Ab Initio Shell Model with a Core: Extending the NCSM to Heavier Nuclei

Bruce R. Barrett
University of Arizona, Tucson

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MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many-body theory

$$H\Psi = E\Psi$$

We cannot, in general, solve the full problem in the complete Hilbert space, so we must truncate to a finite model space

$\Longrightarrow$ We must use effective interactions and operators!

Some current shell-model references

1. 1. E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, and A. P. Zuker, "The Shell Model as a Unified View of Nuclear Structure," *Reviews of Modern Physics* **77**, 427 (2005)
2. 2. B. A. Brown, "The Nuclear Shell Model towards the Drip Lines," *Progress in Particle and Nuclear Physics* **47**, 517 (2001)
3. 3. I. Talmi, "Fifty Years of the Shell Model-The Quest for the
4. Effective Interaction," *Advances in Nuclear Physics*, Vol. **27**,
5. ed. J. W. Negele and E. Vogt (Plenum, NY, 2003)
6. 4. B. R. B., "Effective Operators in Shell-Model Calculations," 10th Indian Summer School of Nuclear Physics:Theory of Many-Fermion Systems, *Czechoslovak Journal of Physics* **49**, 1 (1999)

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)

From few-body to many-body

Ab initio
No Core Shell Model

Realistic NN & NNN forces

↓

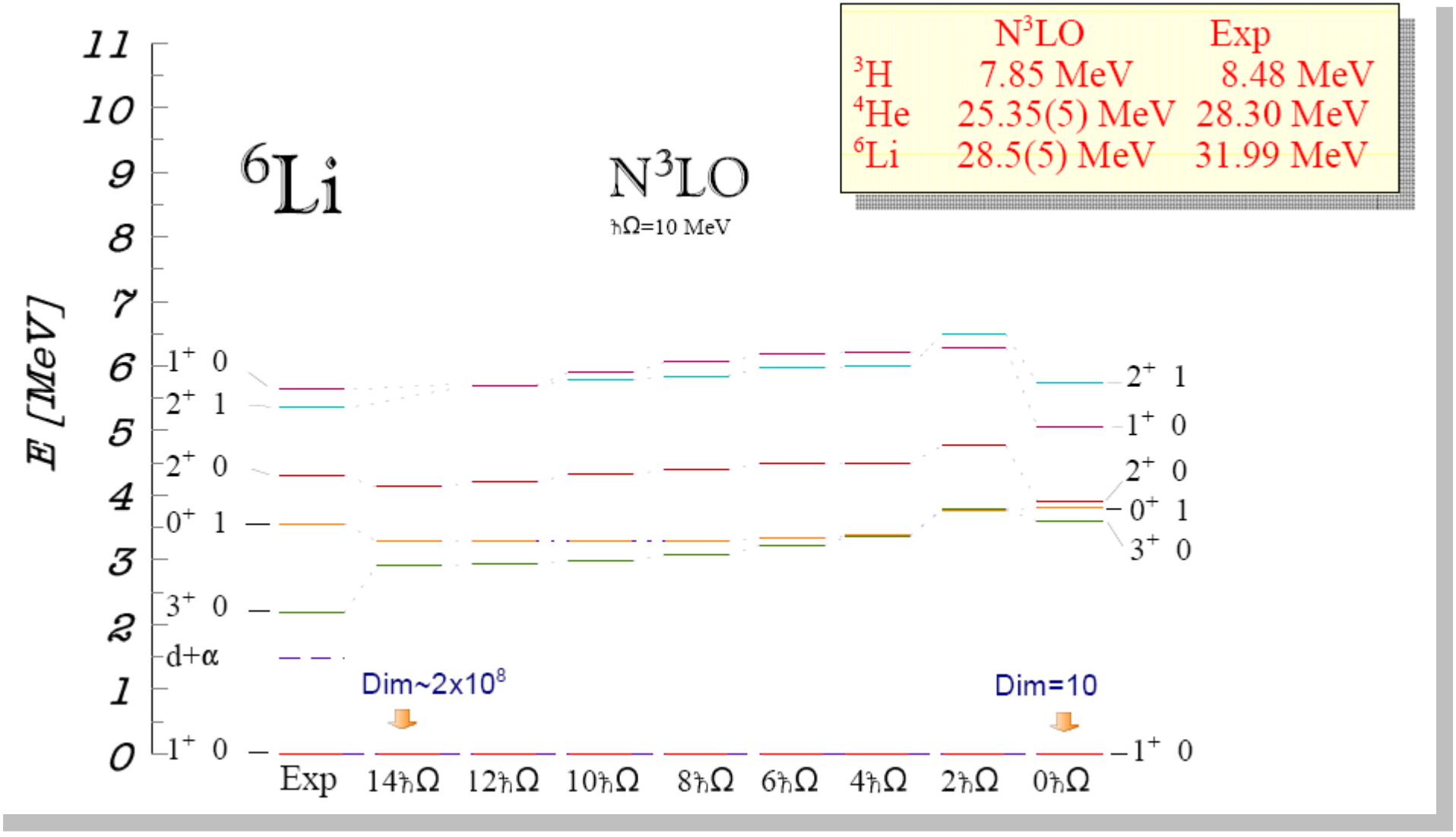
Effective interactions in cluster approximation

