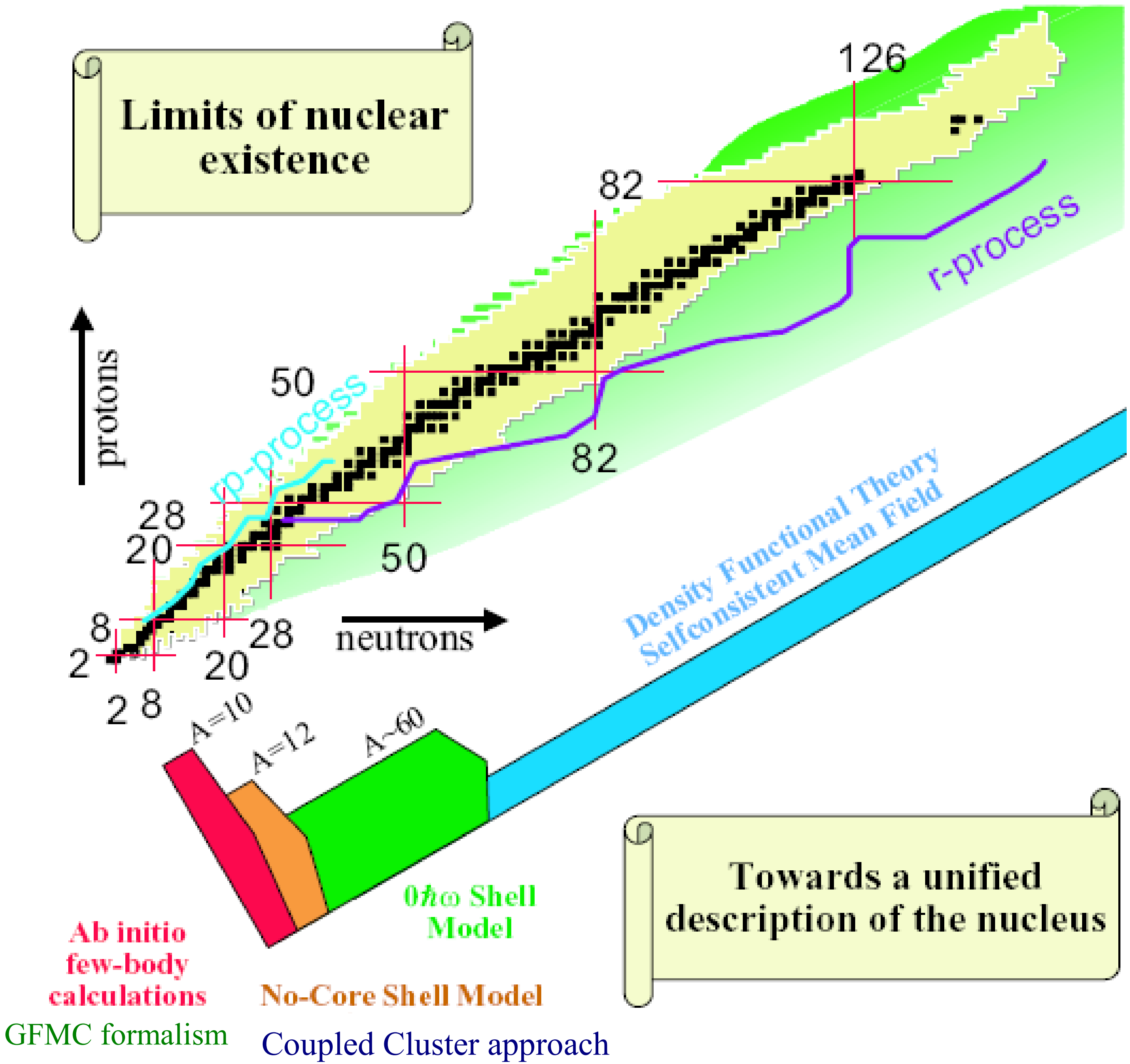
$$\mathcal{H} = \sum_{\beta \epsilon \mathcal{S}} |\Phi_\beta > E_\beta < \tilde{\Phi}_\beta|$$



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



-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N_max
4He
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

