Deriving the Nuclear Shell Model Microscopically

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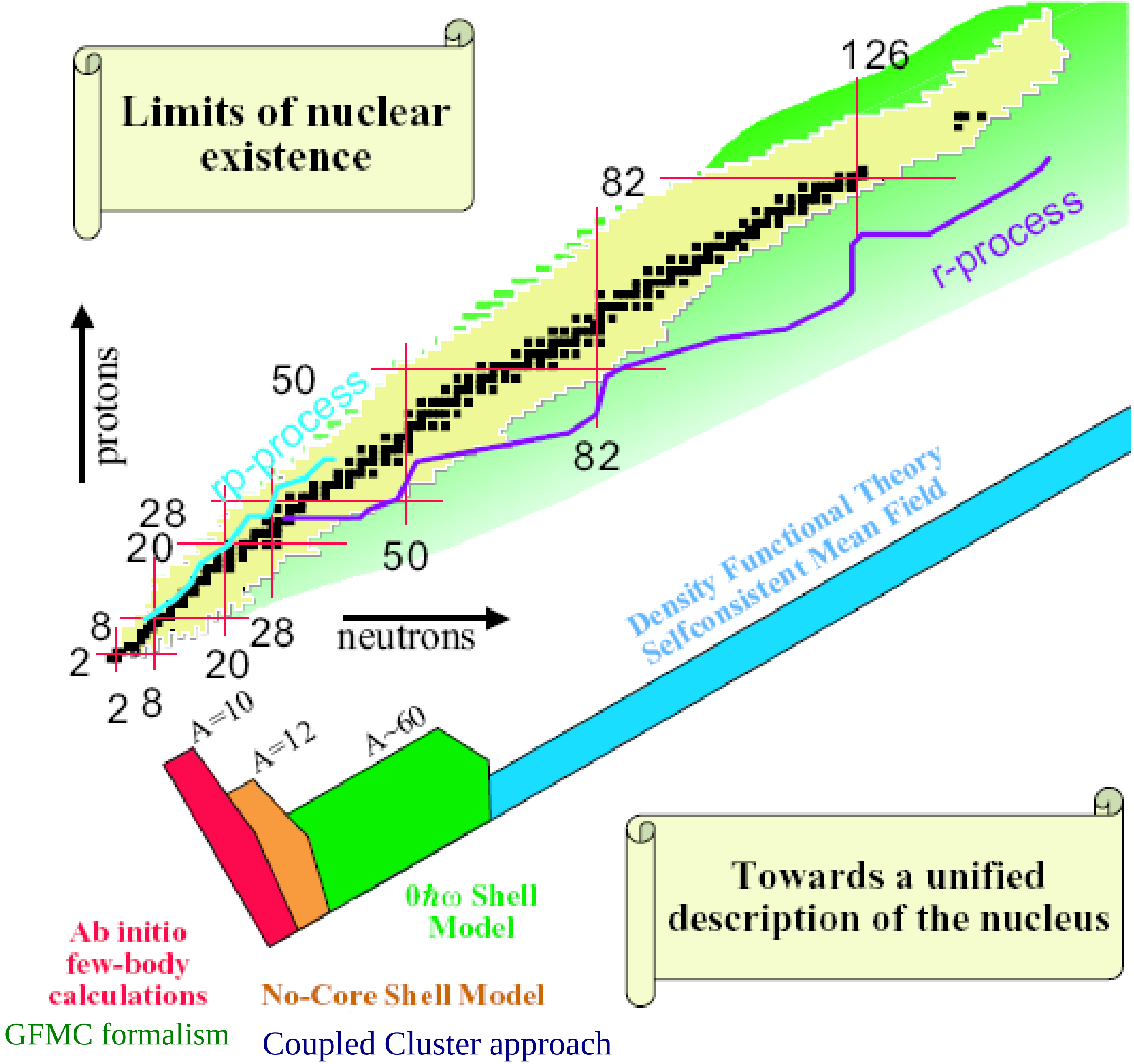
Ab Initio Nuclear Structure and Reaction Theory

Tremendous progress has been made in the last 10 to 15 years in calculating the properties of nuclei microscopically due to:

1. Improved NN and NNN interactions based on Chiral EFT

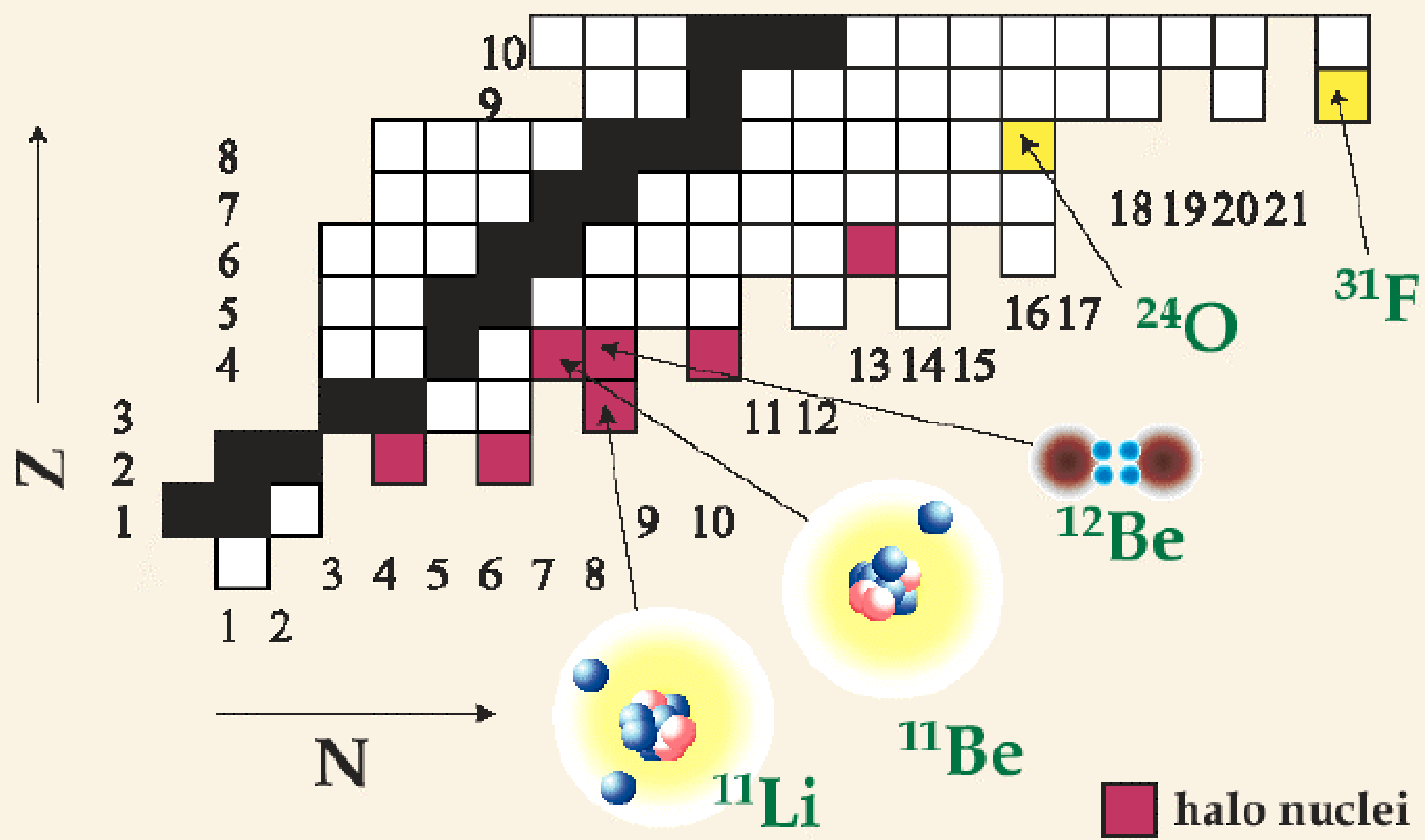
2. New approaches for accurately solving the nuclear many-body problem, e.g., No-Core Shell Model (NCSM), Coupled Cluster method (CC), In-Medium Similarity Renormalization Group technique (IM-SRG), Gorkov-Greens Function theory (GGF), etc.

3. Huge advances in computer technology and computing power.



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
Ab initio few-body calculations
No-Core Shell Model
0ħω Shell Model
GFMC formalism
Coupled Cluster approach
Towards a unified description of the nucleus

Light drip line nuclei



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: $A \geq 60$

OUTLINE

I. 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. 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

$$H_A \Psi^A = E_A \Psi^A$$

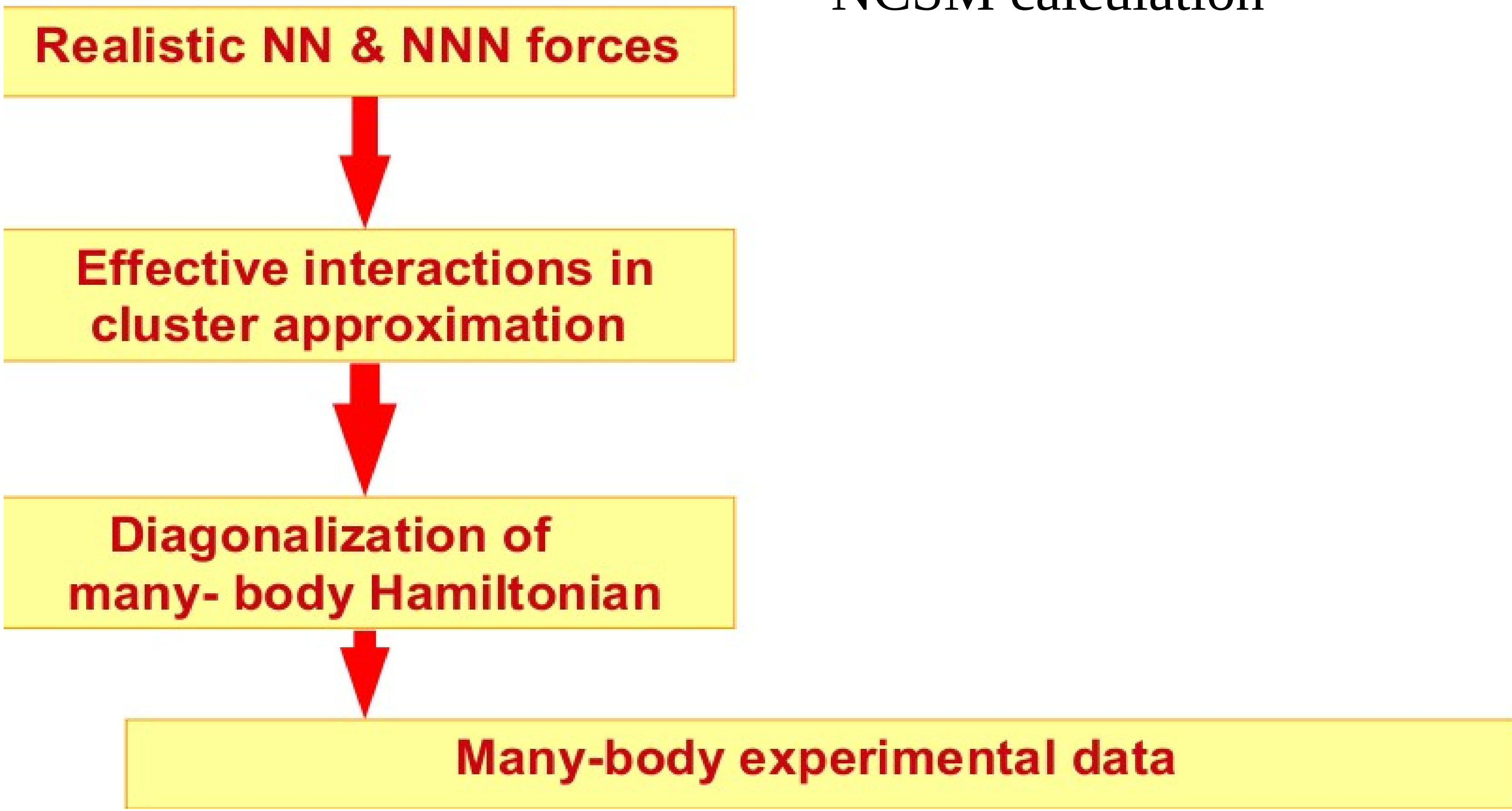
P. Navrátil, J.P. Vary, B.R.B., PRC <u>62,</u> 054311 (2000)