↓

Diagonalization of many- body Hamiltonian

↓

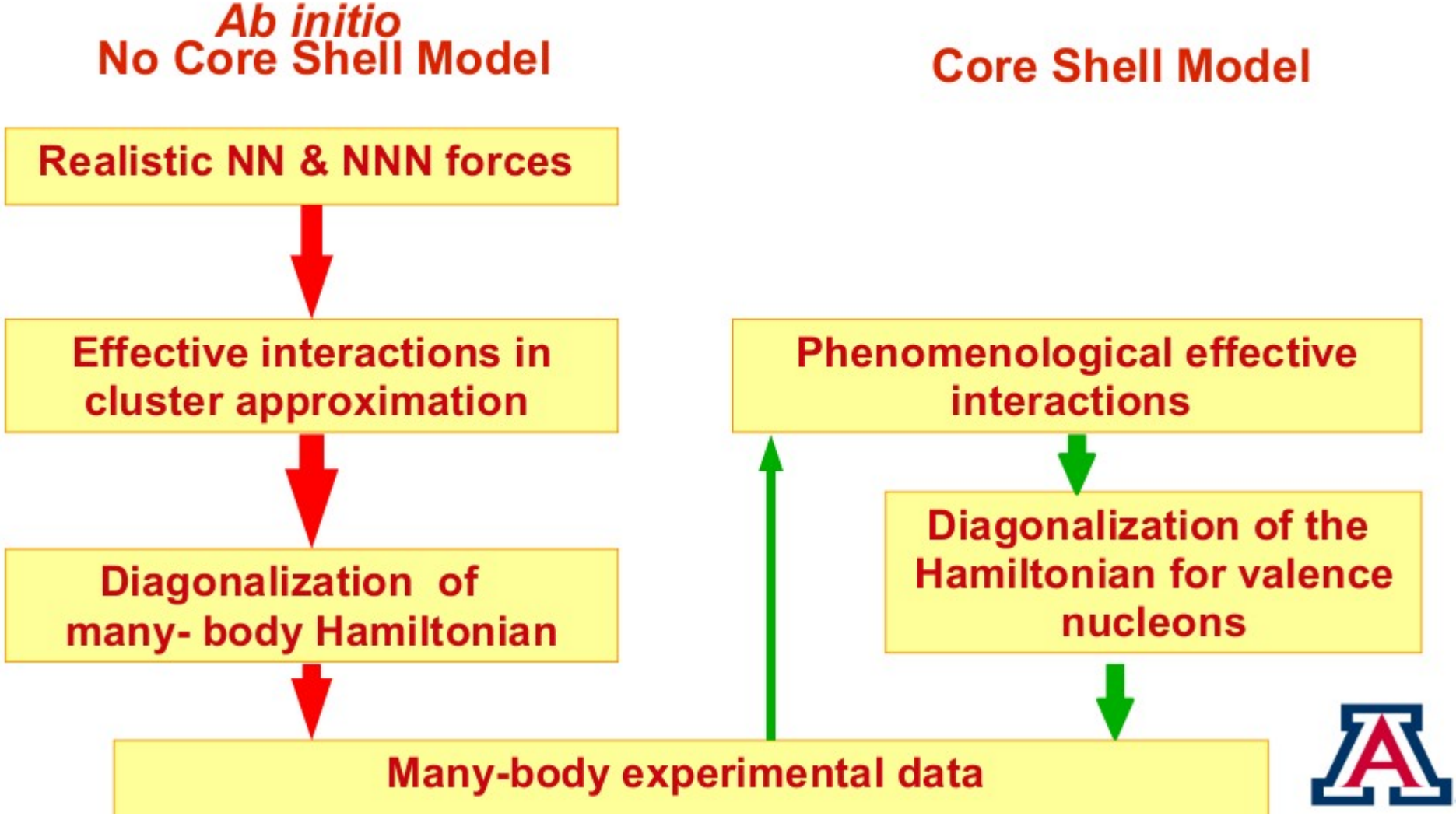
Many-body experimental data