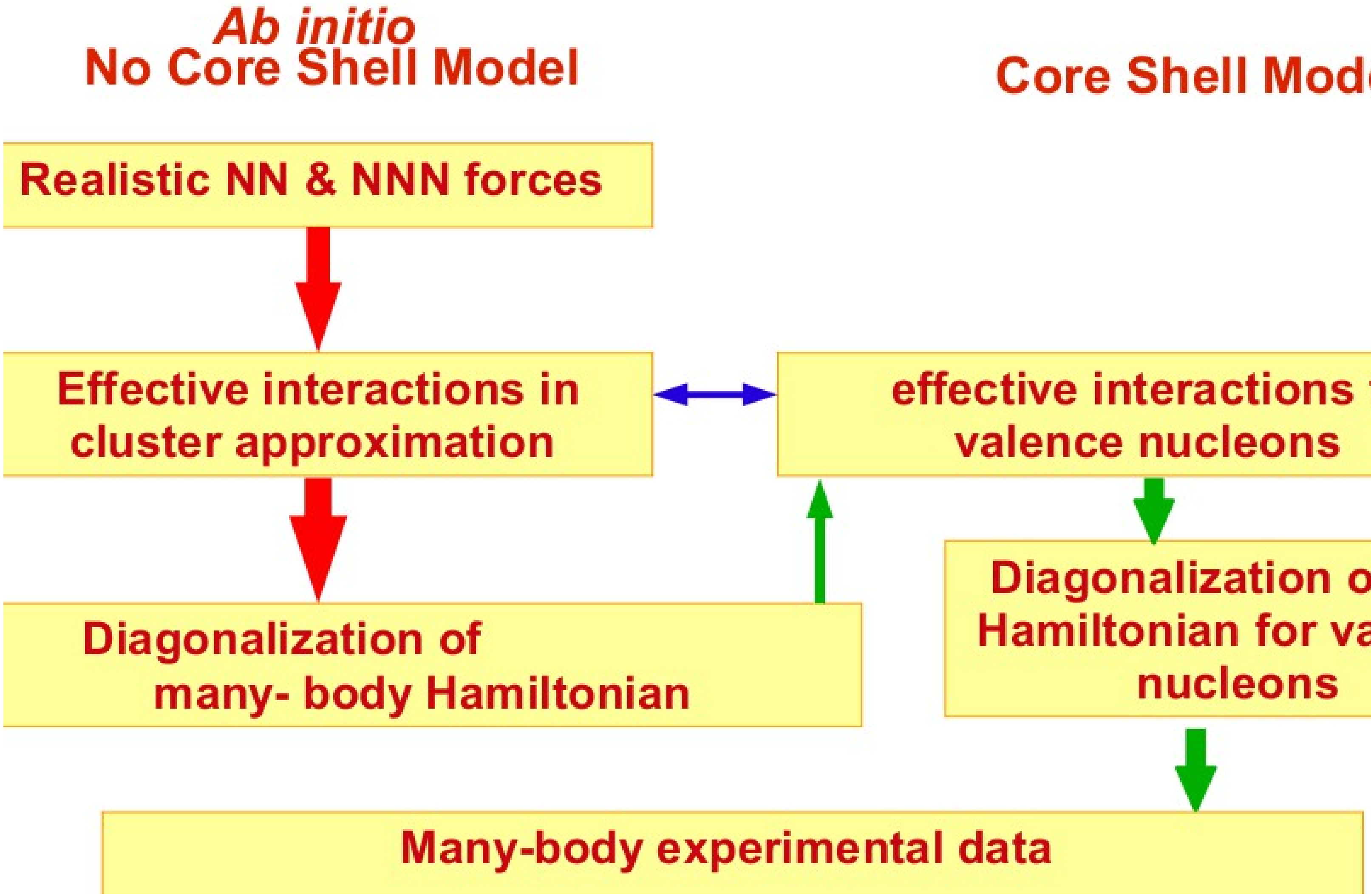


Limits of nuclear existence
protons
neutrons
126
82
50
28
20
8
2
2 8
20
28
50
82
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
Ab initio few-body calculations
GFMC formalism
No-Core Shell Model
Coupled Cluster approach
0ħω Shell Model
Towards a unified description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