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

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 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

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

Effective interaction in a projected model space

$H\Psi_\alpha = E_\alpha \Psi_\alpha$ 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;

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

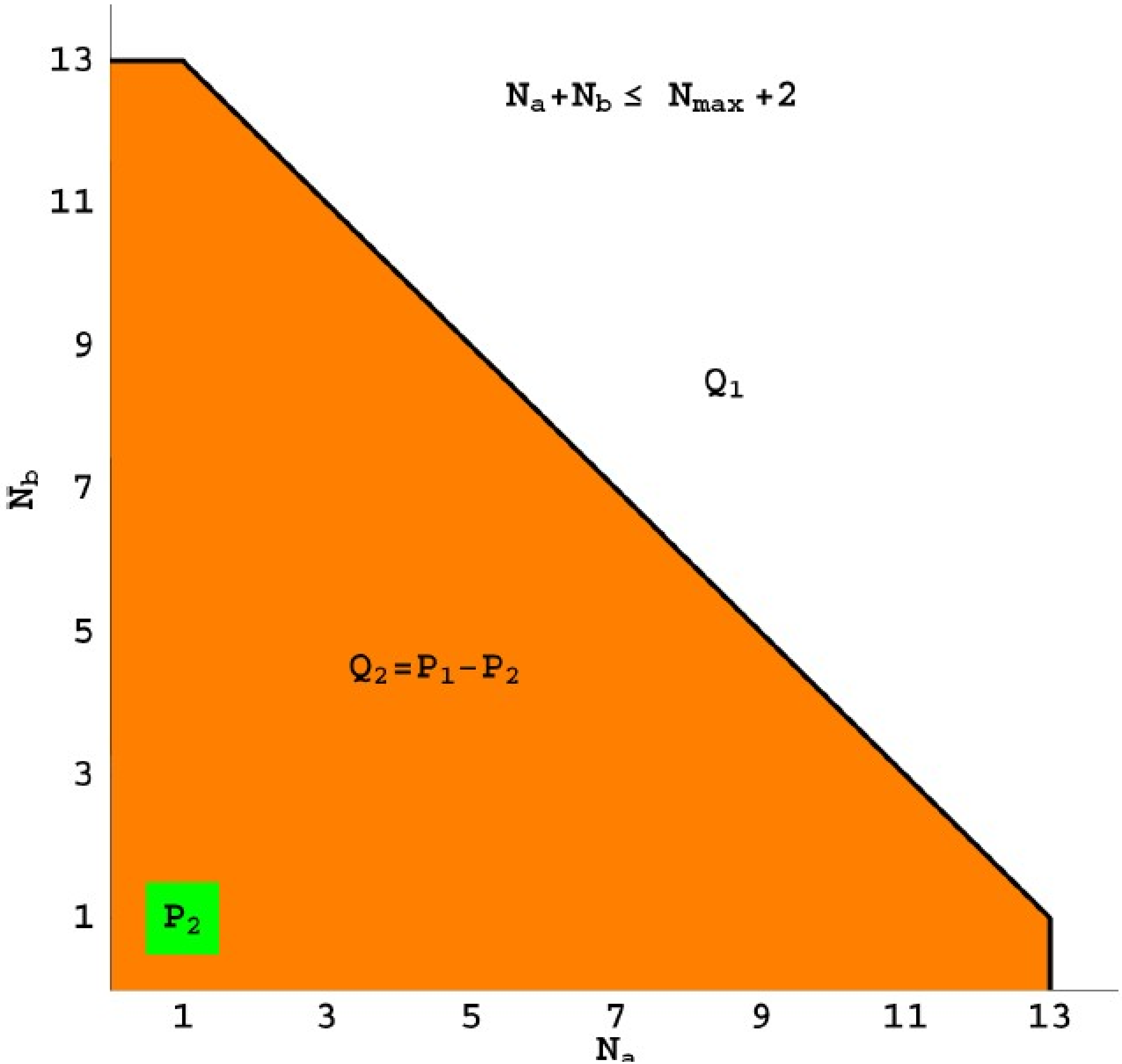
$$U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} E^{\Omega}_{A,2,P} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

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

Two ways of convergence:

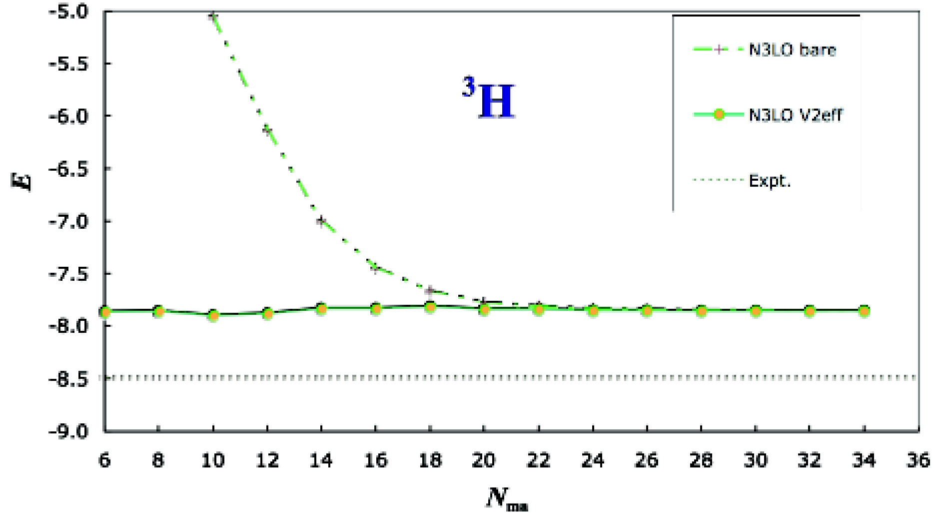
1) For P → 1 and fixed a: $H^{eff}_{A,a=2} \rightarrow H_A$

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



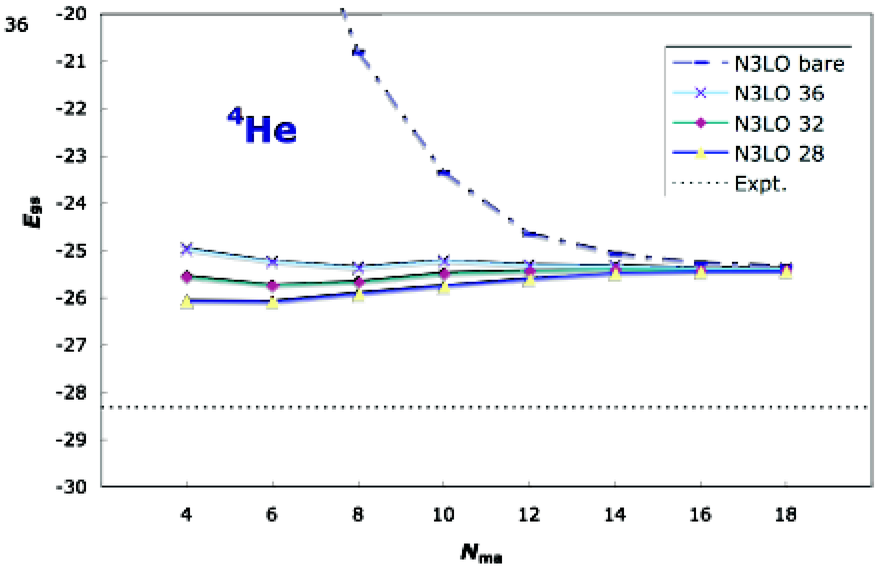
$N_a + N_b \leq N_{max} + 2$
Q_1
$Q_2 = P_1 - P_2$
P_2
N_b
N_a
1
3
5
7
9
11
13

- NCSM convergence test
  - Comparison to other methods



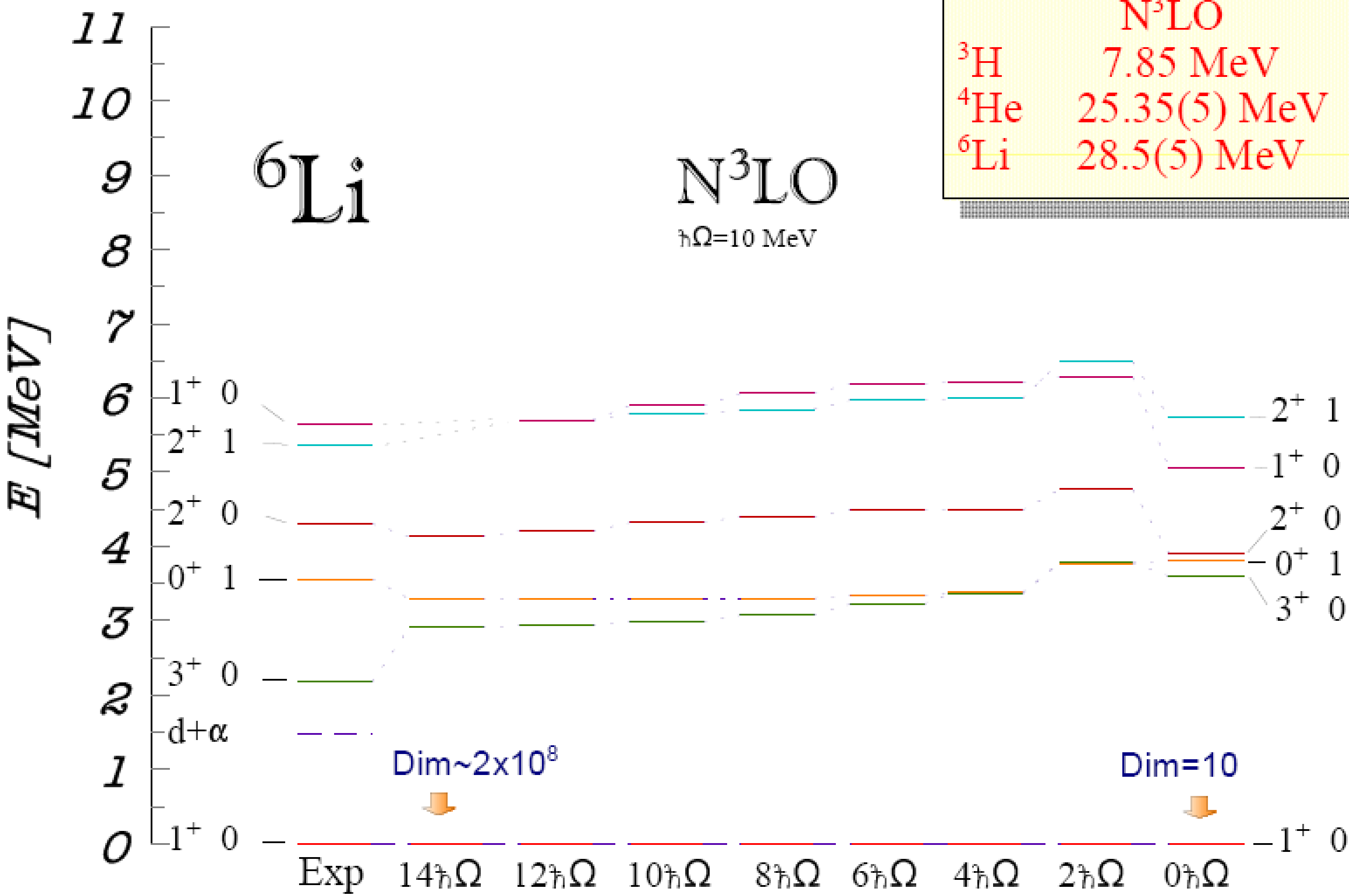
N^{3}LO NN	NCSM	FY	HH
^{3}H	7.852(5)	7.854	7.854
^{4}He	25.39(1)	25.37	25.38