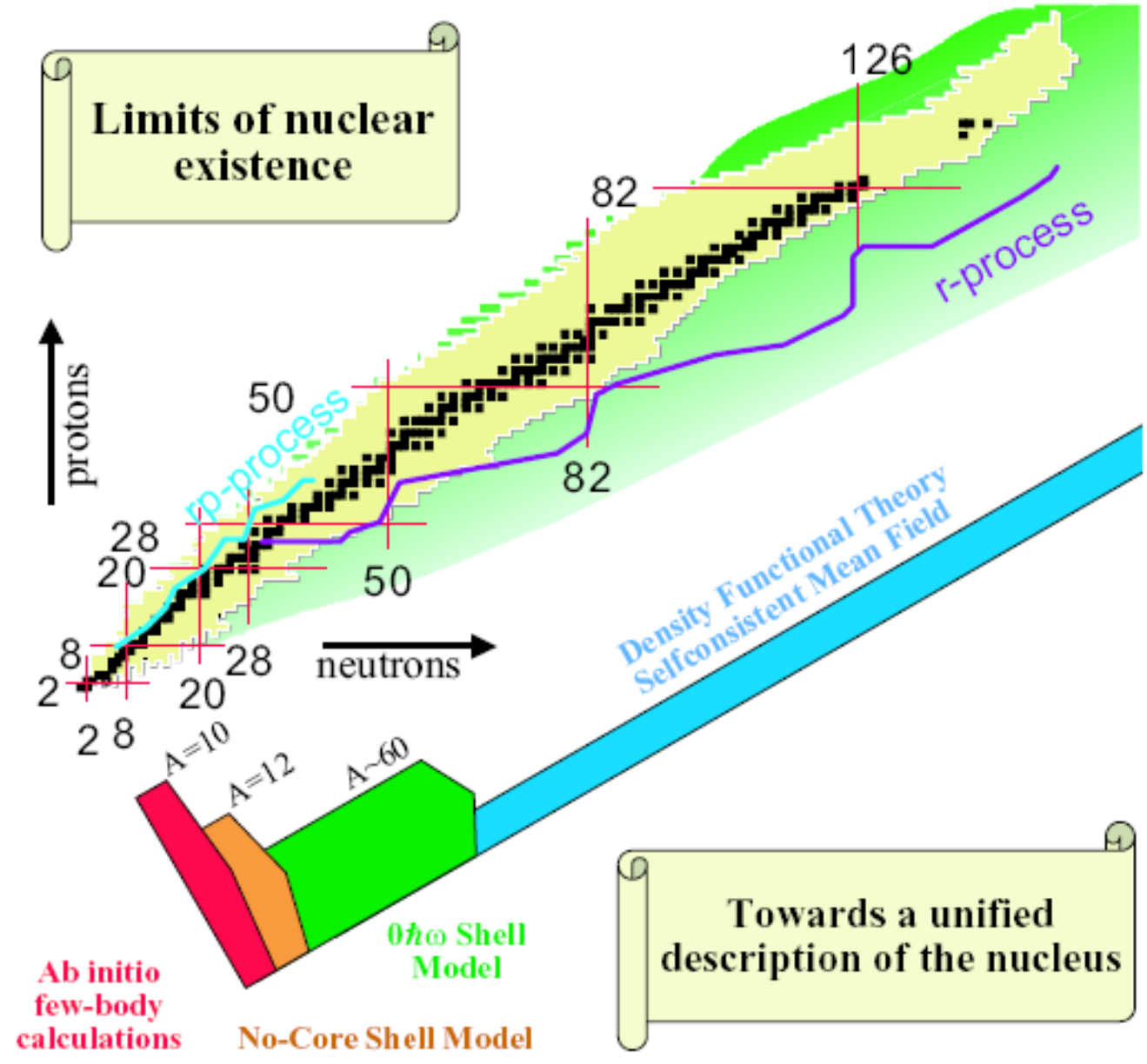


	N^{3}LO	Exp
^{3}H	7.85 MeV	8.48 MeV
^{4}He	25.35(5) MeV	28.30 MeV
^{6}Li	28.5(5) MeV	31.99 MeV

