Microscopic Shell-Model Calculations in the sd-shell

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May 21, 2015

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Towards a unified description of the nucleus

The goal of nuclear structure theory:

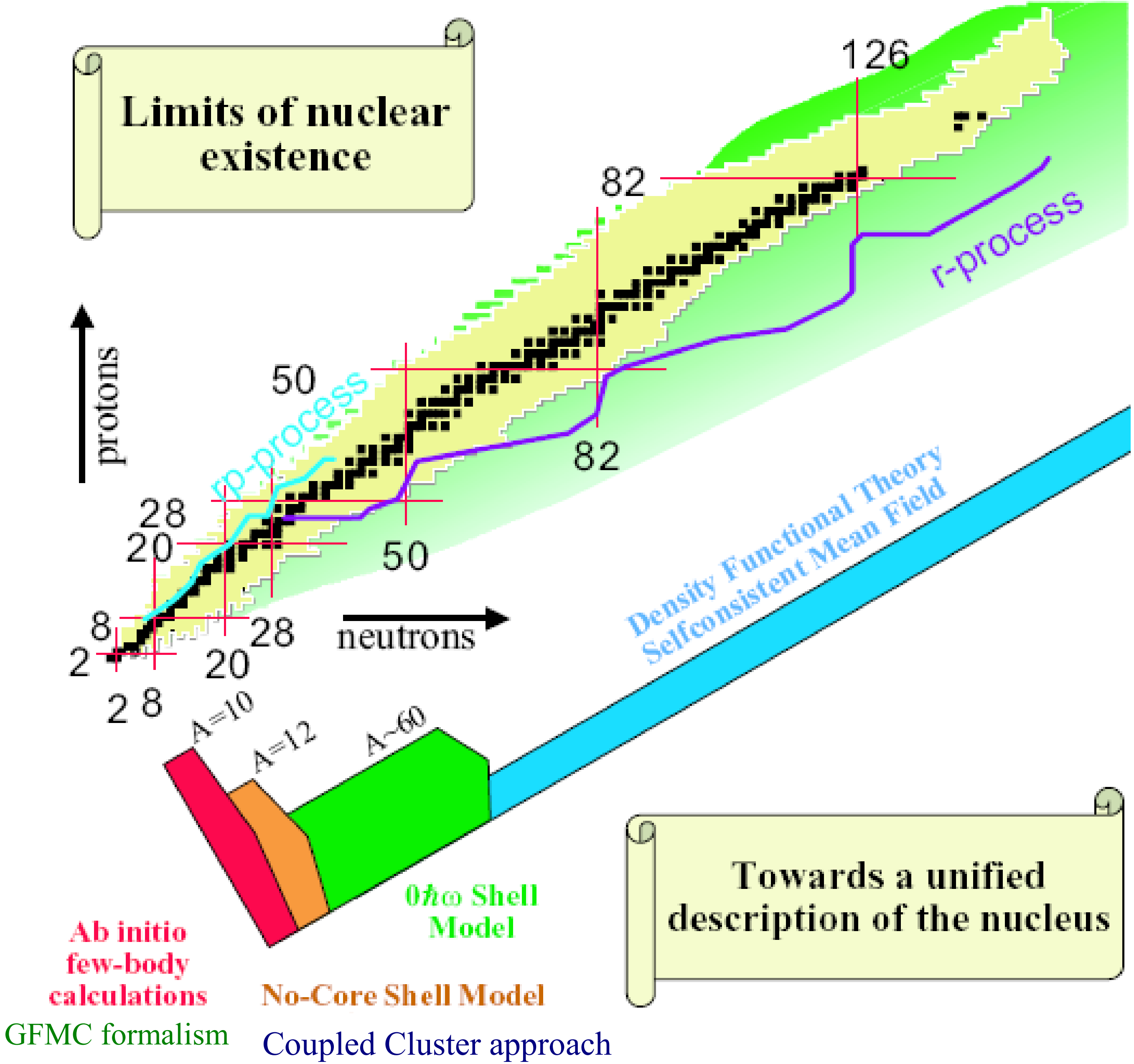
exact treatment of nuclei based on NN, NNN,... interactions

⇨ need to build a bridge between:

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

$0\hbar\Omega$ Shell Model calculations: $16 \leq A \leq 60$

Density Functional Theory calculations: $A \geq 60$



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

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 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)

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

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 <u>no</u> phenomenological s.p. energies!

Can use <u>any</u> NN potentials

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 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

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

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 $\mathcal{S}$

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

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

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;

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

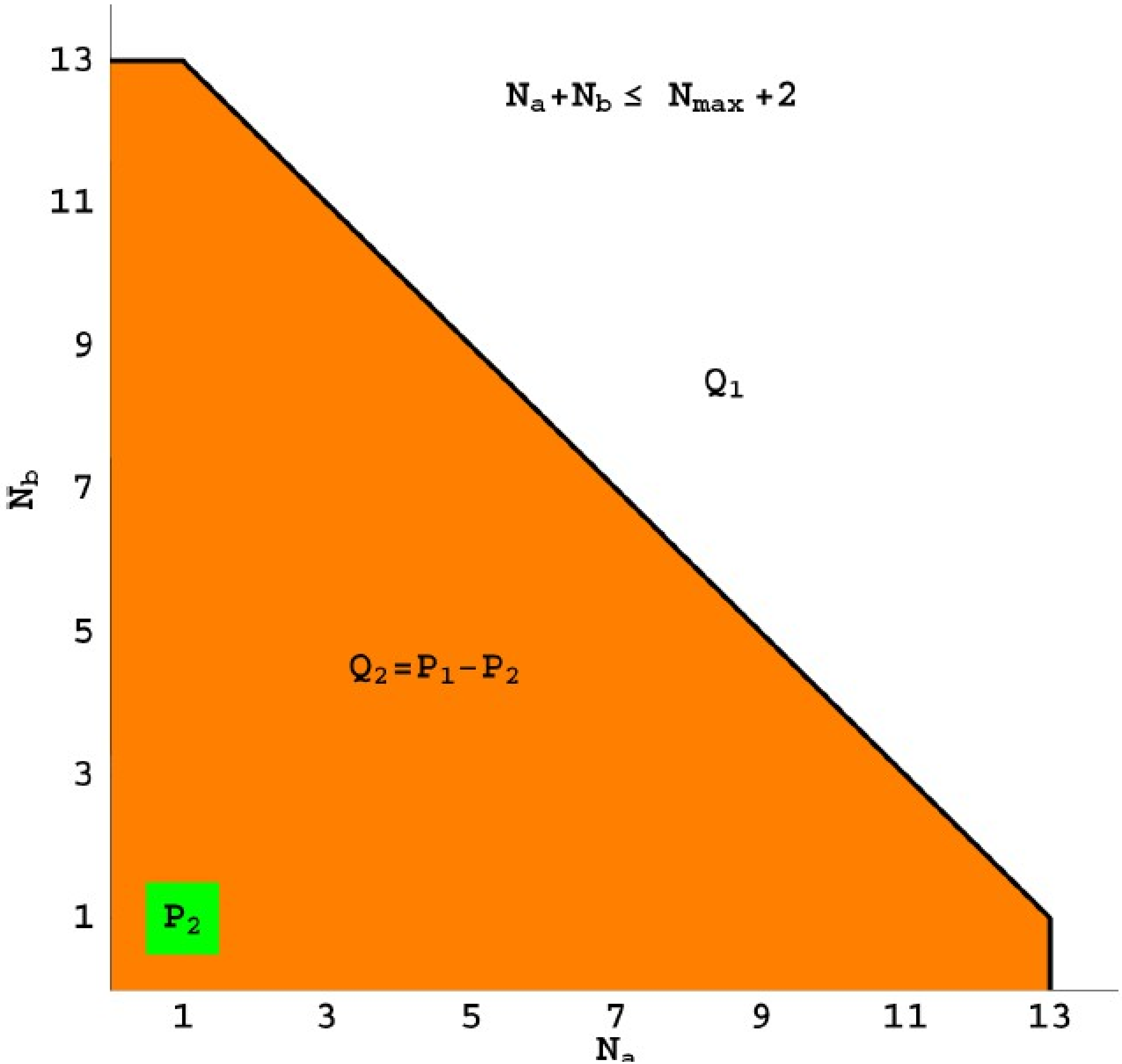
$$U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} E^{\Omega}_{A,2,P} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

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

Two ways of convergence:

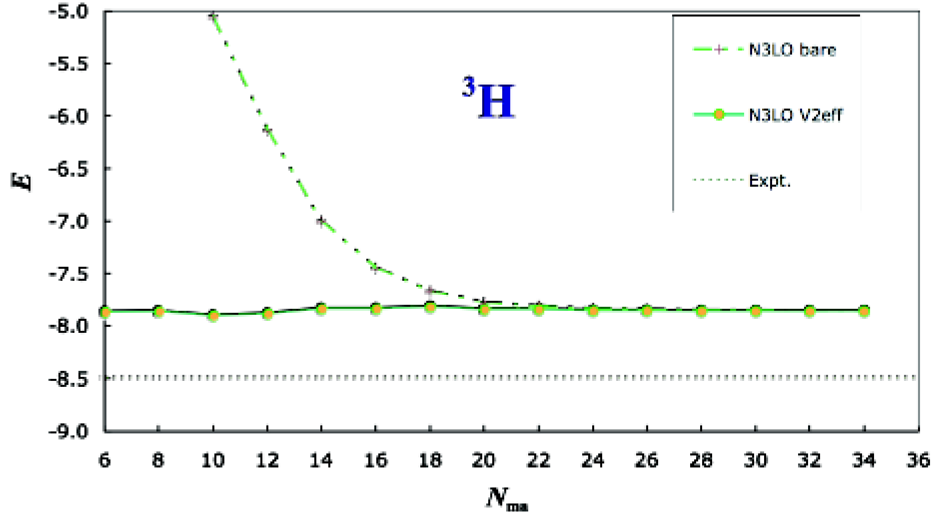
1) For $P \rightarrow 1$ and fixed a: $H^{eff}_{A,a=2} \rightarrow H_A$