- ➢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

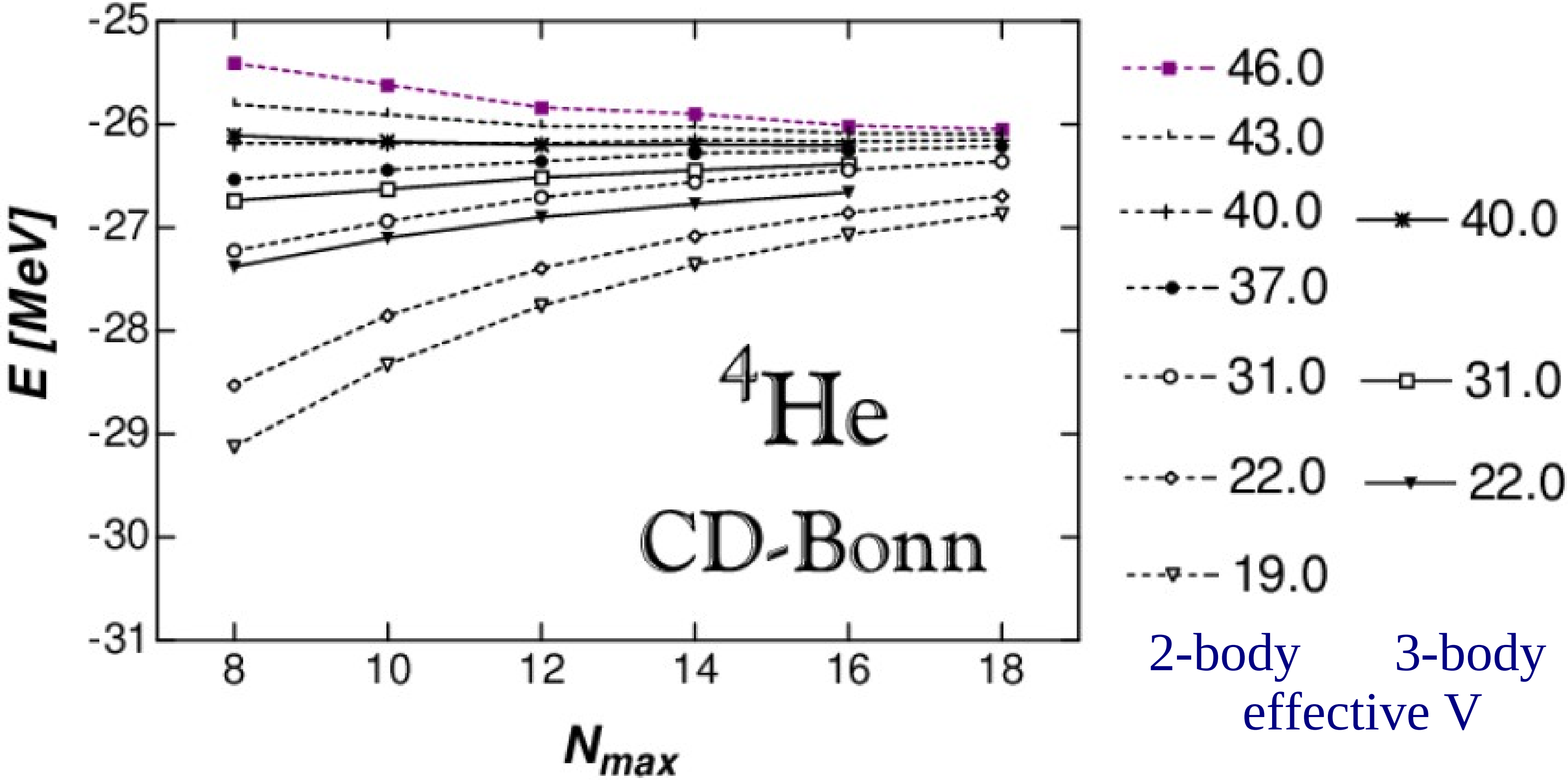


P. Navratil, INT Seminar, November 13, 2007, online

	N³LO	Exp
^3H	7.85 MeV	8.48 MeV
^4He	25.35(5) MeV	28.30 MeV
^6Li	28.5(5) MeV	31.99 MeV



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

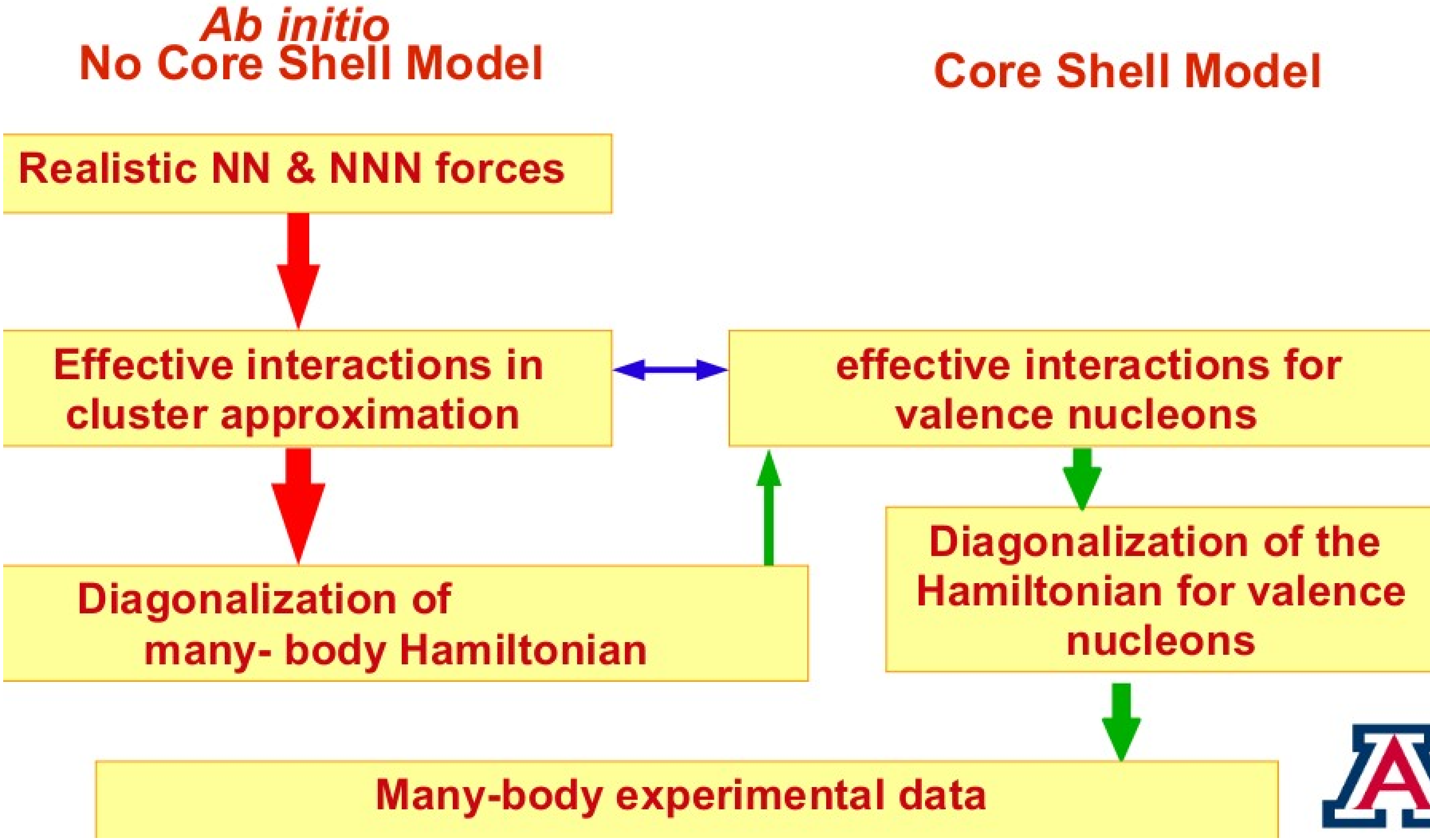


-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N_{max}
^{4}He
CD-Bonn
46.0
43.0
40.0
37.0
31.0
22.0
19.0
40.0
31.0
22.0
2-body
3-body
effective V

II. Ab Initio Shell Model with a Core Approach

From few-body to many-body

Using the NCSM to calculate the shell model input



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)