P. Navrátil and E. Caurier, Phys. Rev. C **6 9**, 014311 (2004)

From few-body to many-body

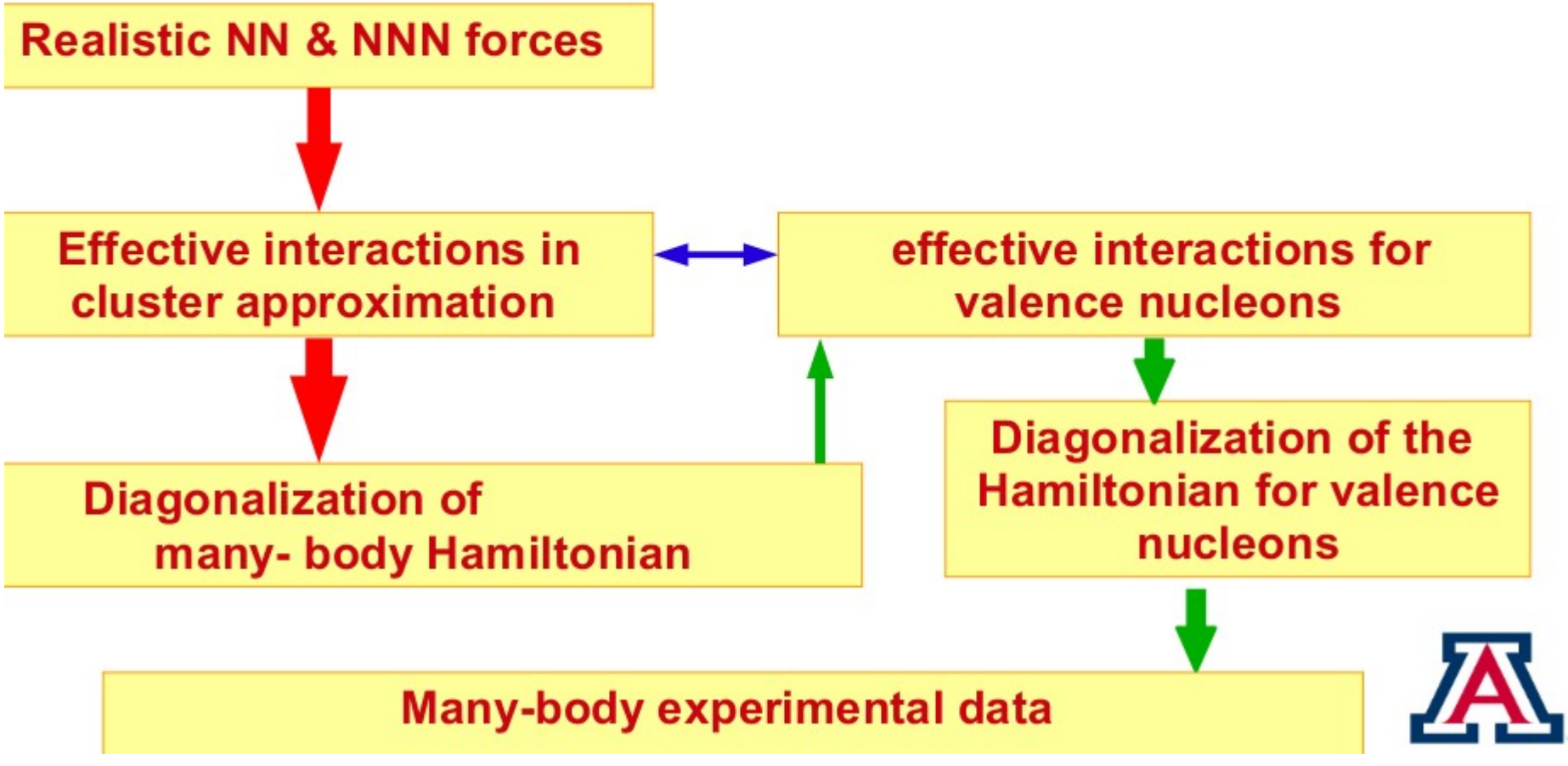



Limits of nuclear existence
126
82
82
50
50
28
20
28
20
8
2
2 8
protons
neutrons
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
0ħω Shell Model
Ab initio few-body calculations
No-Core Shell Model
Towards a unified description of the nucleus

From few-body to many-body

Ab initio
No Core Shell Model

Core Shell Model



No Core Shell Model

Starting Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A} V_{NN}(\vec{r}_i - \vec{r}_j) + \sum_{i<j<k}^{A} V_{ijk}^{3b}$$

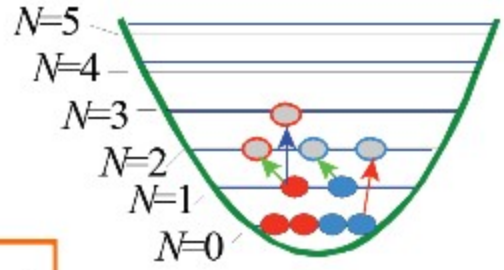
Realistic NN and NNN potentials

Coordinate space – Argonne V18, AV18', CD-Bonn, chiral N^{3}LO, NNN Tucson - Melbourne

Momentum space – NNN chiral N^{2}LO

Binding center-of-mass HO potential (Lipkin 1958)

$$\frac{1}{2} A m\Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$



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

<HO|V$_{NN}$(,A)|HO>

Cluster Expansion:

Two-body cluster approximation

$$H_2^{\Omega} = \sum_{i=1}^{2} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{2} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

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;