II. Ab Initio Shell Model with a Core Approach

From few-body to many-body

Using the NCSM to calculate the shell model input



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*
[3]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[4]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*
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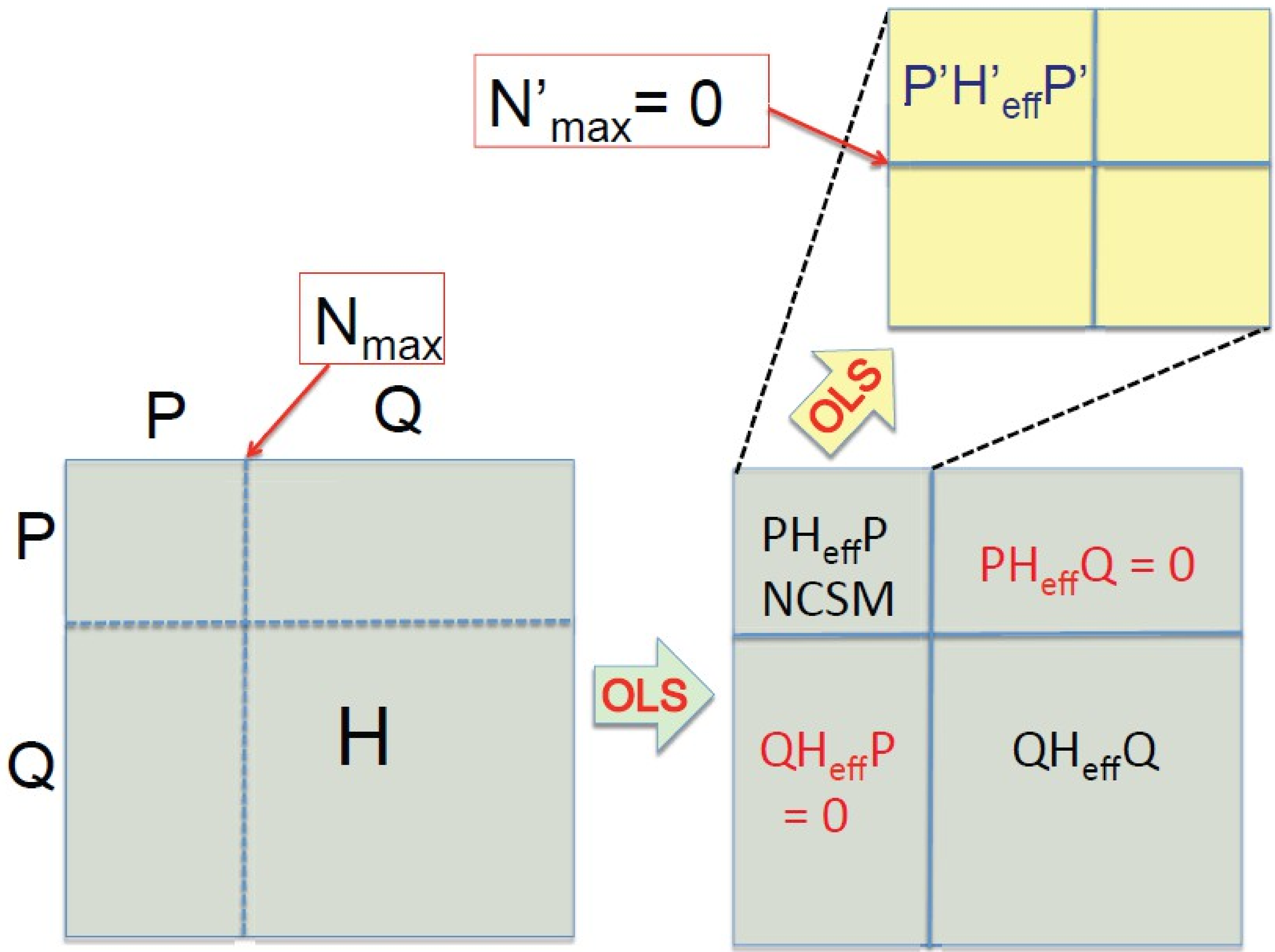
We construct effective two- and three-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ *ab initio* no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians 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.