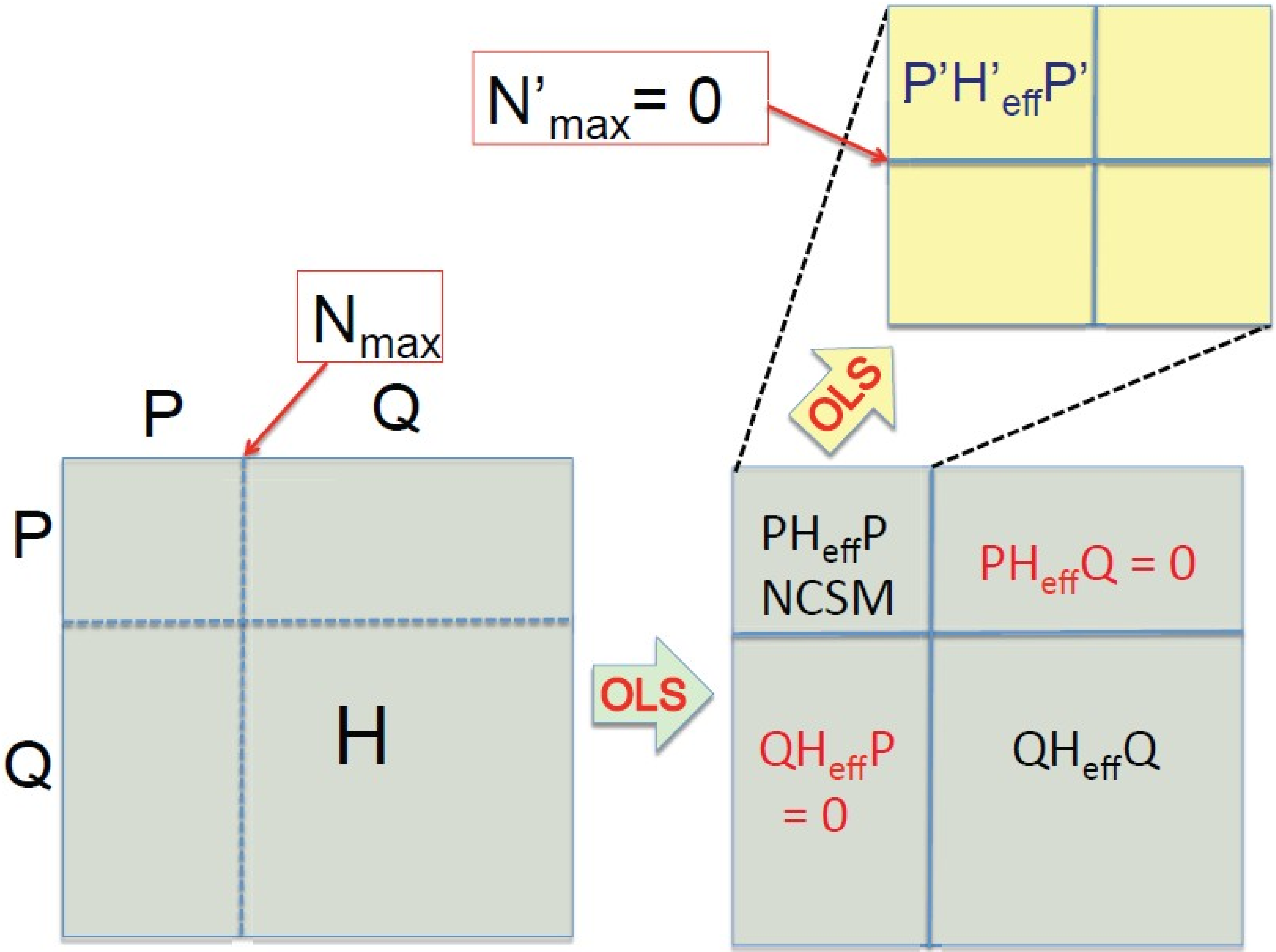
We construct effective two- and three-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ *ab initio* no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians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

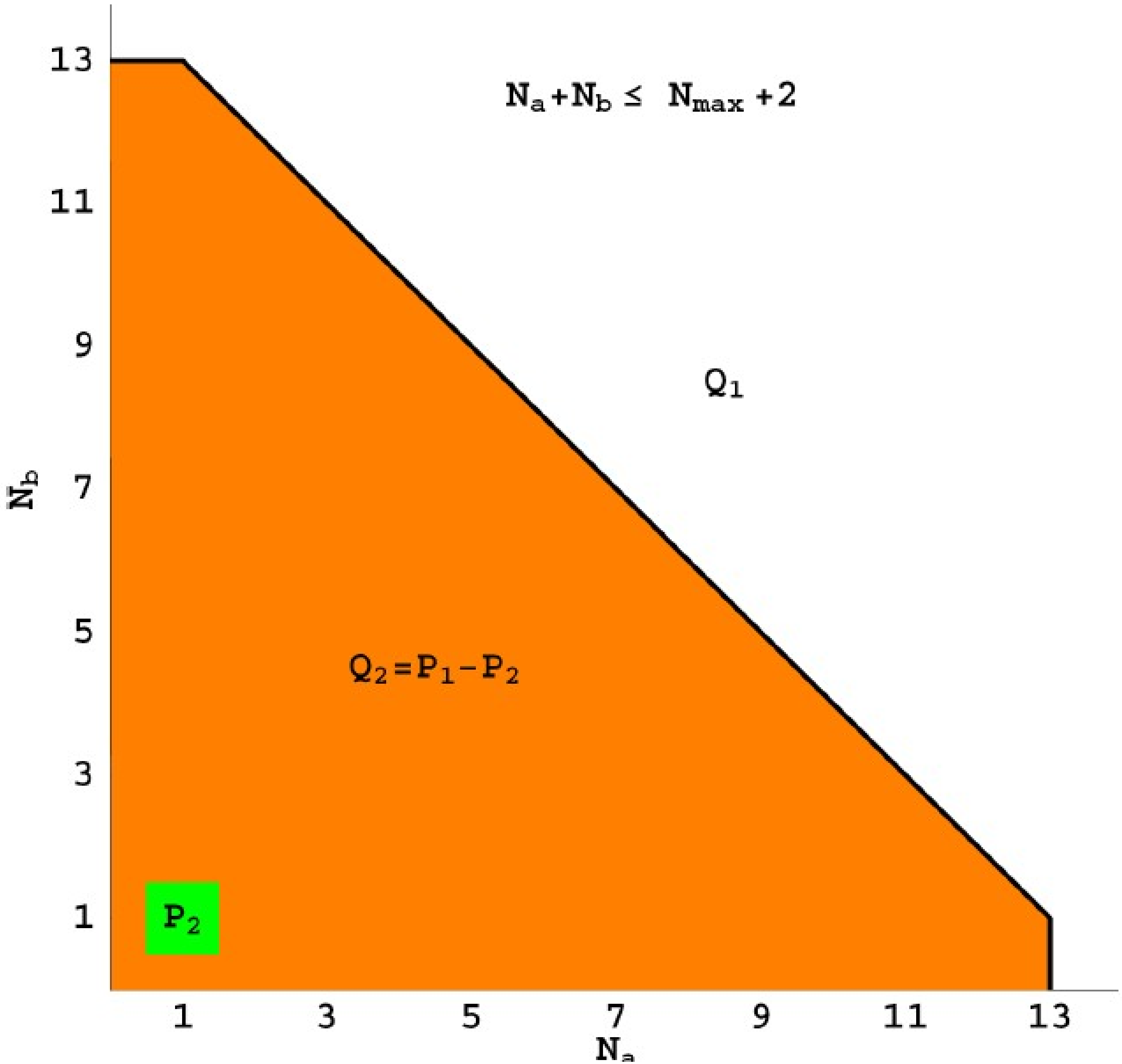
P. Navratil, M. Thoresen and B.R.B., Phys. Rev. C 55, R573 (1997)

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
13
11
9
7
5
3
1

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;

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

III. Results: sd-shell nuclei

Accepted for publication in PRC

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

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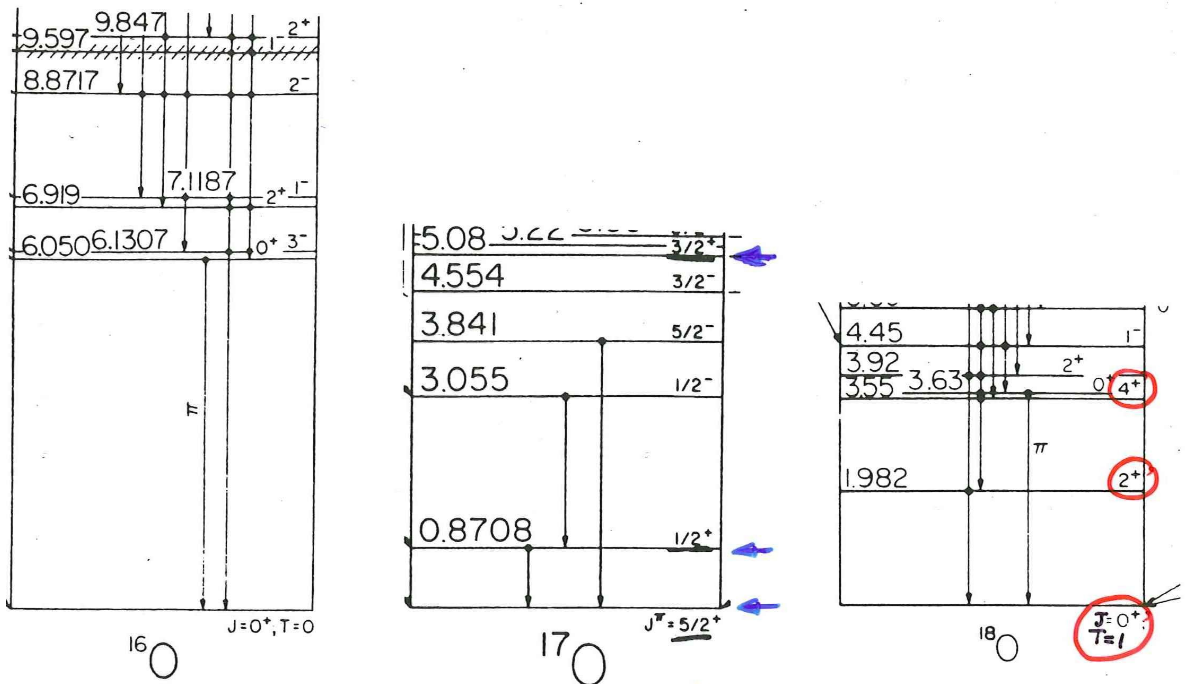
(Dated: February 3, 2015)

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

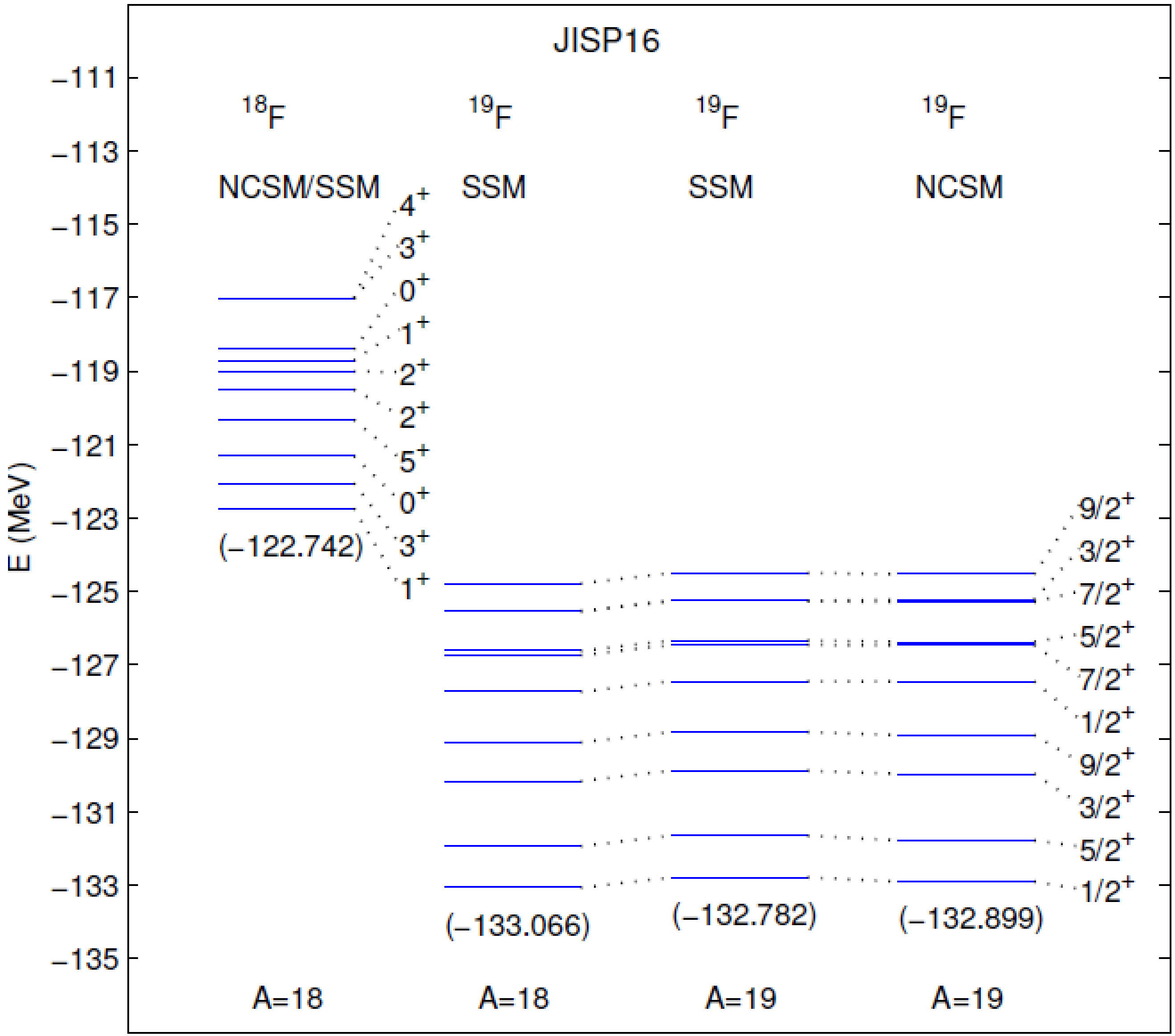
- Next, add CM harmonic-oscillator Hamiltonian