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



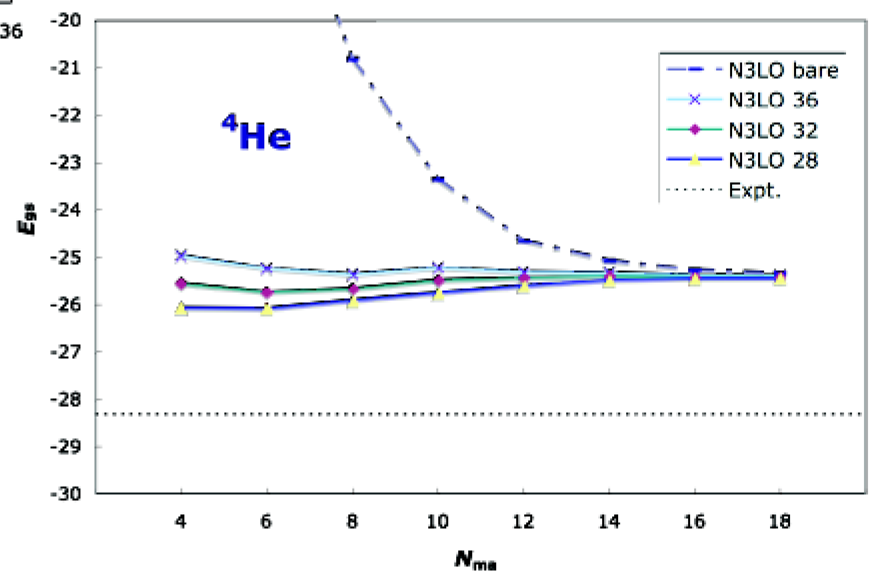
13
11
9
7
5
3
1
N_b
$N_a + N_b \leq N_{max} + 2$
Q_1
$Q_2 = P_1 - P_2$
P_2
1
3
5
7
9
11
13
N_a

- NCSM convergence test
  - Comparison to other methods

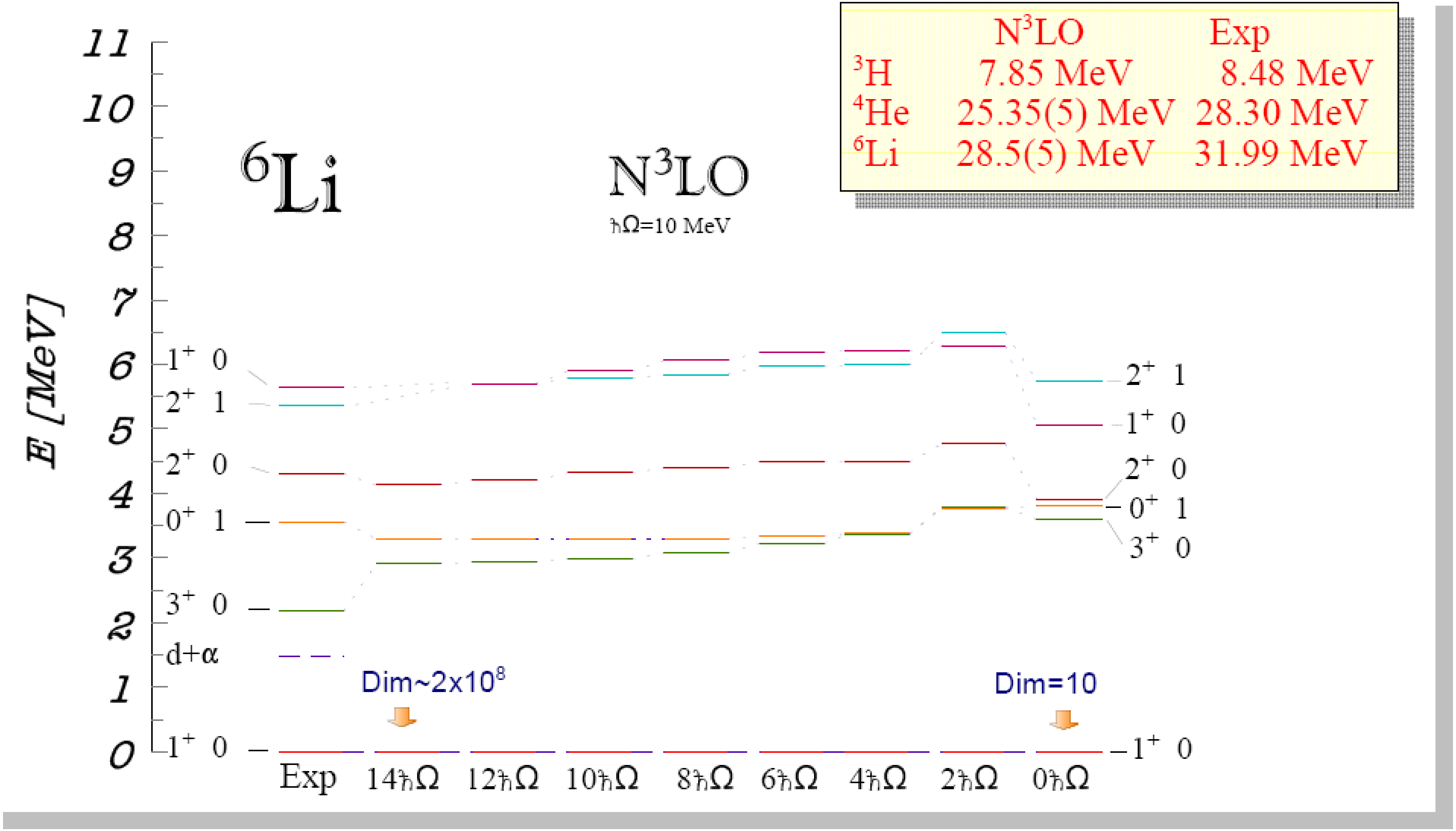


N³LO NN	NCSM	FY	HH
^{3}H	7.852(5)	7.854	7.854
^{4}He	25.39(1)	25.37	25.38

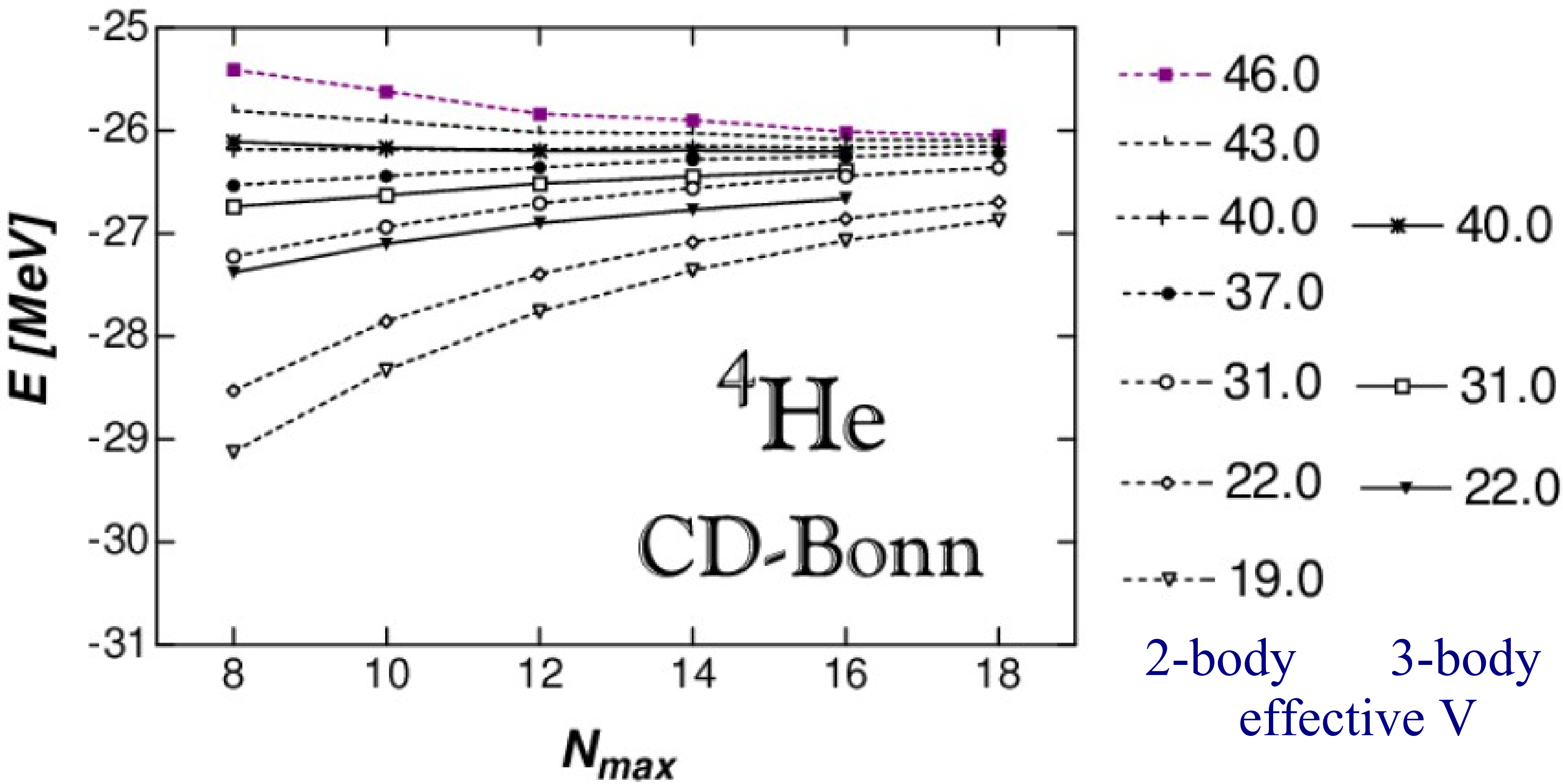
- ➢Short-range correlations ⇒ effective interaction
- ➢Medium-range correlations ⇒ multi-$h\Omega$ model space
- ➢Dependence on
  - ▪size of the model space (N_{max})
  - ▪HO frequency ($h\Omega$)
- ➢Not a variational calculation
- ➢Convergence OK
- ➢NN interaction insufficient to reproduce experiment