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

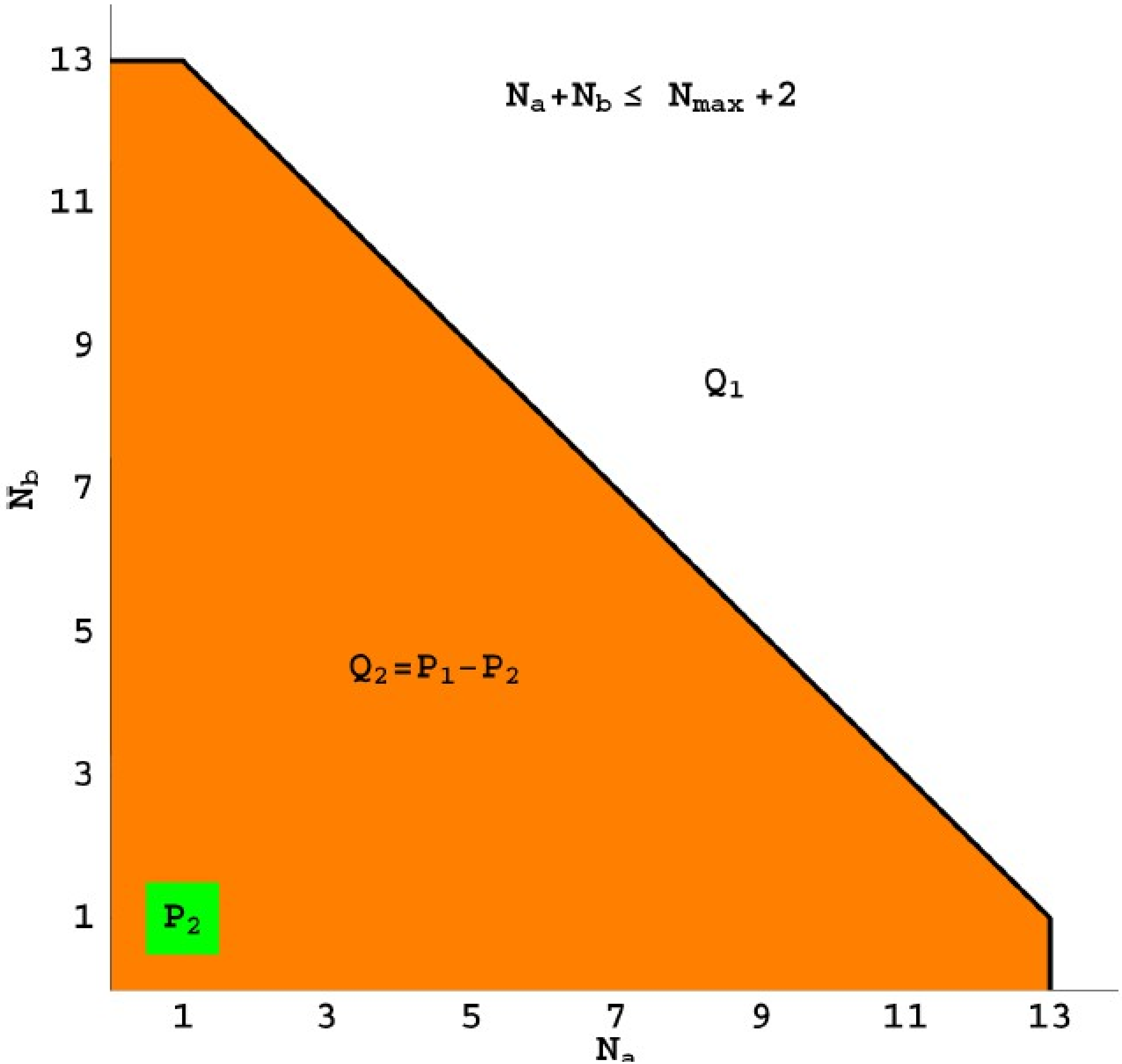
Also P. Navratil, M. Thoresen and B.R.B., PRC 55, R573 (1997)

FORMALISM

1. Perform a large basis NCSM for a core + 2N system, e.g., 18^F.
2. Use Okubo-Lee-Suzuki transformation to project these results into a single major shell to obtain effective 2-body matrix elements.
3. Separate these 2-body matrix elements into a core term, single-particle energies and residual 2-body interactions, i.e., the standard input for a normal Shell Model calculation.
4. Use these values for performing SM calculations in that shell.



N'max= 0
P'H'effP'
Nmax
OLS
P
Q
P
Q
H
OLS
PHeffP
NCSM
PHeffQ = 0
QHeffP
= 0
QHeffQ



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

How to calculate the Shell Model 2-body effective interaction:

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;