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

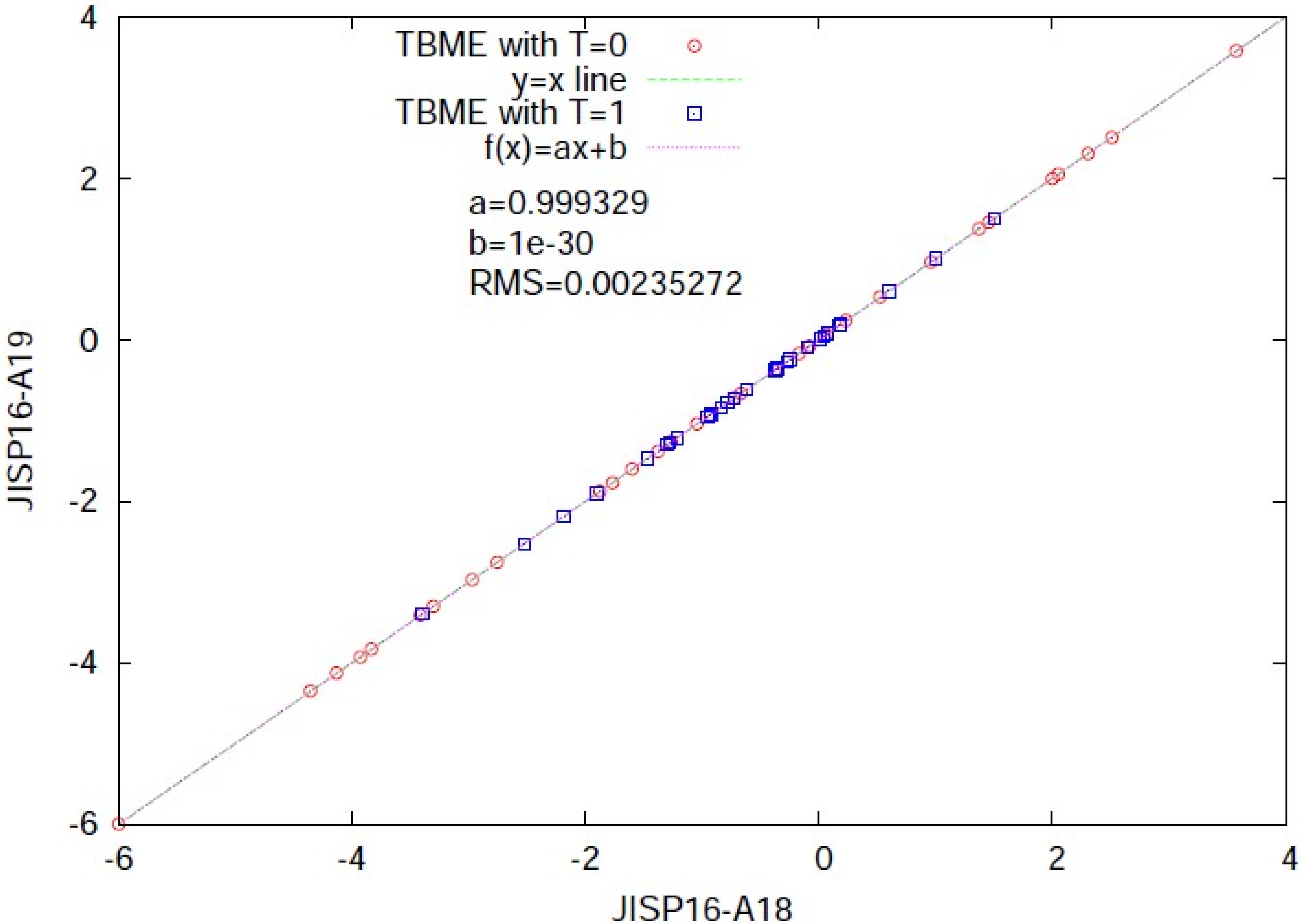
To H_A, yielding

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

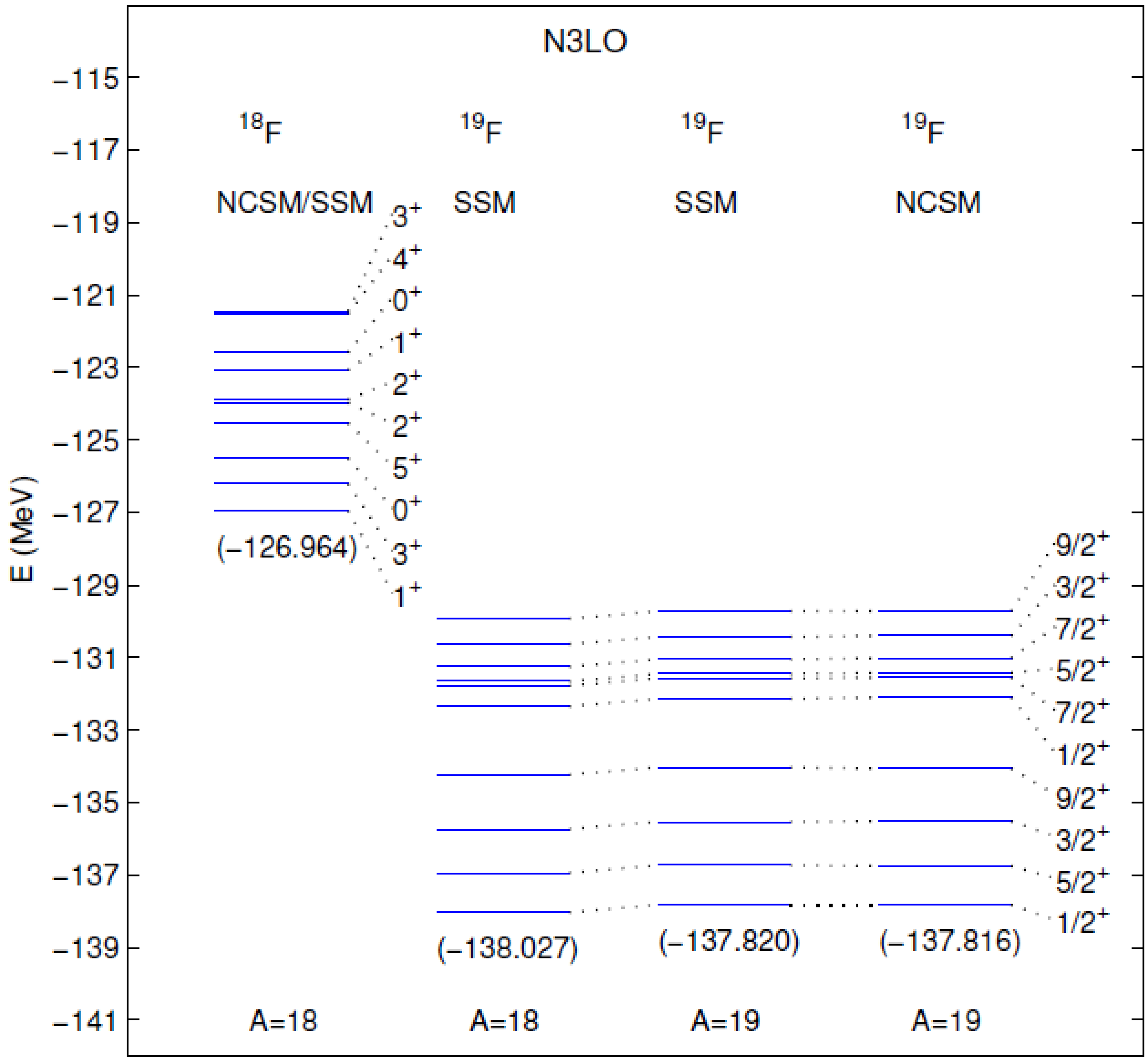
Defines a basis (*i.e.* HO) for evaluating V_{ij}