P. Navratil, INT Seminar, November 13, 2007, online



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

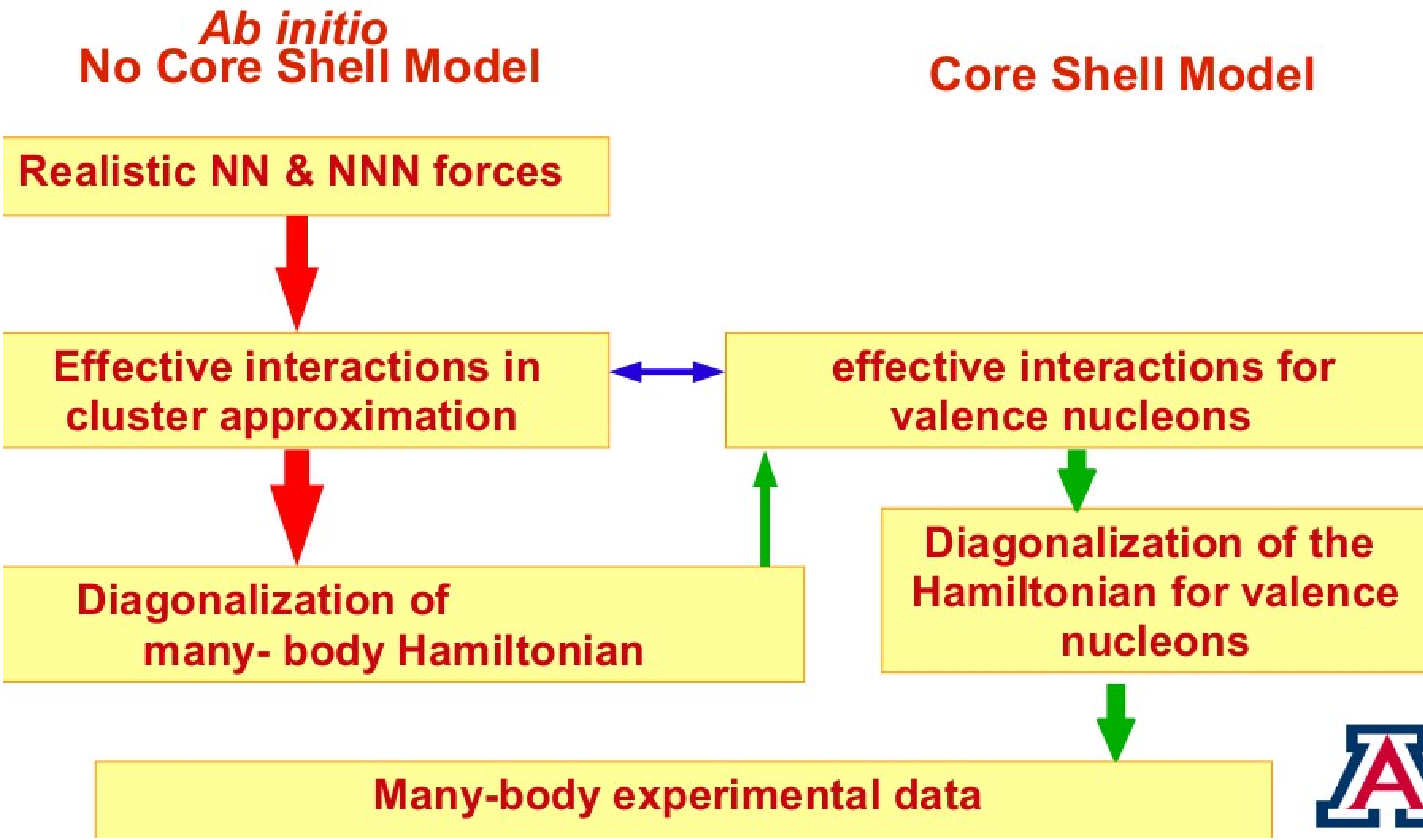


-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N_{max}
^{4}He
CD-Bonn
46.0
43.0
40.0
37.0
31.0
22.0
19.0
40.0
31.0
22.0
2-body
3-body
effective V

II. Ab Initio Shell Model with a Core Approach

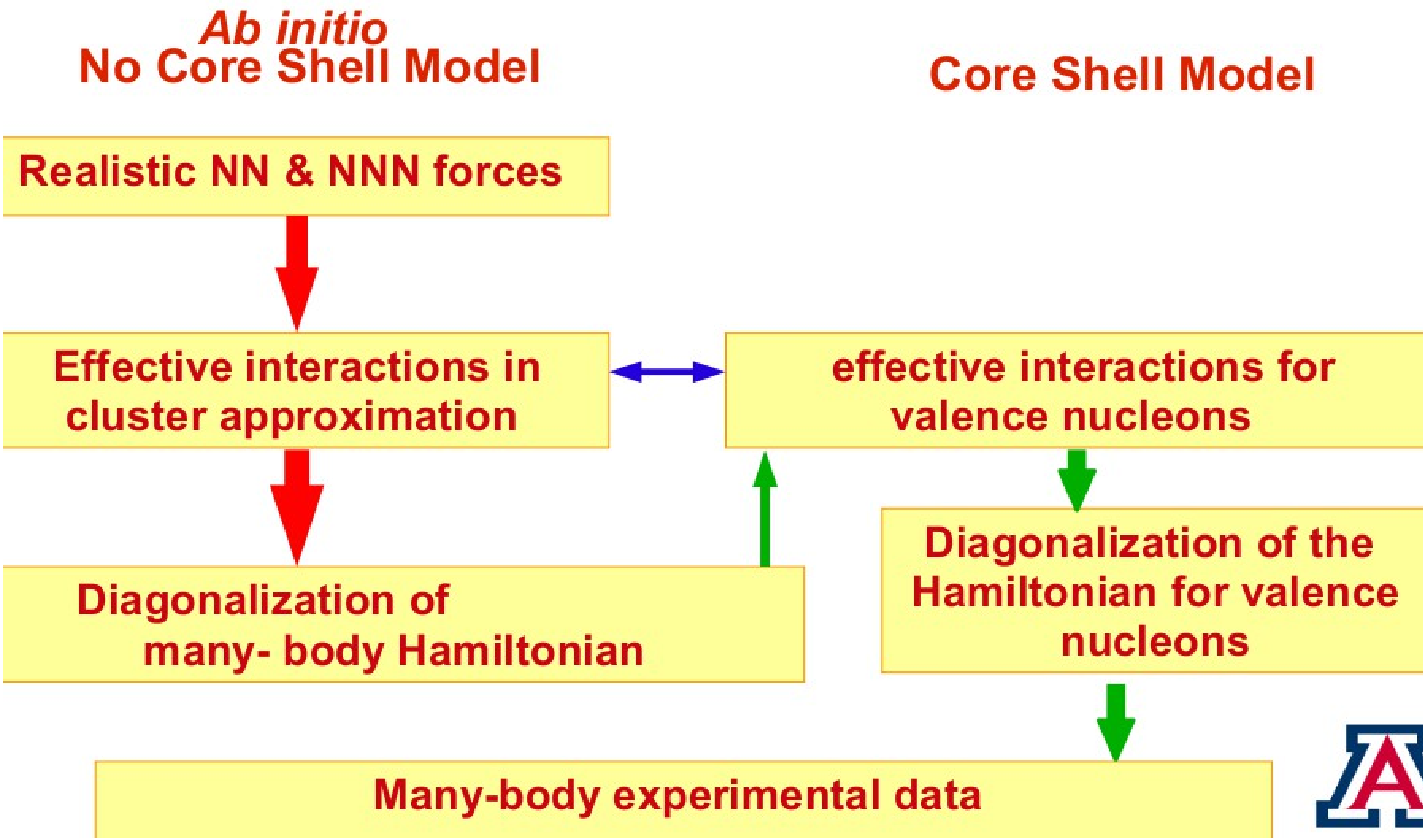
From few-body to many-body

Using the NCSM to calculate the shell model input



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

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(Received 20 June 2008; published 10 October 2008)