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

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

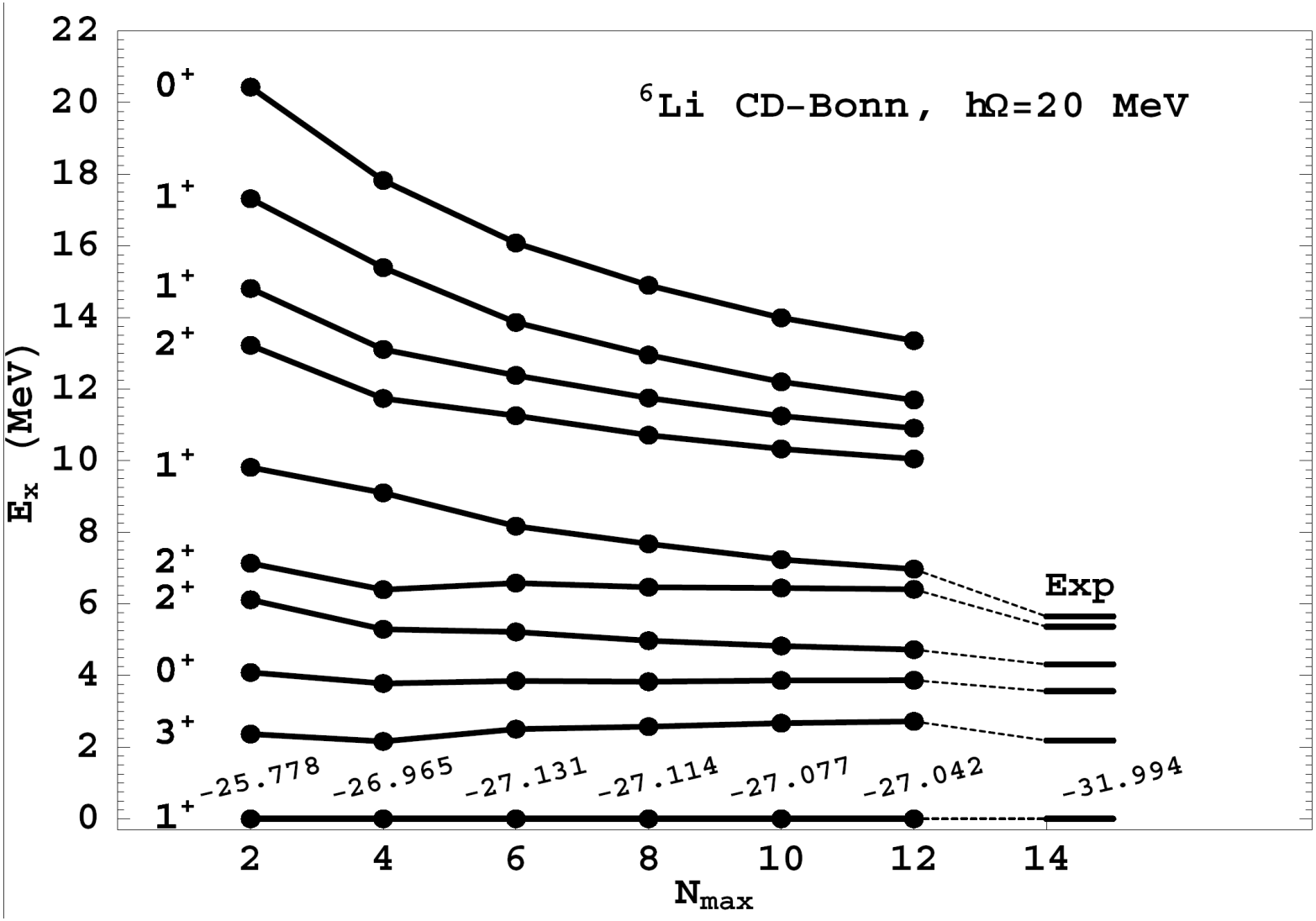
Two ways of convergence:

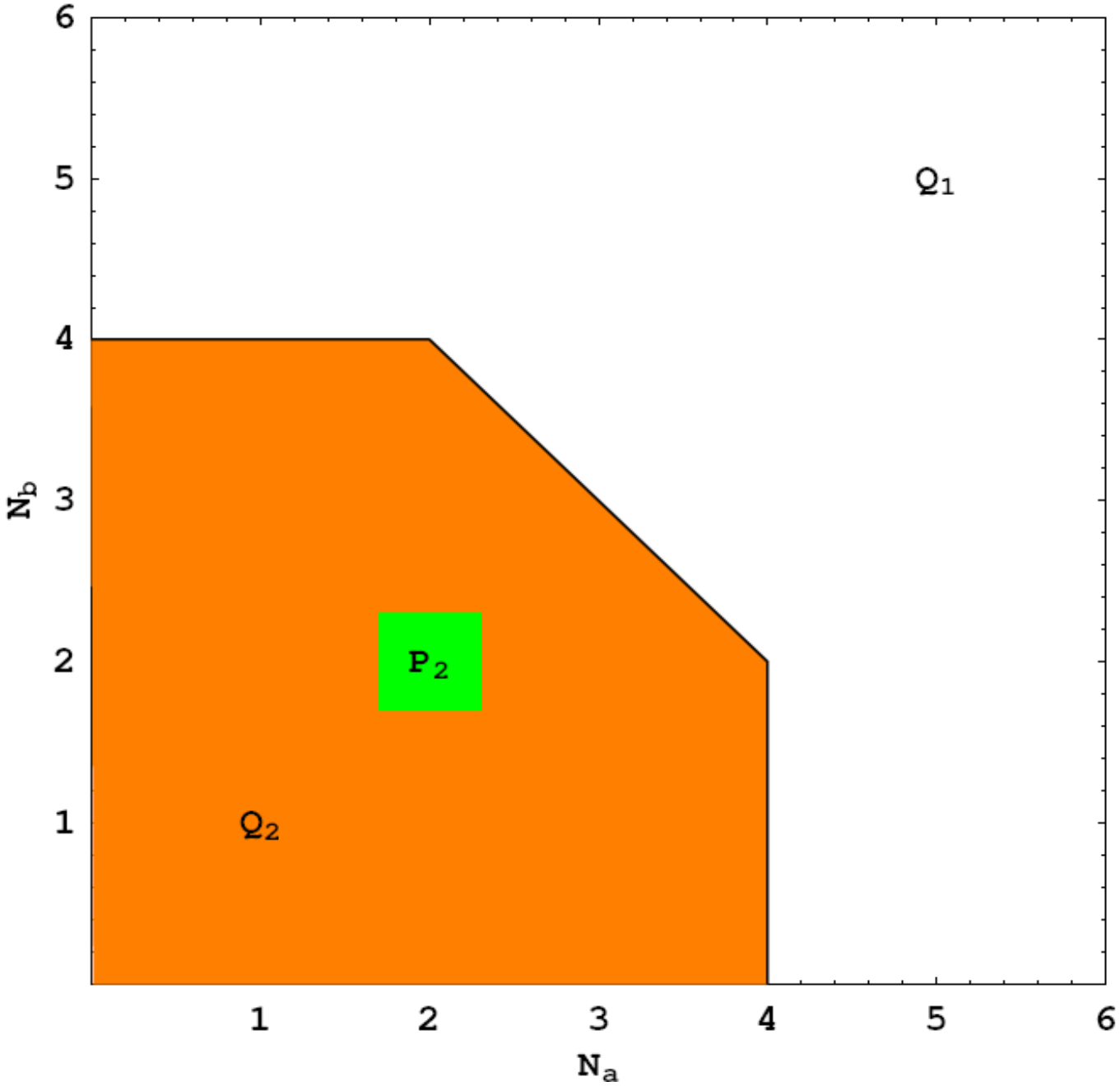
1) For $P \to 1$ and fixed a: $H^{\mathrm{eff}}_{A,a=2} \to H_A$

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




6
5
4
3
2
1
N_b
Q_1
P_2
Q_2
1
2
3
4
5
6
N_a

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;