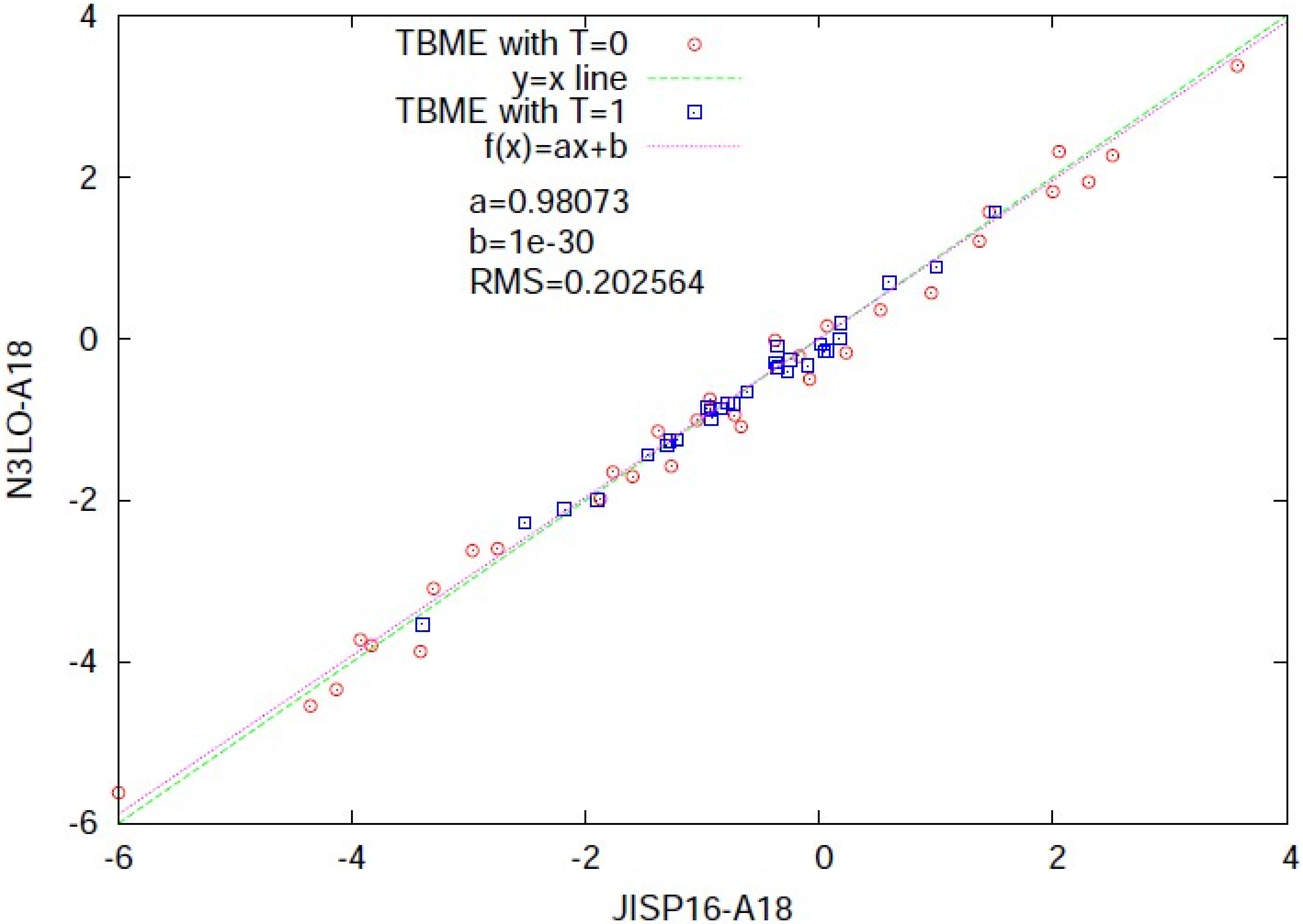
JISP16
E (MeV)
−111
−113
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
18F
19F
19F
19F
NCSM/SSM
SSM
SSM
NCSM
(−122.742)
(−133.066)
(−132.782)
(−132.899)
4+
3+
0+
1+
2+
2+
5+
0+
3+
1+
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
A=18
A=18
A=19
A=19



Preliminary Results



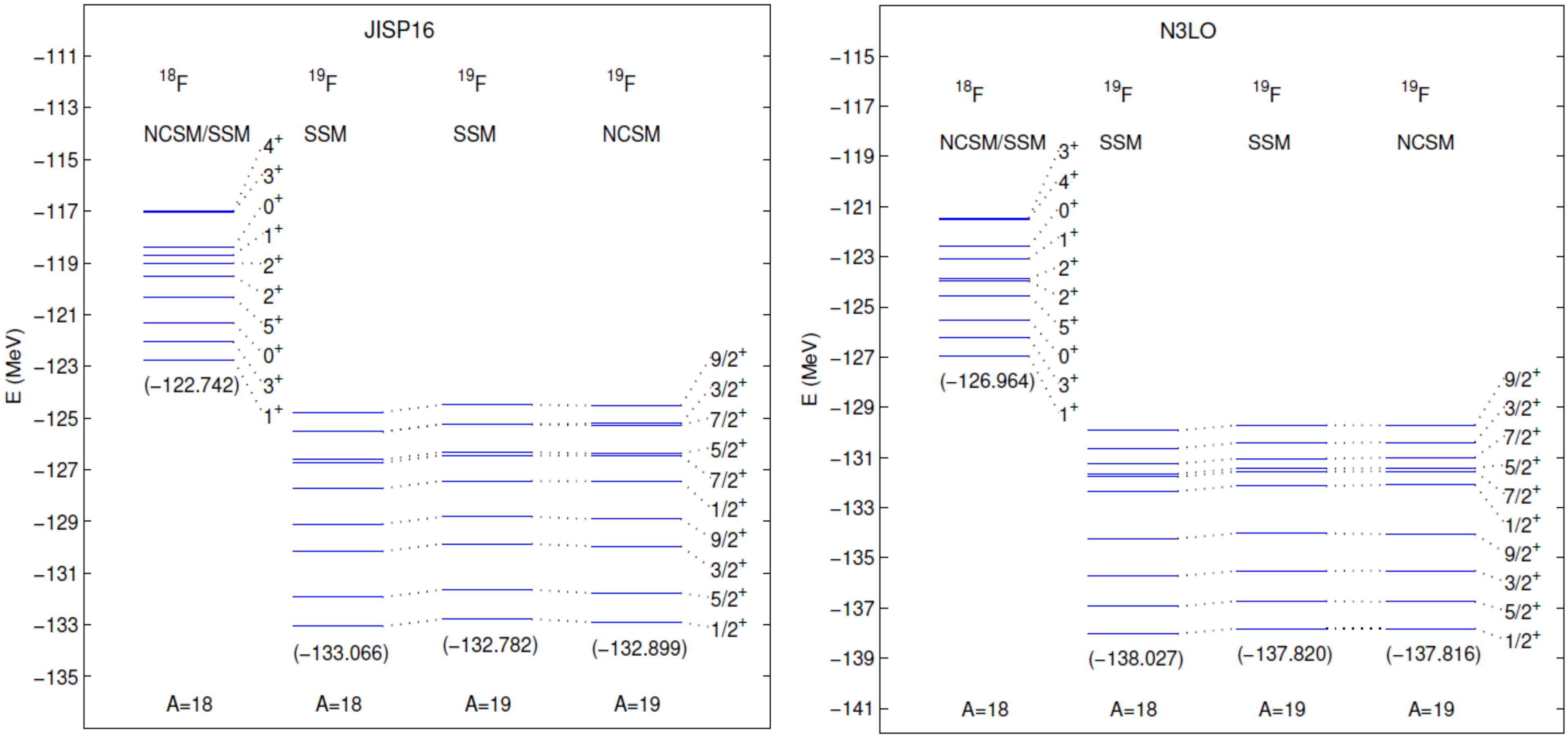
N3LO
E (MeV)
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
−137
−139
−141
18F
NCSM/SSM
19F
SSM
19F
SSM
19F
NCSM
3+
4+
0+
1+
2+
2+
5+
0+
3+
1+
(−126.964)
(−138.027)
(−137.820)
(−137.816)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
A=18
A=18
A=19
A=19