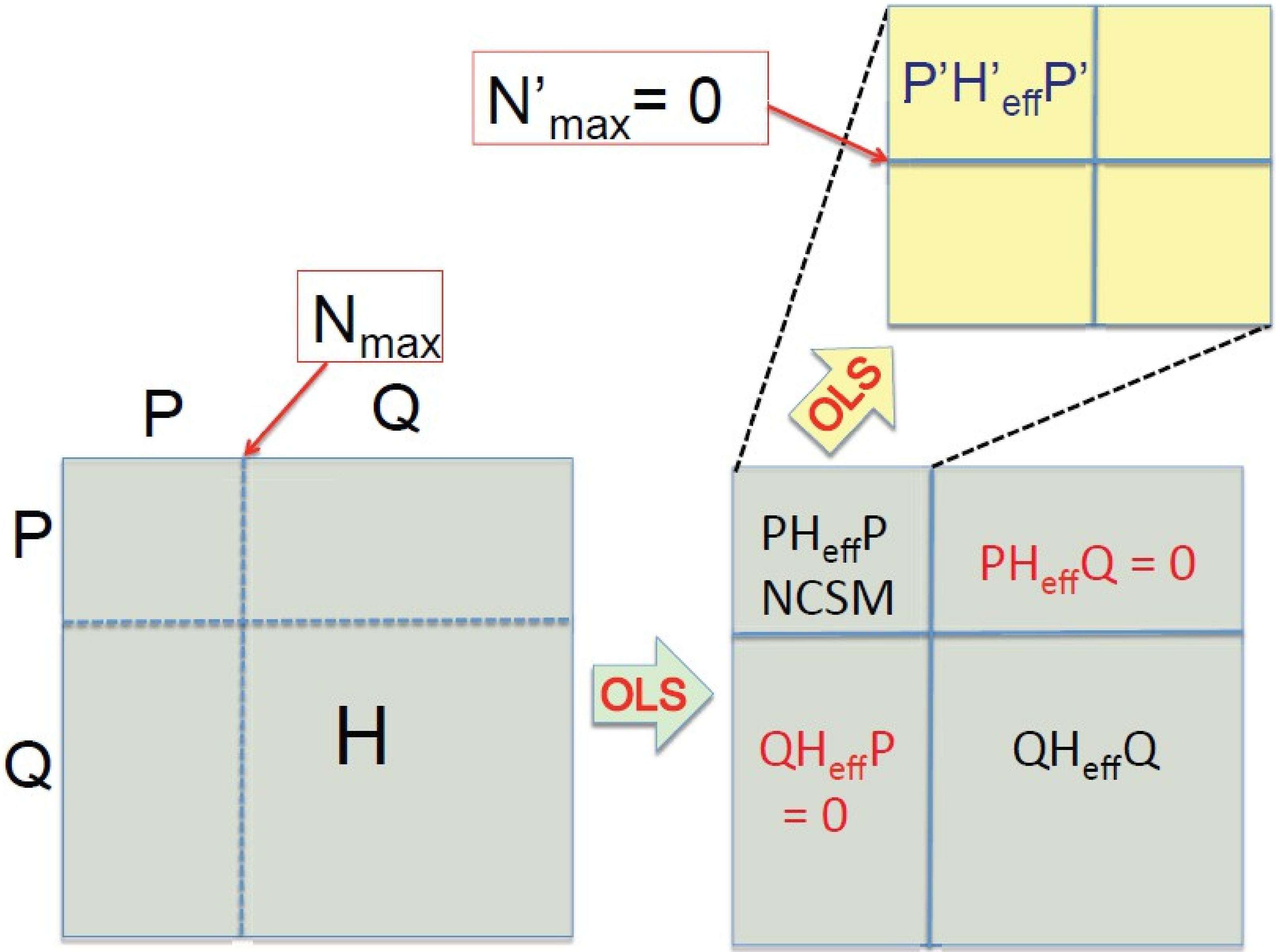
We construct effective two- and three-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ *ab initio* no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians 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.

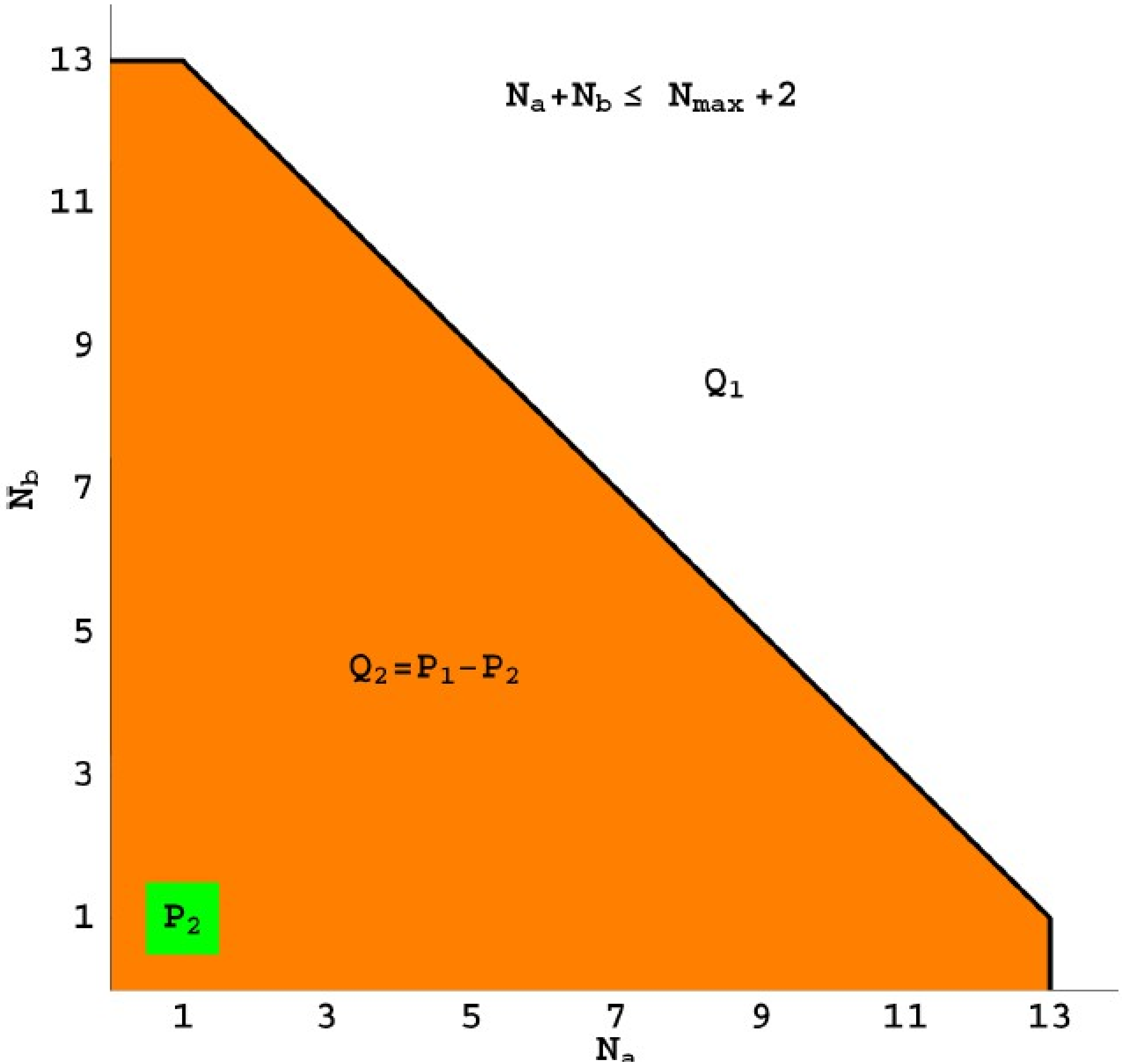
DOI: 10.1103/PhysRevC.78.044302 PACS number(s): 21.10.Hw, 21.60.Cs, 23.20.Lv, 27.20.+n

P. Navratil, M. Thoresen and B.R.B., Phys. Rev. C 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



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

Effective Hamiltonian for SSM

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

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;

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

III. Results: sd-shell nuclei

Accepted for publication in PRC

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

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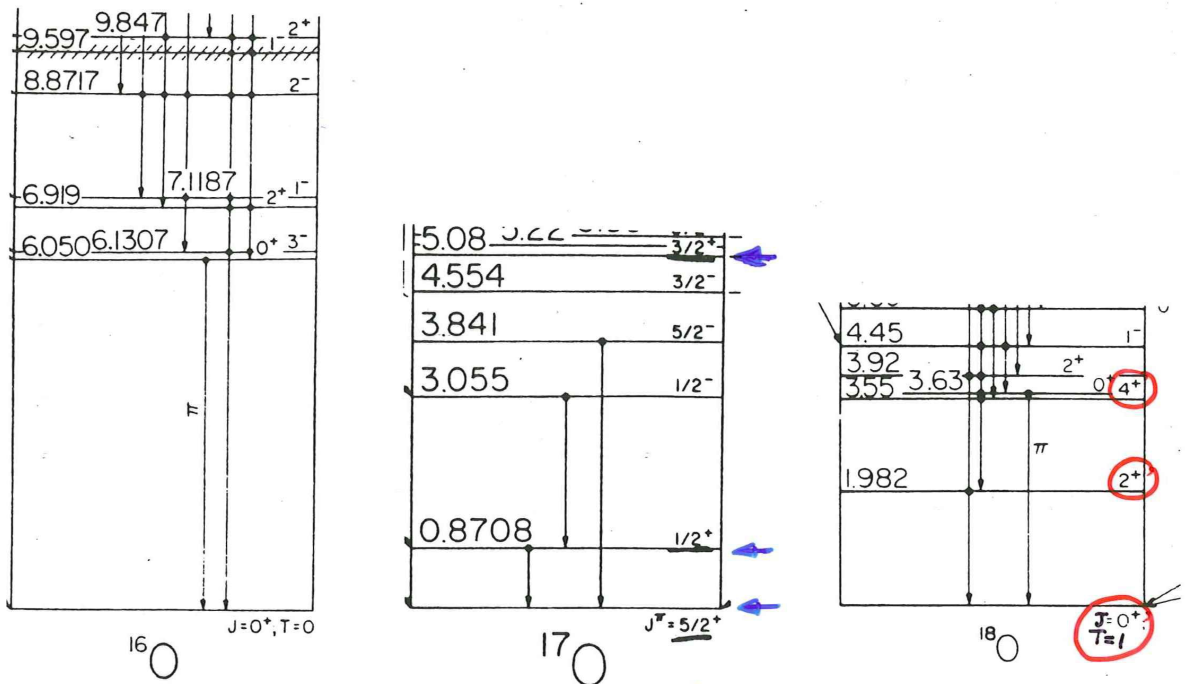
(Dated: February 3, 2015)

We perform *ab initio* no core shell model calculations for $A = 18$ and 19 nuclei in a $4\hbar\Omega$, or $N_{\rm max} = 4$, 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 $A = 19$.