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

III. Results: sd-shell nuclei

Submitted for publication

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

E. Dikmen,[1,2,*] A. F. Lisetskiy,[2,†] B. R. Barrett,[2,‡] P. Maris,[3,§] A. M. Shirokov,[3,4,5,¶] and J. P. Vary[3,**]

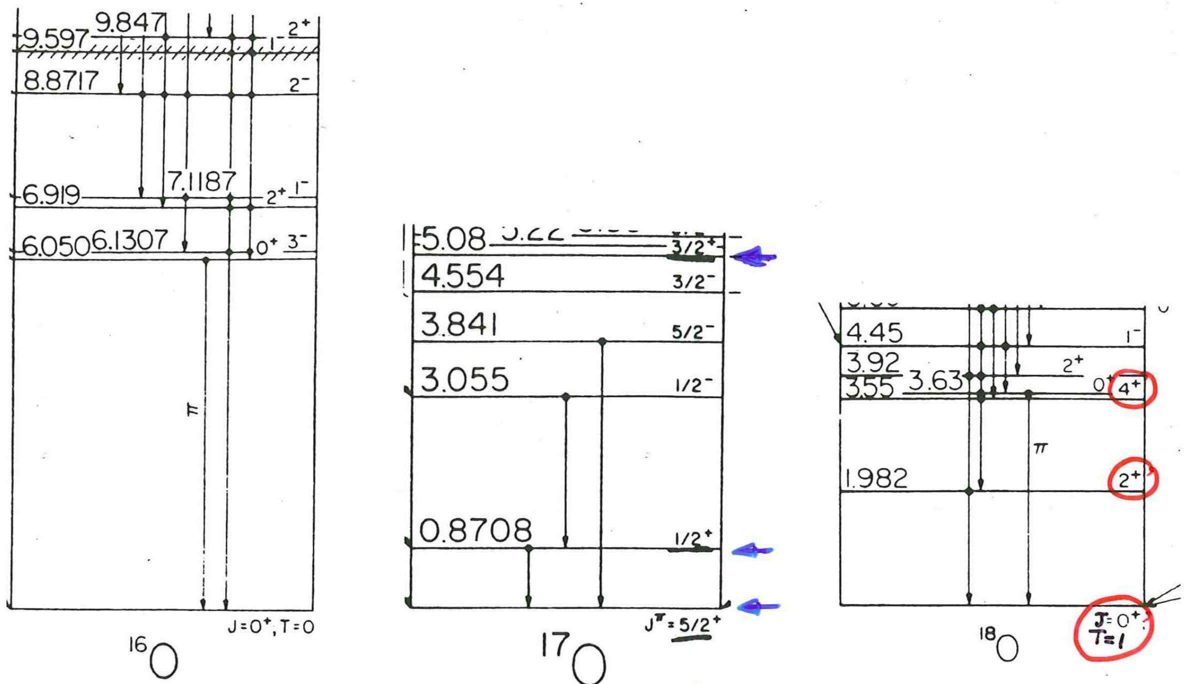
[1] *Department of Physics, Suleyman Demirel University, Isparta, Turkey*
[2] *Department of Physics, University of Arizona, Tucson, Arizona 85721*
[3] *Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011*
[4] *Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia*
[5] *Pacific National University, 136 Tikhookeanskaya st., Khabarovsk 680035, Russia*

(Dated: February 3, 2015)

We perform *ab initio* no core shell model calculations for $A = 18$ and 19 nuclei in a $4\hbar\Omega$, or $N_{\max} = 4$, model space using the effective JISP16 and chiral N3LO nucleon-nucleon potentials and transform the many-body effective Hamiltonians into the $0\hbar\Omega$ model space to construct the A-body effective Hamiltonians in the *sd*-shell. We separate the A-body effective Hamiltonians with $A = 18$ and $A = 19$ into inert core, one- and two-body components. Then, we use these core, one- and two-body components to perform standard shell model calculations for the $A = 18$ and $A = 19$ systems with valence nucleons restricted to the *sd*-shell. Finally, we compare the standard shell model results in the $0\hbar\Omega$ model space with the exact no core shell model results in the $4\hbar\Omega$ model space for the $A = 18$ and $A = 19$ systems and find good agreement.

ArXiv: Nucl-th 1502.00700

Empirical Single-Particle Energies



$$\varepsilon_{0d_{5/2}} = 0.0 \text{ MeV}$$

$$\varepsilon_{1s_{1/2}} = 0.87 \text{ MeV}$$

$$\varepsilon_{0d_{3/2}} = 5.08 \text{ MeV}$$

$$H^{sd}(P\Psi)^{sd} = \left\{ \sum_i^{sd} \varepsilon_i + v_{eff}^{sd} \right\} (P\Psi)^{sd}$$