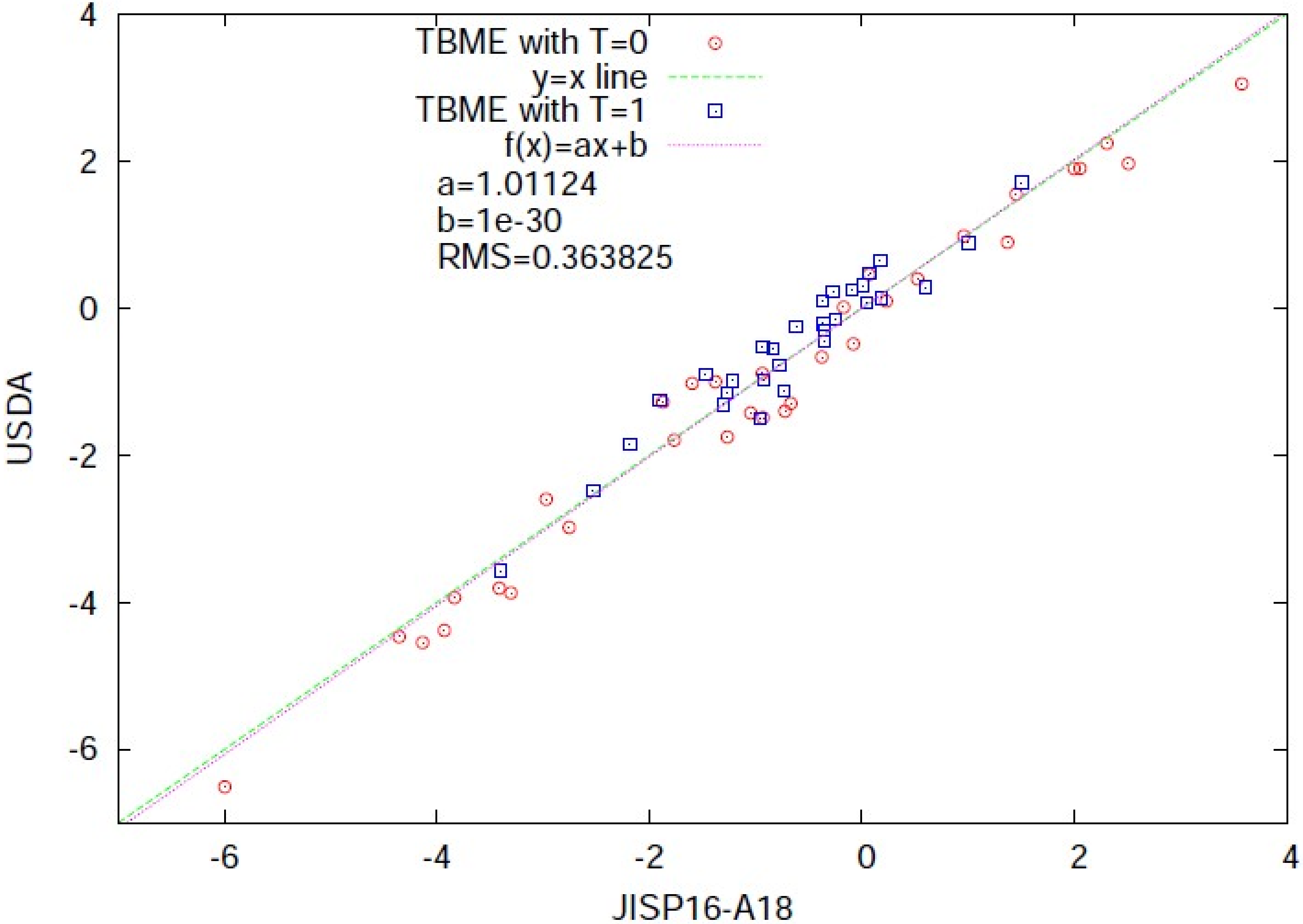


Preliminary Results

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

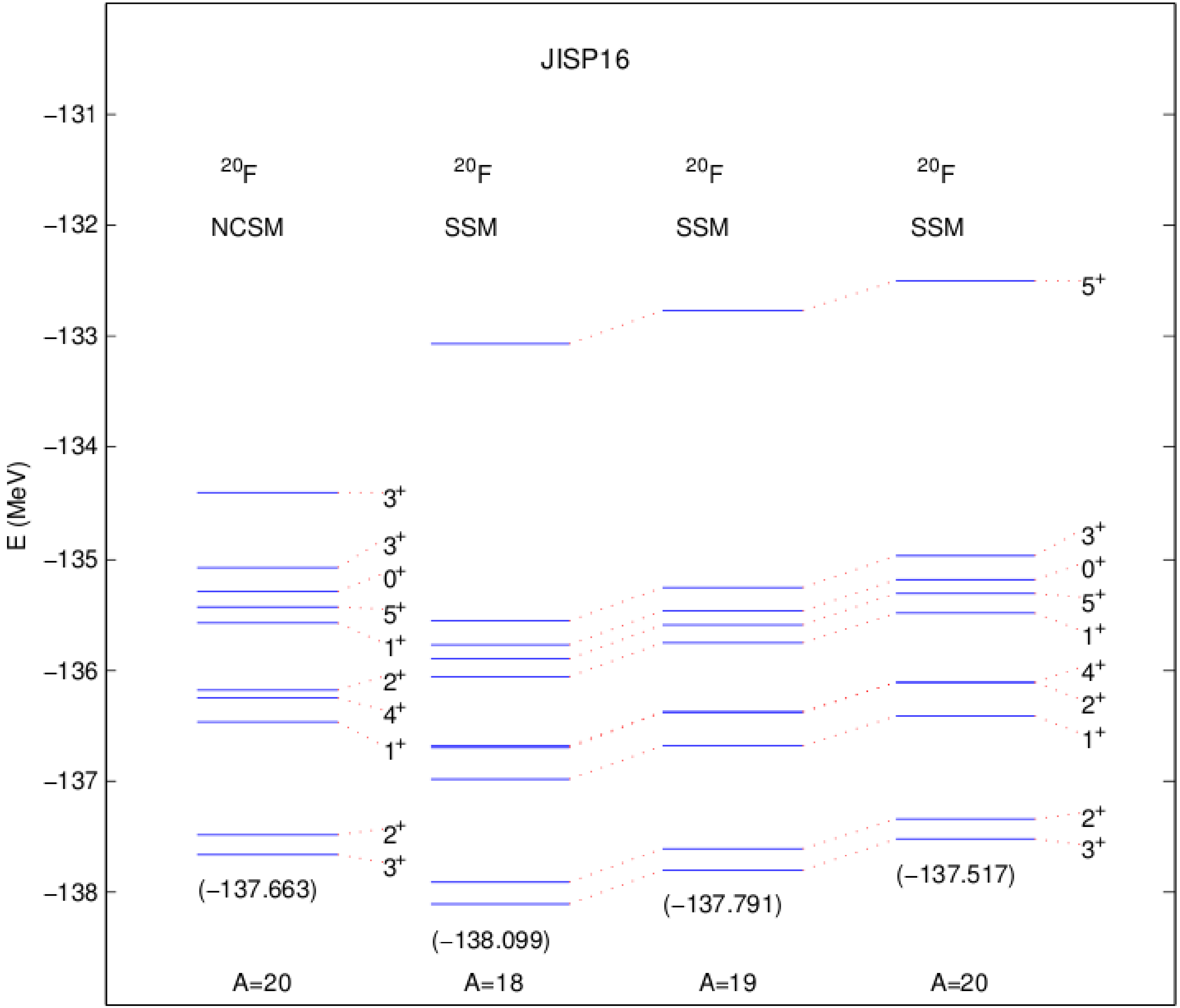

JISP16
E (MeV)
−111
−113
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
18F
19F
19F
19F
NCSM/SSM
SSM
SSM
NCSM
4+
3+
0+
1+
2+
2+
5+
0+
3+
1+
(−122.742)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
(−133.066)
(−132.782)
(−132.899)
A=18
A=18
A=19
A=19
N3LO
E (MeV)
−115
−117
−119
−121
−123
−125
−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)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
(−138.027)
(−137.820)
(−137.816)
A=18
A=18
A=19
A=19



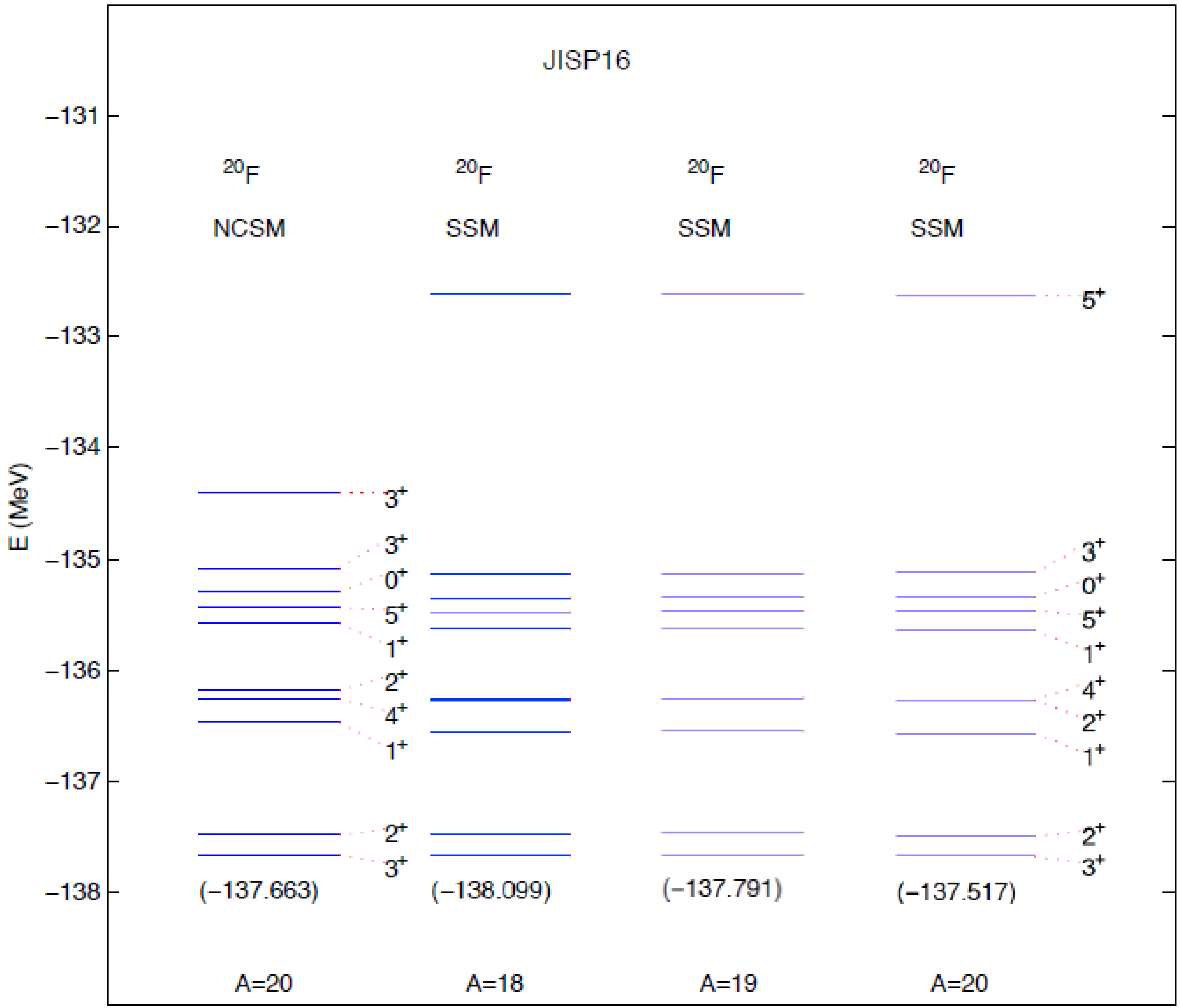
Comparison of effective TBMEs in the sd-shell: JISP16 vs USDA by Alex Brown et al.

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.

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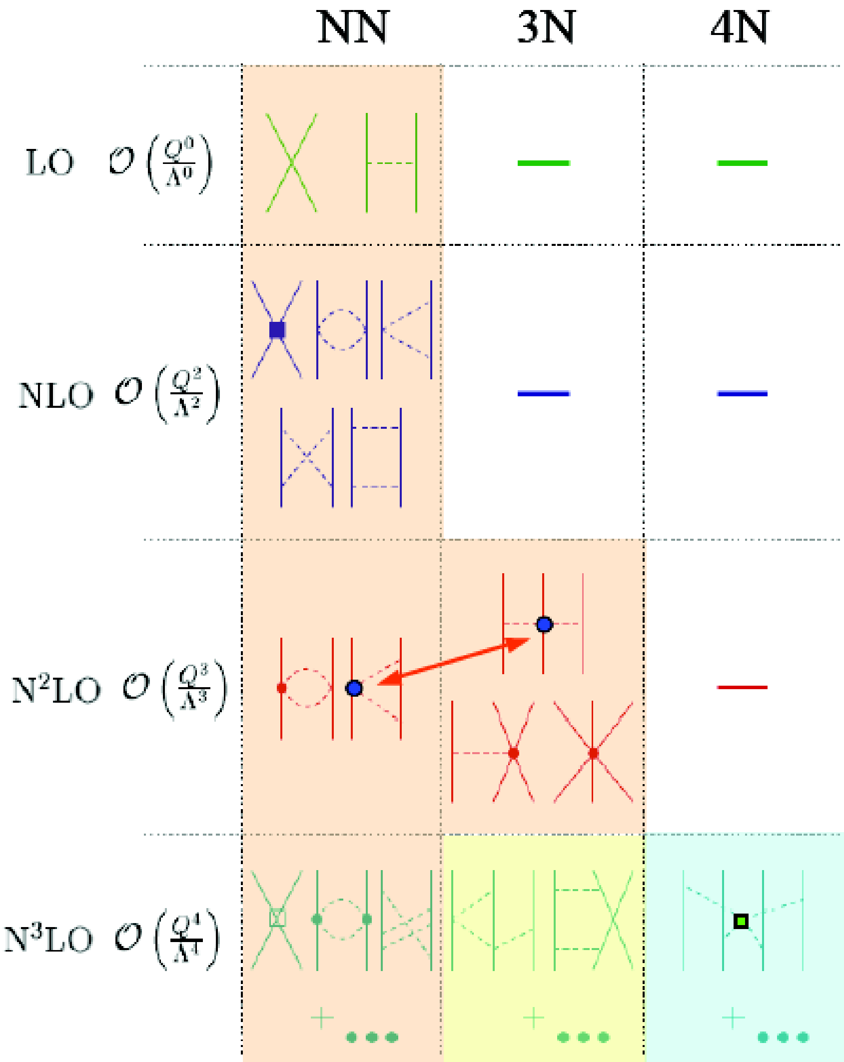
Chiral effective field theory (EFT) for nuclear forces

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

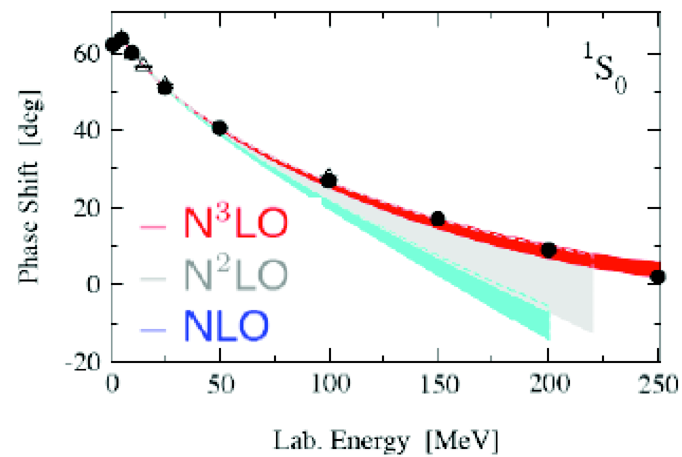


explains pheno hierarchy:
NN > 3N > 4N > …

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

3N,4N: 2 new couplings to N^{3}LO!