	$A = 18$, $E_{\rm core} = -115.529$			$A = 19$, $E_{\rm core} = -115.319$		
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 $A = 19$.

	$A = 18$, $E_{\rm core} = -118.469$			$A = 19$, $E_{\rm core} = -118.306$		
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.

No-Core Shell-Model Approach

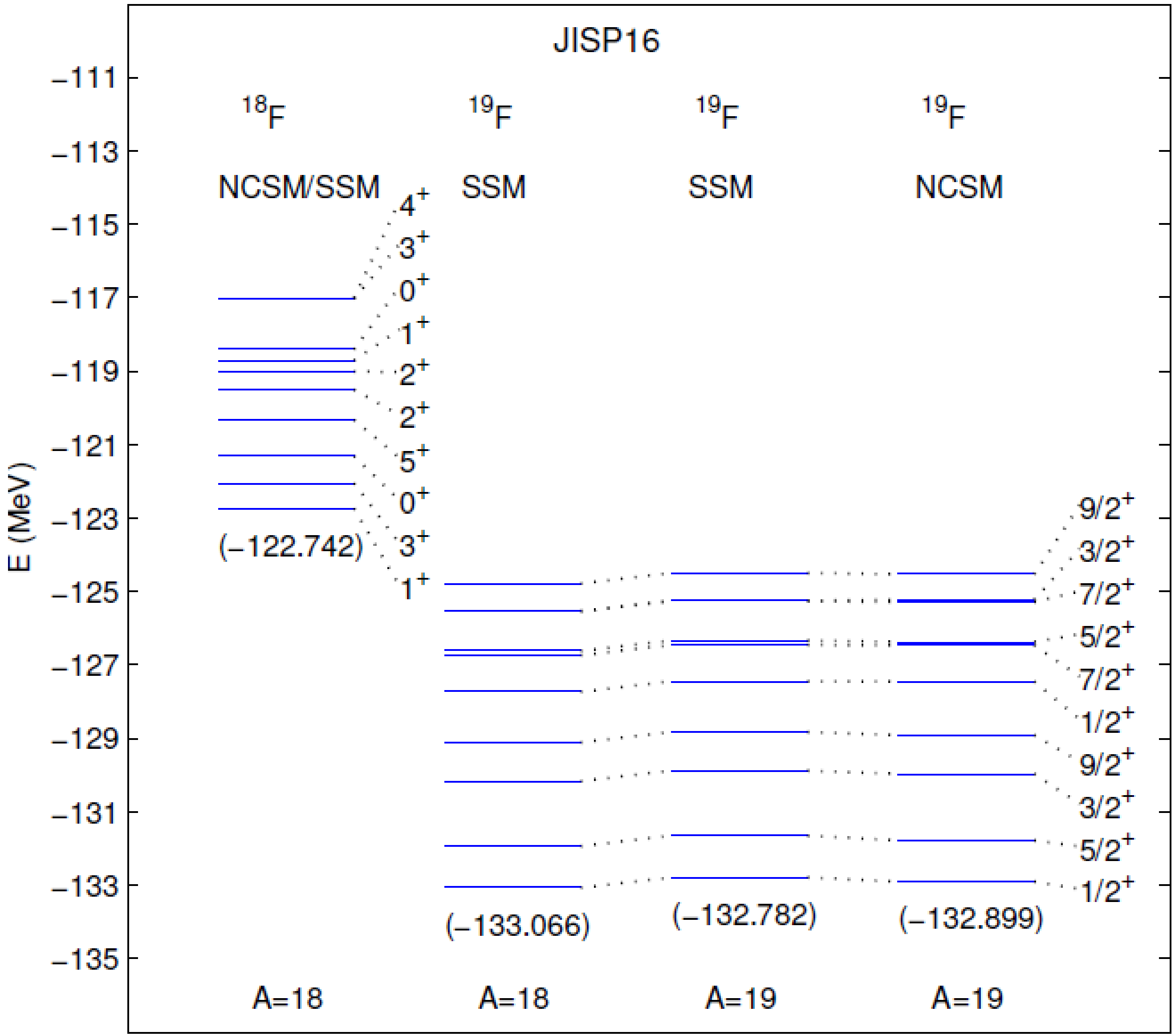
- Next, add CM harmonic-oscillator Hamiltonian