$$\left\{ H_0 + V_{eff}^{sd} \right\} (P\Psi)^{sd} = E^{sd} (P\Psi)^{sd}$$

Input: The results of N_max = 4 and hw = 14 MeV NCSM calculations

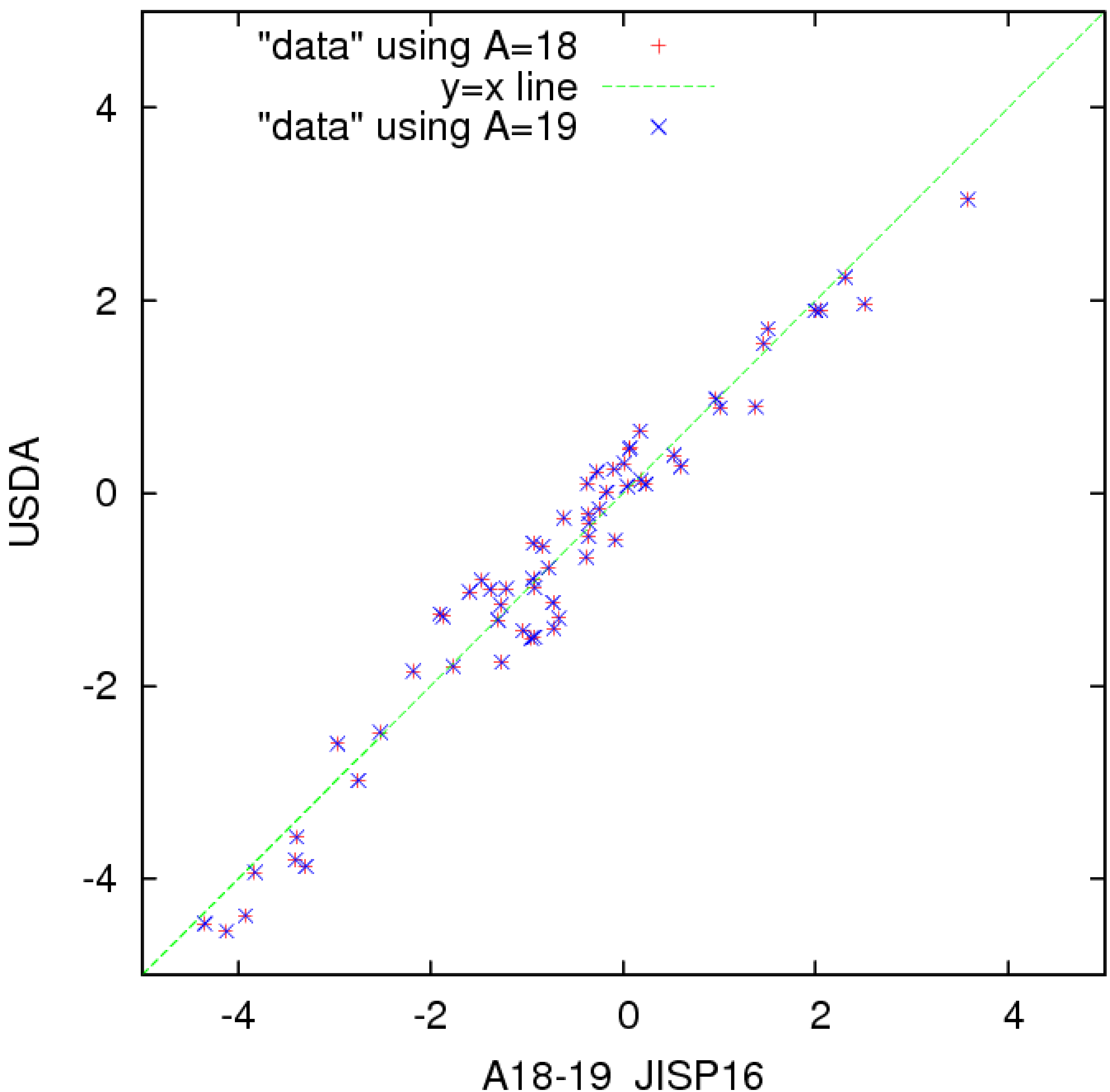
TABLE II: Proton and neutron single-particle energies (in MeV) for JISP16 effective interaction obtained for the mass of $A = 18$ and $A = 19$.

	$A = 18$, $E_{\text{core}} = -115.529$			$A = 19$, $E_{\text{core}} = -115.319$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon^n_{j_i}$	-3.068	-2.270	6.262	-3.044	-2.248	6.289
$\epsilon^p_{j_i}$	0.603	1.398	9.748	0.627	1.419	9.774