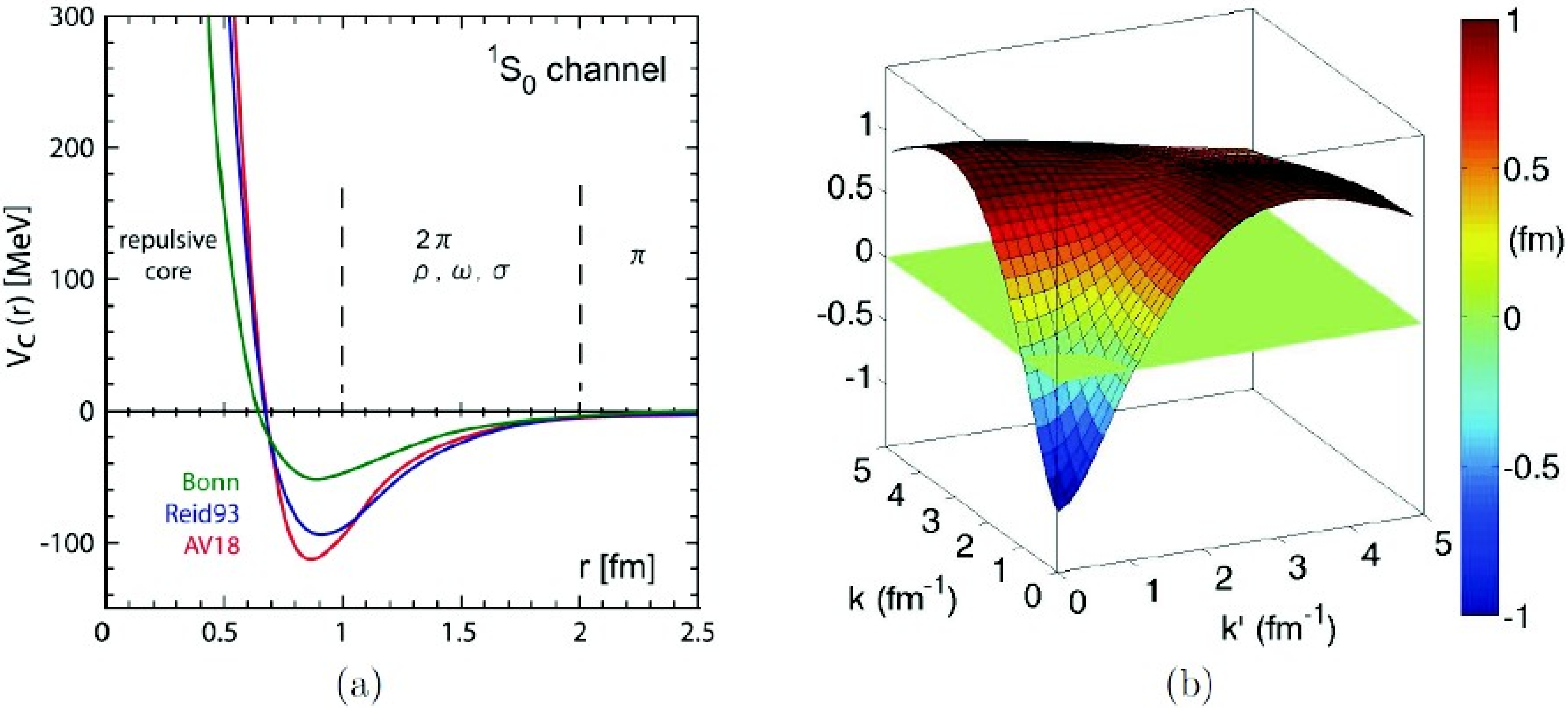
theoretical error estimates



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

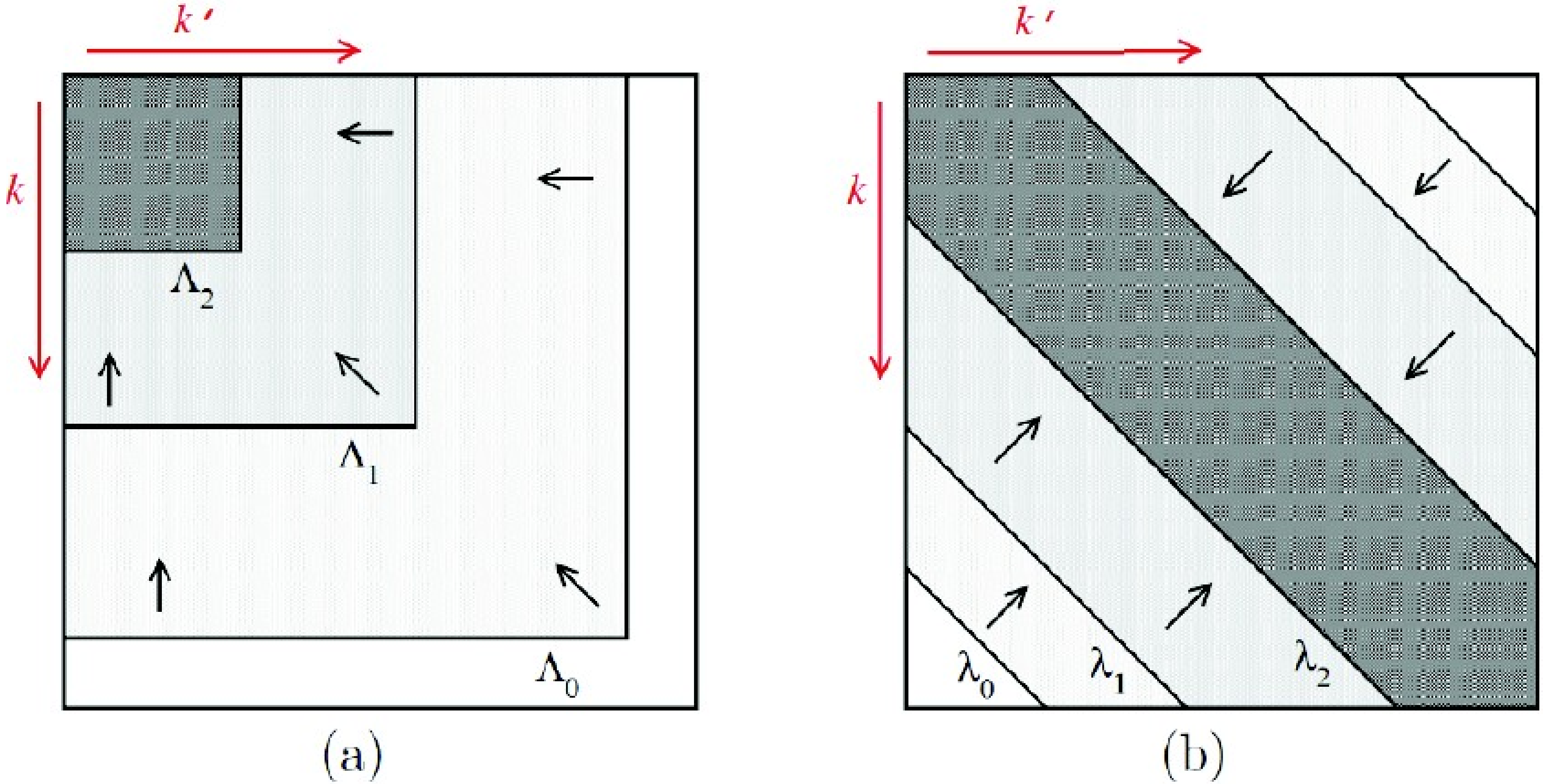
A. Schwenk

Realistic two-body potentials in coordinate and momentum space



Repulsive core makes calculations difficult

Illustration on how the high momentum nodes are integrated out in the Vlowk (a) and in the SRG (b) RG methods



→ Need to decouple high/low momentum modes
✓ Achieved by V_{low-k} or Similarity RG approaches (e.g. SRG)

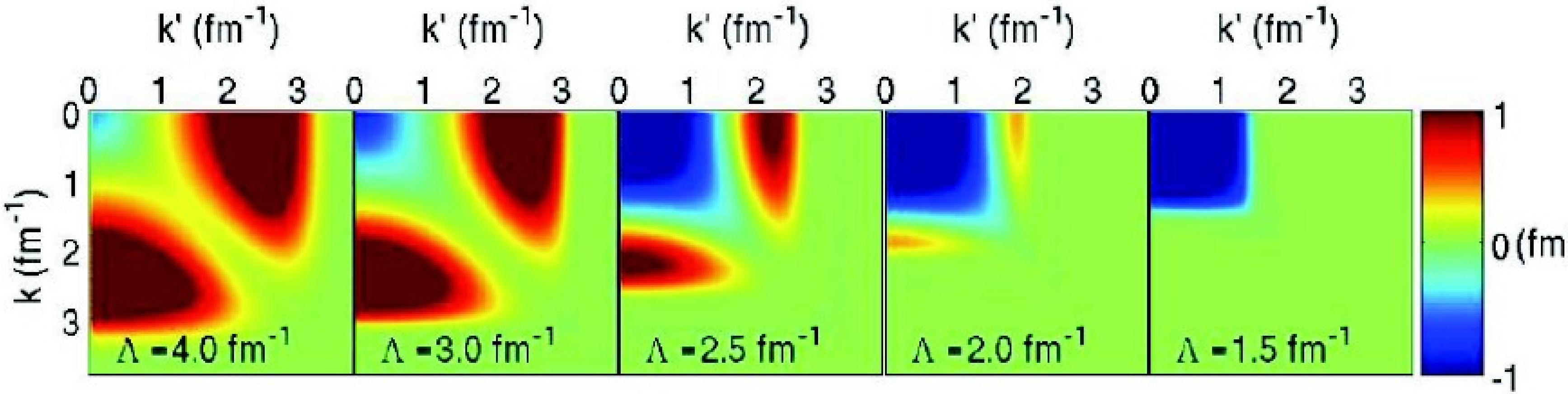


Fig. from S. Bogner et al Prog.Part.Nucl.Phys.65:94-147,2010

→ Observable physics is preserved (e.g. NN phase shifts) AND calculations become easier (work with the relevant degrees of freedom)

→ One has to deal with "induced" many-body forces...

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 !!!

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

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

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

Ab-initio coupled-cluster effective interactions for the shell model: Application to neutron-rich oxygen and carbon isotopes

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We derive and compute effective valence-space shell-model interactions from ab-initio coupled-cluster theory and apply them to open-shell and neutron-rich oxygen and carbon isotopes. Our shell-model interactions are based on nucleon-nucleon and three-nucleon forces from chiral effective-field theory. We compute the energies of ground and low-lying states, and find good agreement with experiment. In particular our calculations are consistent with the $N = 14, 16$ shell closures in ^{22,24}O, while for ^{20}C the corresponding $N = 14$ closure is weaker. We find good agreement between our coupled-cluster effective-interaction results with those obtained from standard single-reference coupled-cluster calculations for up to eight valence neutrons.

PACS numbers: 21.30.Fe, 21.60.Cs, 21.60.De, 21.10.-k

arXiv: 1402.2563v1 [nuch-th] 11 Feb. 2014

Core energies: A=18, -130.462; A=19, -130.056 (MeV)