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

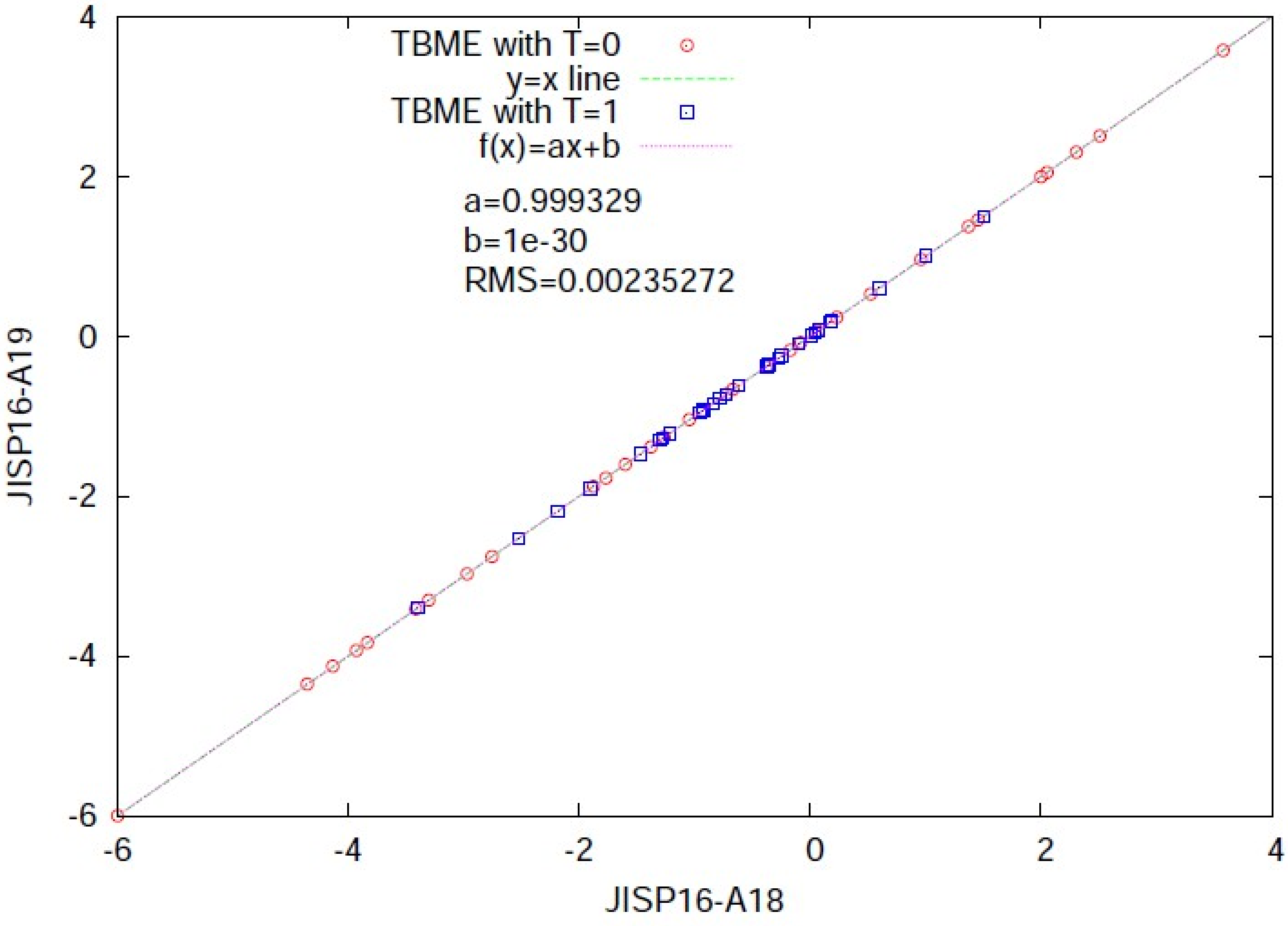
To H_A, yielding

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

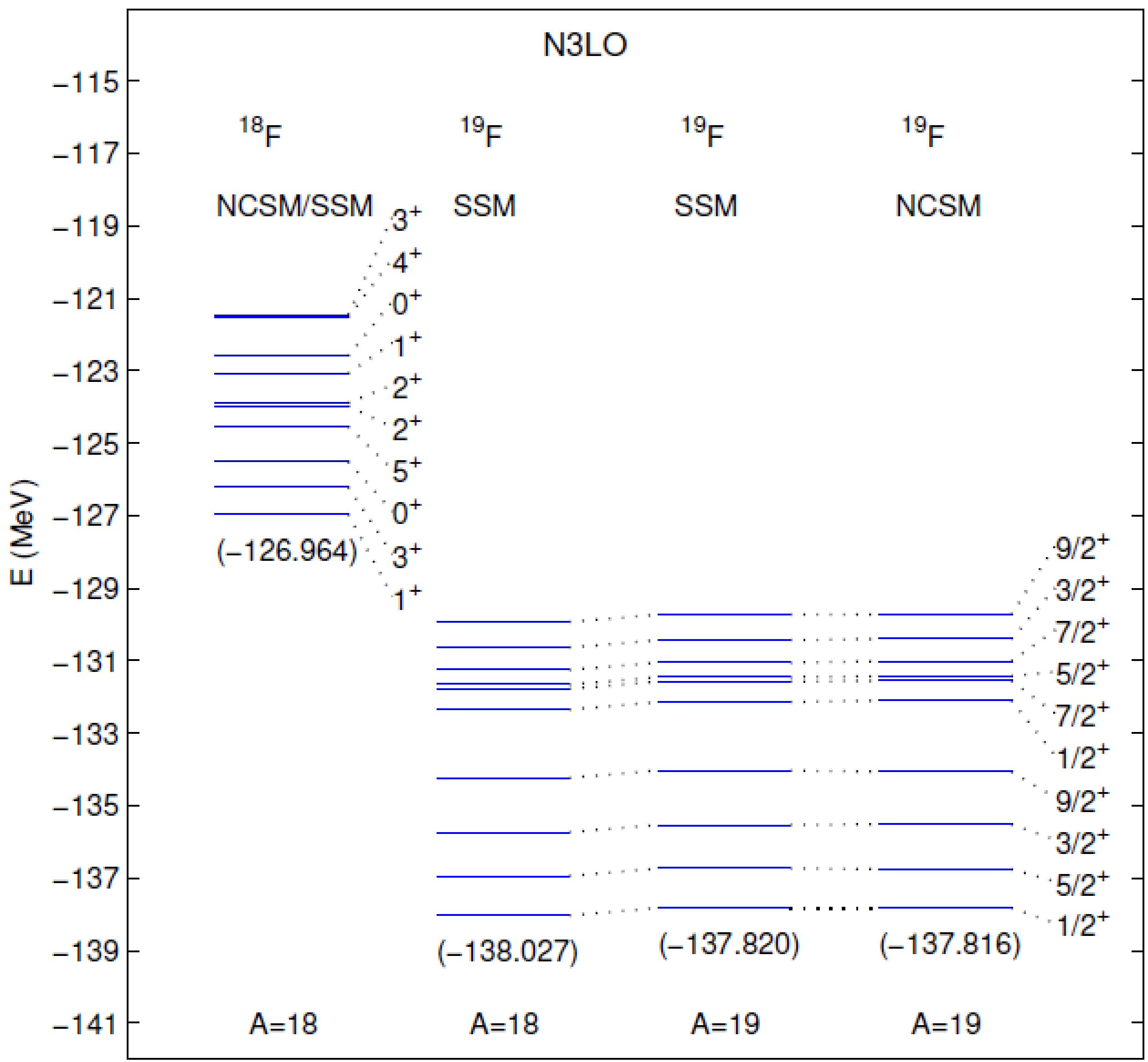
Defines a basis (*i.e.* HO) for evaluating V_{ij}

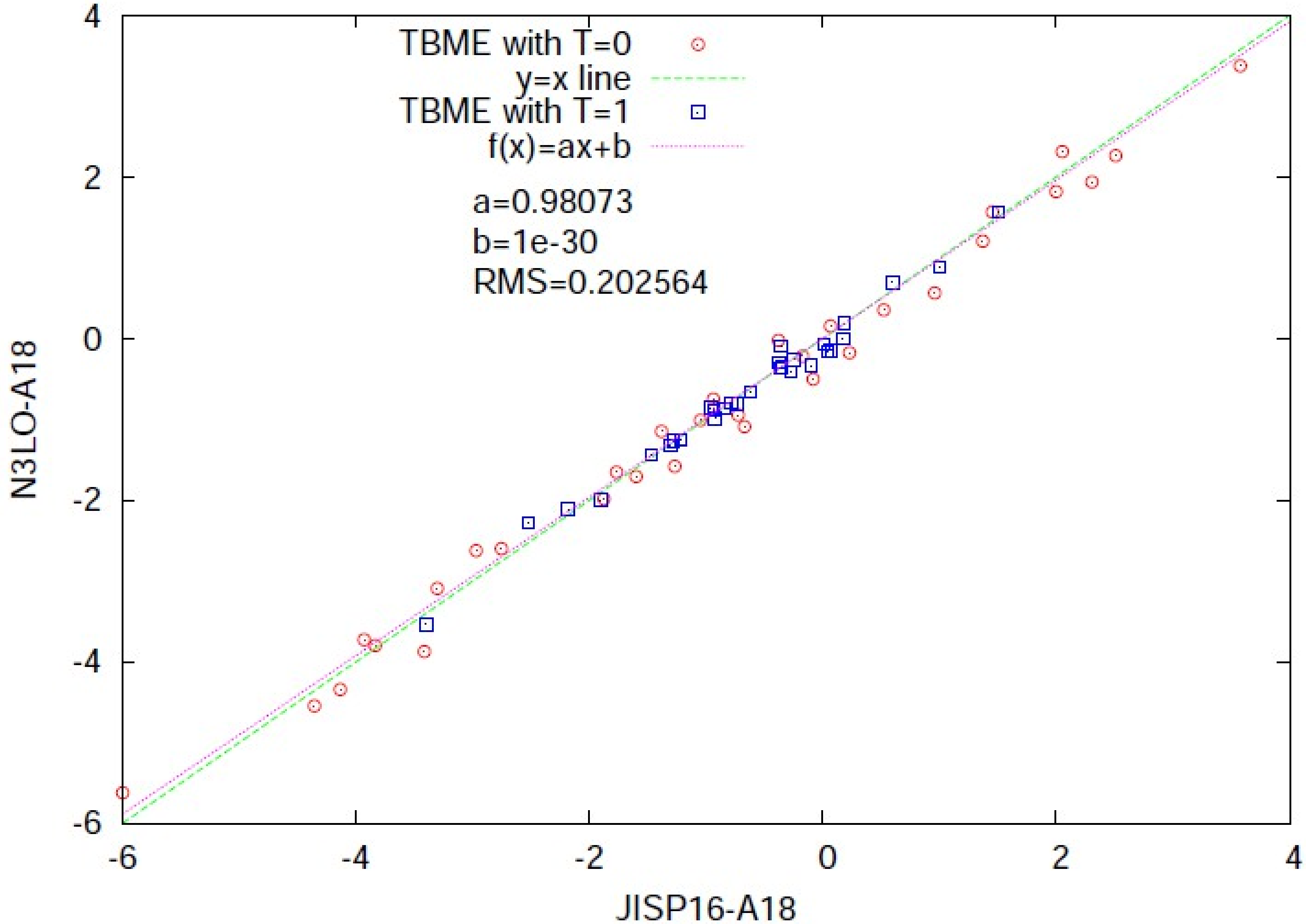


JISP16
E (MeV)
−111
−113
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
^{18}F
NCSM/SSM
(−122.742)
A=18
^{19}F
SSM
(−133.066)
A=18
^{19}F
SSM
(−132.782)
A=19
^{19}F
NCSM
(−132.899)
A=19
4+
3+
0+
1+
2+
2+
5+
0+
3+
1+
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+



Preliminary Results

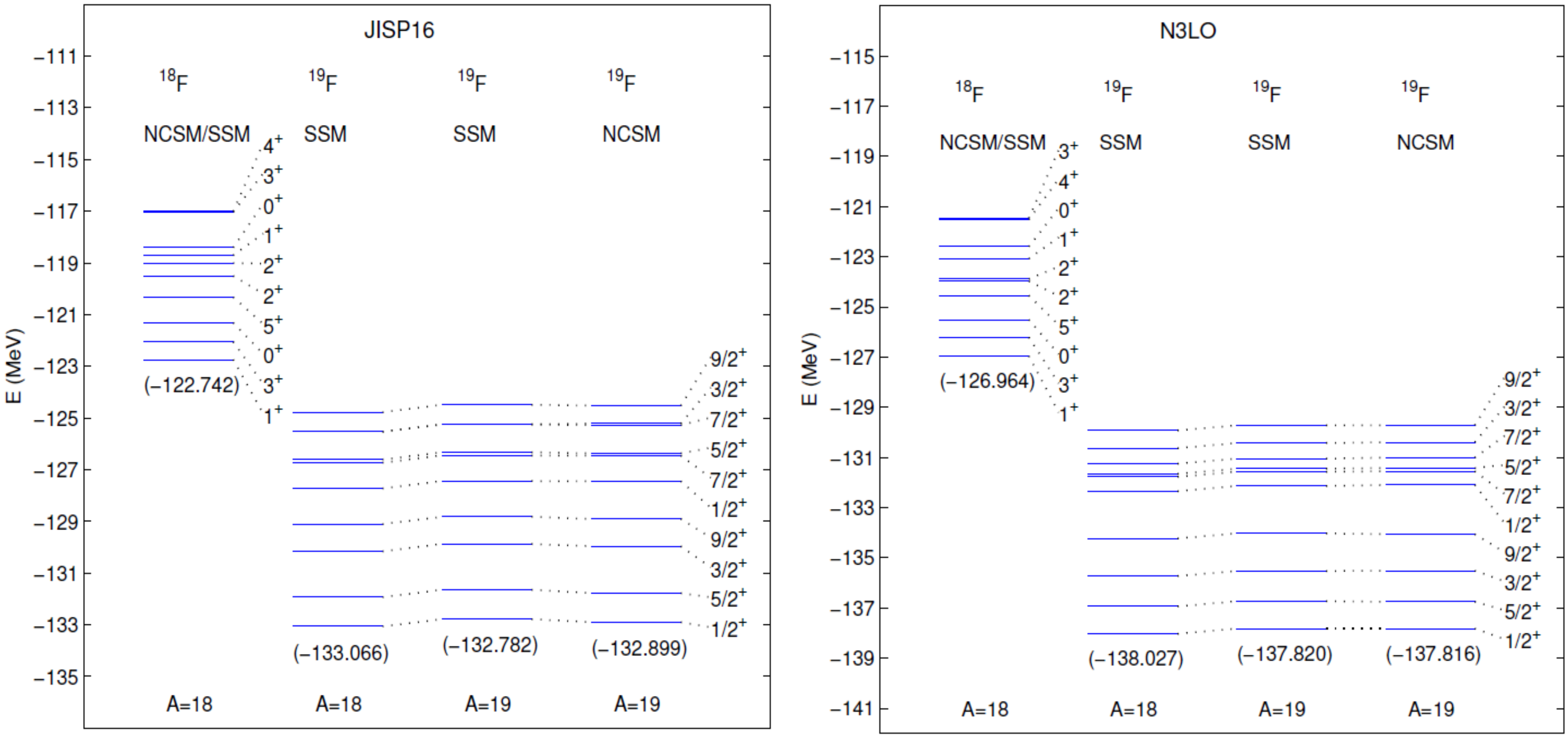

N3LO
E (MeV)
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
−137
−139
−141
18F
19F
19F
19F
NCSM/SSM
SSM
SSM
NCSM
3+
4+
0+
1+
2+
2+
5+
0+
3+
1+
(−126.964)
(−138.027)
(−137.820)
(−137.816)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
A=18
A=18
A=19
A=19