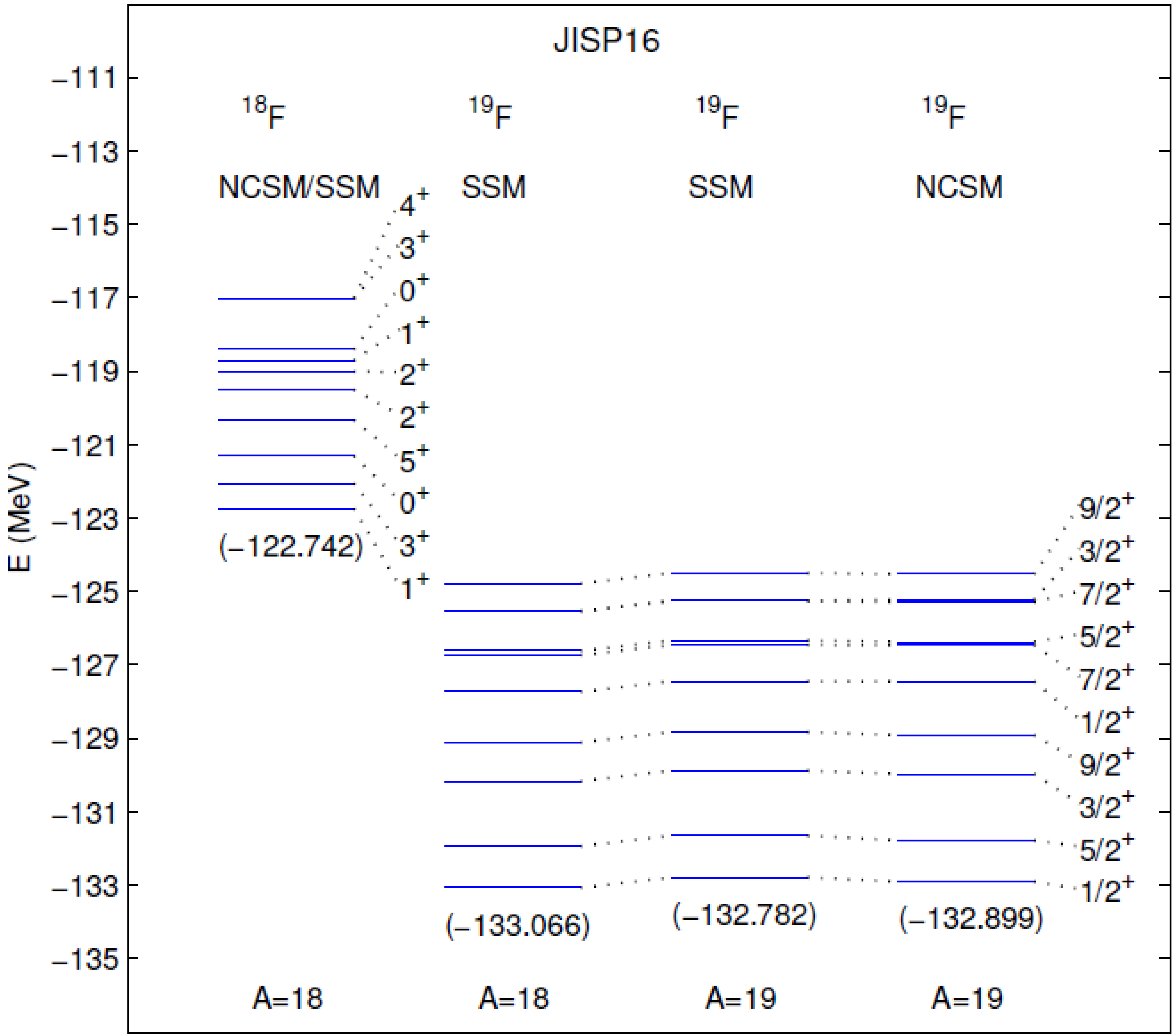
TABLE III: Proton and neutron single-particle energies (in MeV) for chiral N3LO effective interaction obtained for the mass of $A = 18$ and $A = 19$.

	$A = 18$, $E_{\text{core}} = -118.469$			$A = 19$, $E_{\text{core}} = -118.306$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon^n_{j_i}$	-3.638	-3.042	3.763	-3.625	-3.031	3.770
$\epsilon^p_{j_i}$	0.044	0.690	7.299	0.057	0.700	7.307