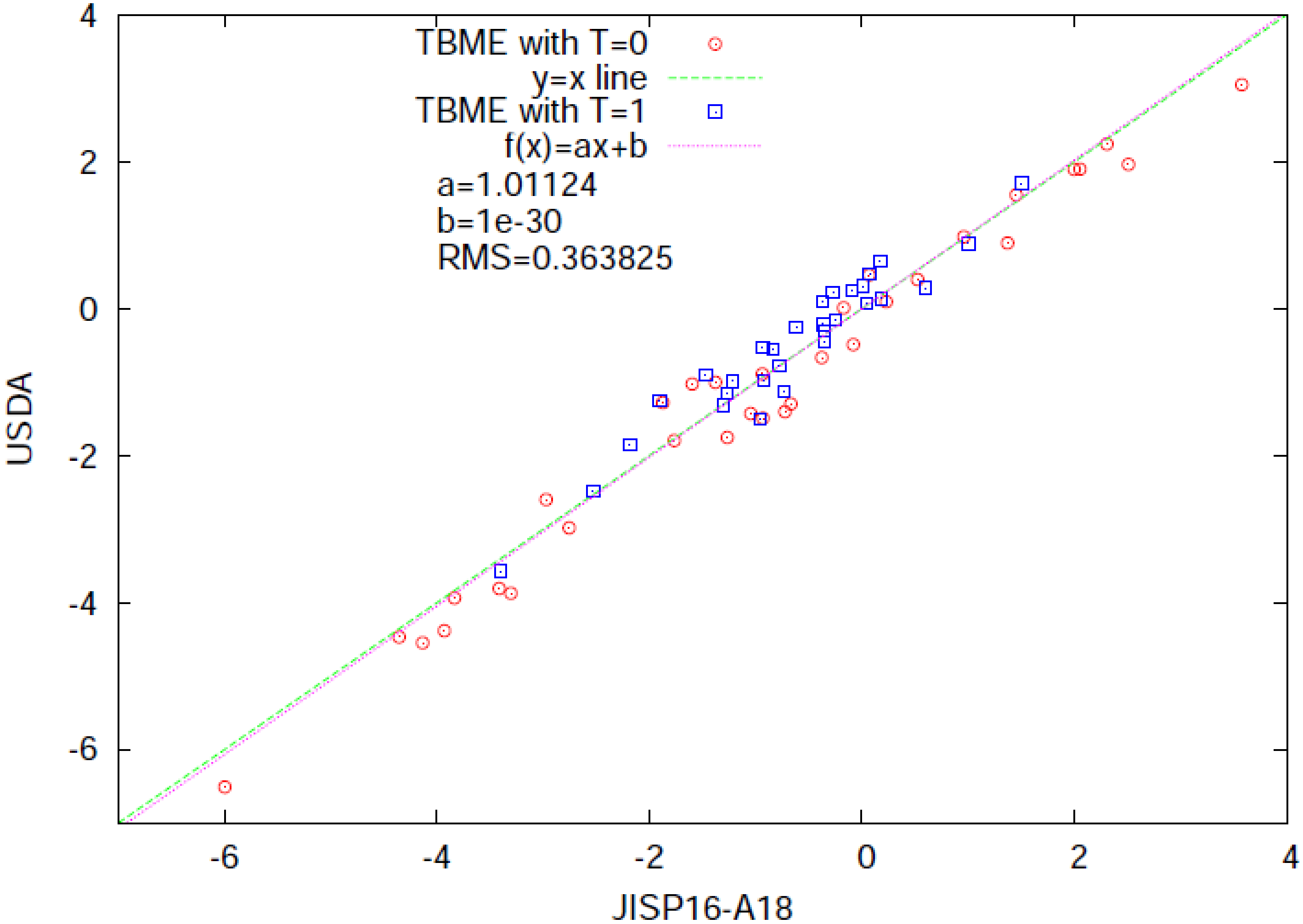


Preliminary Results

TABLE III: The NCSM energies (in MeV) of the lowest 28 states J_i^π of ^{18}F calculated in $4\hbar\Omega$ model space using JISP16 and chiral N3LO NN interactions with $\hbar\Omega = 14$ MeV.

J_i^π	T	JISP16	J_i^π	T	N3LO
1_1^+	0	-122.742	1_1^+	0	-126.964
3_1^+	0	-122.055	3_1^+	0	-126.214
0_1^+	1	-121.320	0_1^+	1	-125.510
5_1^+	0	-120.329	5_1^+	0	-124.545
2_1^+	1	-119.505	2_1^+	1	-123.974
2_2^+	0	-119.011	2_2^+	0	-123.890
1_2^+	0	-118.709	1_2^+	0	-123.077
0_2^+	1	-118.410	0_2^+	1	-122.586
2_3^+	1	-117.211	2_3^+	1	-121.588
3_2^+	1	-117.035	4_1^+	1	-121.512
4_1^+	1	-117.004	3_2^+	1	-121.450
3_3^+	0	-116.765	3_3^+	0	-121.376
1_3^+	0	-113.565	1_3^+	0	-119.658
4_2^+	0	-112.314	4_2^+	0	-118.656
2_4^+	0	-111.899	2_4^+	0	-117.950
1_4^+	0	-110.357	1_4^+	0	-116.106
4_3^+	1	-109.625	4_3^+	1	-115.785
2_5^+	1	-109.292	2_5^+	1	-115.407
1_5^+	1	-108.752	3_4^+	0	-115.309
3_4^+	0	-108.706	1_5^+	1	-114.870
2_6^+	0	-108.485	2_6^+	0	-114.787
1_6^+	1	-108.055	1_6^+	1	-114.392
2_7^+	1	-108.041	3_5^+	1	-114.258
3_5^+	1	-107.874	2_7^+	1	-114.176
3_6^+	0	-101.528	3_6^+	0	-109.316
1_7^+	0	-99.946	1_7^+	0	-107.798
0_3^+	1	-99.848	2_8^+	1	-107.473
2_8^+	1	-99.607	0_3^+	1	-107.436

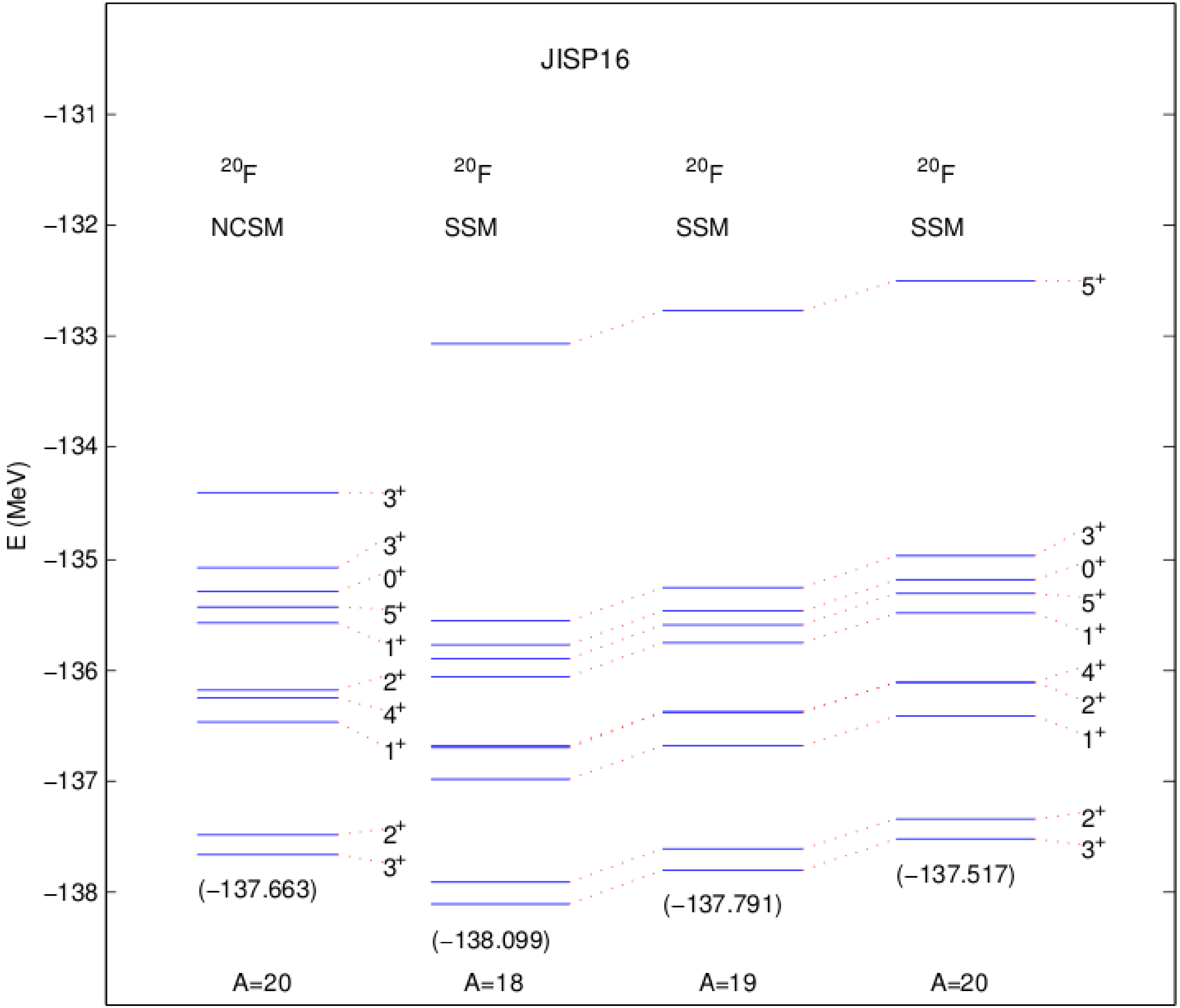

JISP16
18F NCSM/SSM
19F SSM
19F SSM
19F NCSM
E (MeV)
4+
3+
0+
1+
2+
2+
5+
0+
3+
1+
(−122.742)
(−133.066)
(−132.782)
(−132.899)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
A=18
A=18
A=19
A=19
N3LO
18F NCSM/SSM
19F SSM
19F SSM
19F NCSM
3+
4+
0+
1+
2+
2+
5+
0+
3+
1+
(−126.964)
(−138.027)
(−137.820)
(−137.816)
A=18
A=18
A=19
A=19



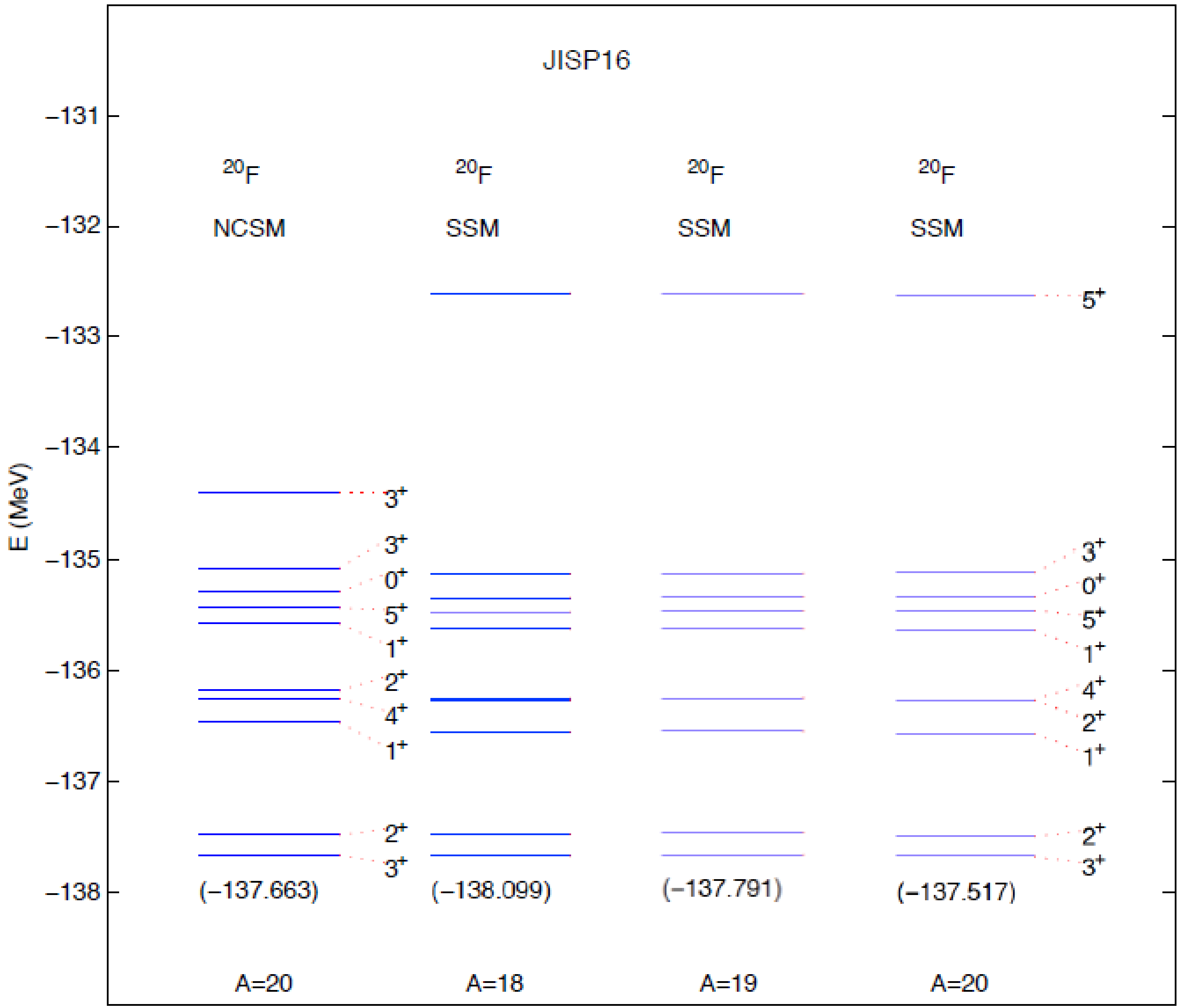
Comparison of effective TBMEs in the sd-shell: JISP16 vs USDA by Alex Brown et al.

Preliminary Results

PRELIMINARY RESULTS



Preliminary Results



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.

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 !!!

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

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

^{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 !!!

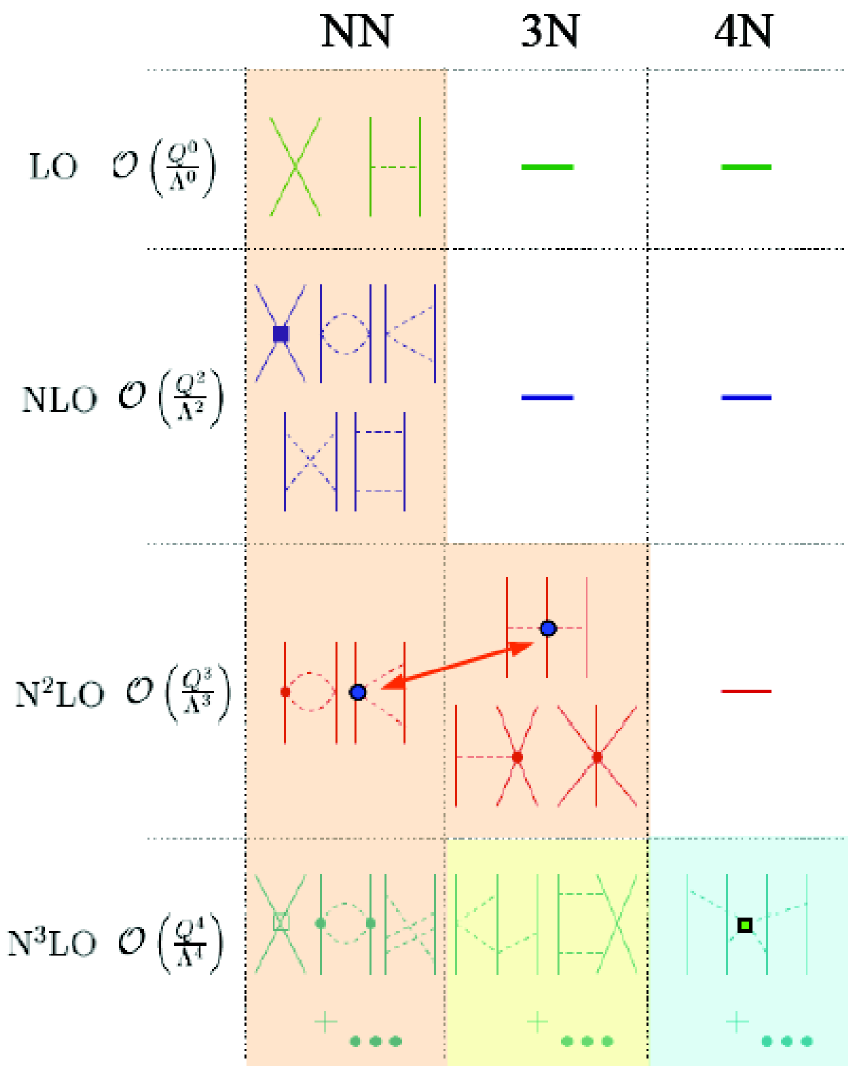
$$H_{A\;\;\;,2}^{N_{\max},\Omega,\text{eff}}$$

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

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

Chiral effective field theory (EFT) for nuclear forces

Separation of scales: low momenta $\frac{1}{\lambda} = Q \ll \Lambda_b$ breakdown scale Λ_b

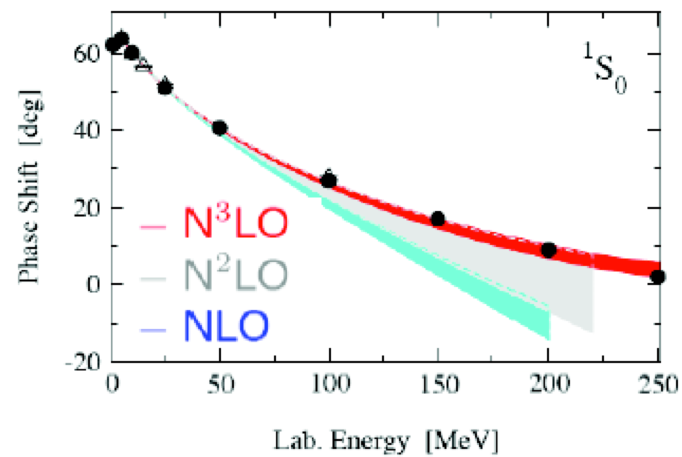


explains pheno hierarchy:
NN > 3N > 4N > …

NN-3N, πN, ππ, electro-weak,…
consistency

3N,4N: 2 new couplings to N³LO!

theoretical error estimates



Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Meissner, Nogga, Machleidt,…

A. Schwenk