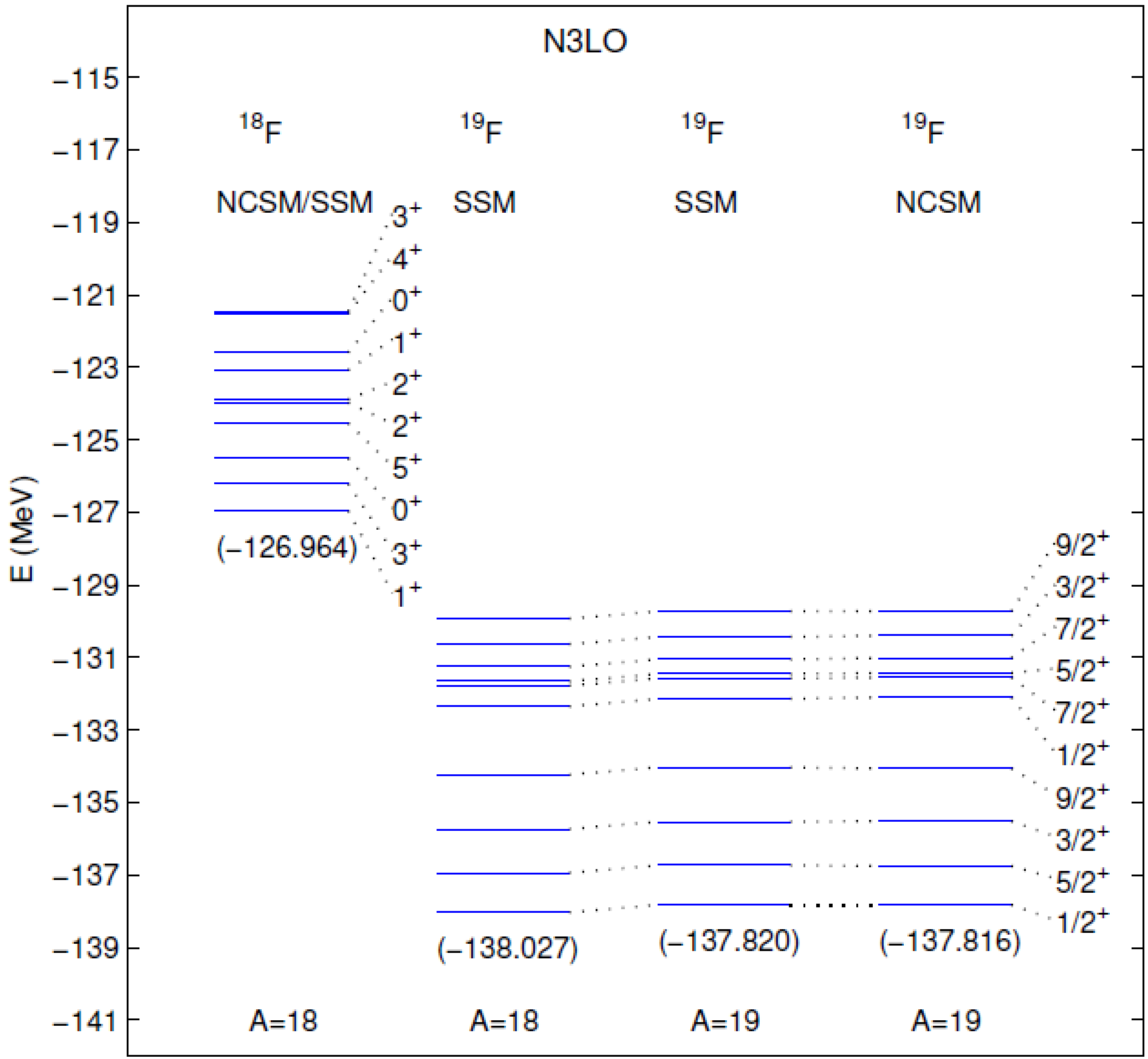
	A = 18	A = 19	
Coupled Cluster, E_core: Idaho NN N3LO + 3N N2LO	-130.462	-130.056	from G.R. Jansen et al. PRL 113, 142502 (2014)
IM-SRG, E_core: Idaho NN N3LO + 3N N2LO	-130.132	-129.637	from H. Hergert private comm.



Comparison of 2-body effective matrx elements in the sd-shell: JISP16 vs USDA by Alex Brown et al.



JISP16
E (MeV)
−111
−113
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
18F
19F
19F
19F
NCSM/SSM
SSM
SSM
NCSM
4+
3+
0+
1+
2+
2+
5+
0+
3+
1+
(−122.742)
(−133.066)
(−132.782)
(−132.899)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
A=18
A=18
A=19
A=19



N3LO
E (MeV)
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
−137
−139
−141
18F
19F
19F
19F
NCSM/SSM
SSM
SSM
NCSM
3+
4+
0+
1+
2+
2+
5+
0+
3+
1+
(−126.964)
(−138.027)
(−137.820)
(−137.816)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
A=18
A=18
A=19
A=19

Summary

Perform a converged NCSM calculation with a NN or NN+NNN interaction for a closed core + 2 valence nucleon system.

An OLS transformation of the results of the above NCSM calculation into a single major shell allows one to obtain core and single-particle energies and two-body residual matrix elements appropriate for shell model calculations in that shell, which have only a weak A-dependence.

The core and single-particle energies and two-body residual matrix elements obtained by this procedure can be used in Standard Shell Model calculations in the sd-shell, yielding results in good agreement with the full space NCSM results. The core and s.p. energies + 2-body effective interactions for A=18 give also good results for A=19 and 20.

Additional calculations are being performed with other NN interactions and for heavier nuclei in the sd-shell.

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}

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: $H^{\mathrm{eff}}_{A,a} \rightarrow H_A$