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

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

$$V_2^{6,6} = \mathcal{H}^{0,N_{\max}}_{6,6} - \mathcal{H}^{0,N_{\max}}_{6,5}$$

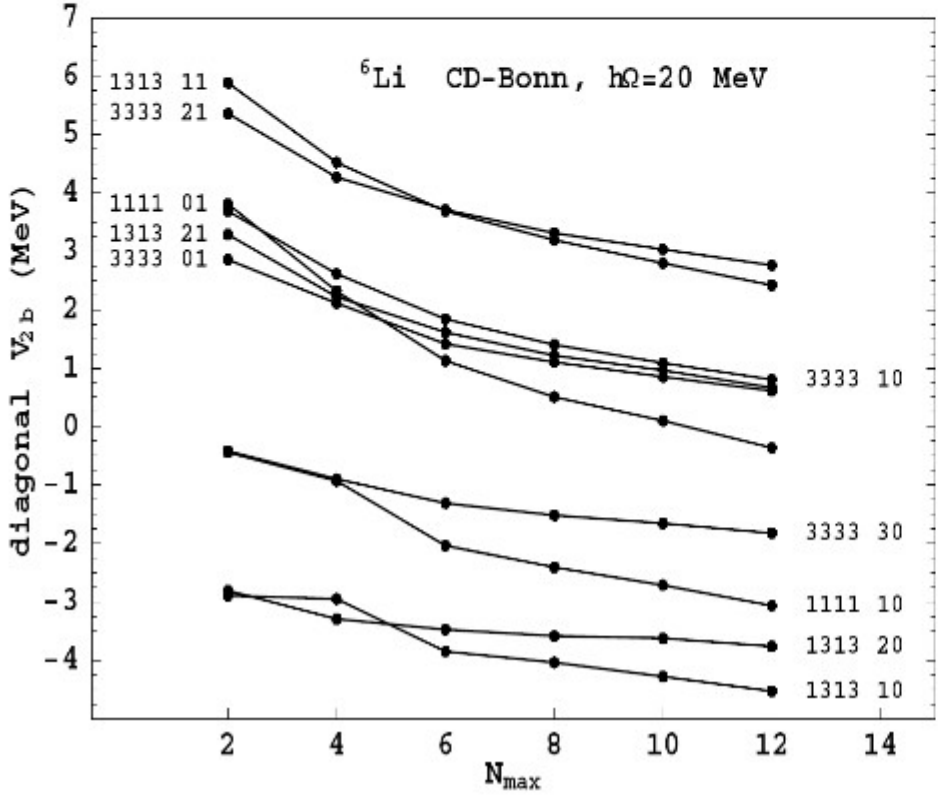
TBMEs:

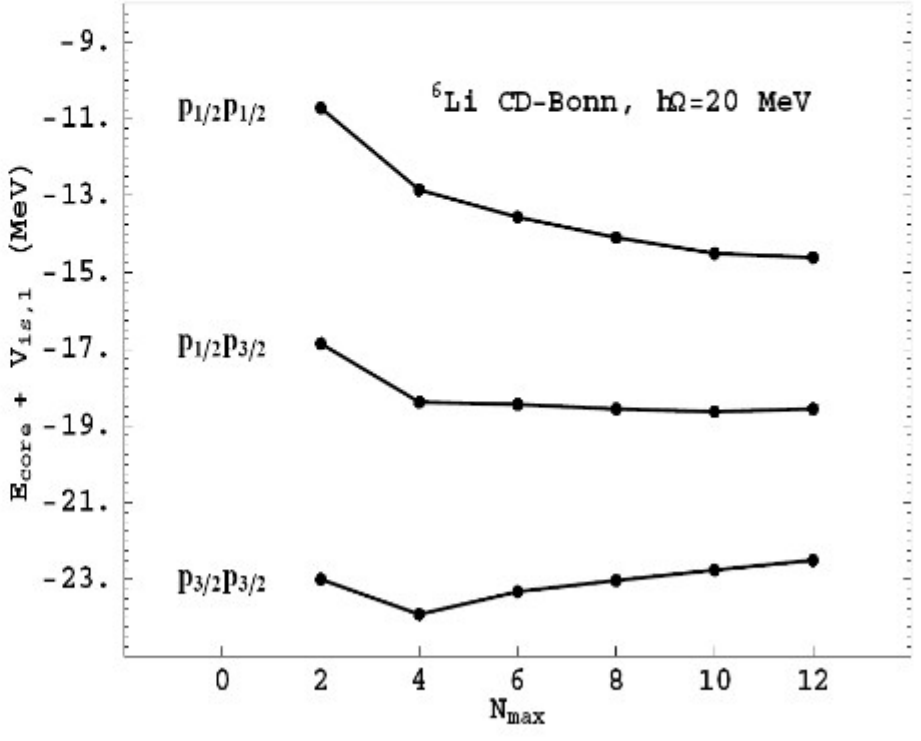
$\langle p_{3/2}p_{3/2}|V_2^{6,6}|p_{3/2}p_{3/2}\rangle_{J=3,T=0}$ = -1.825 MeV

$\langle p_{3/2}p_{3/2}|V_2^{6,6}|p_{3/2}p_{3/2}\rangle_{J=2,T=1}$ = 2.762 MeV

2-body Valence Cluster approximation for A>6

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





2-body Valence Cluster approximation for A=6

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

Need NCSM results in N_{max} space for

$V_0^{6,4}$: ^{4}He

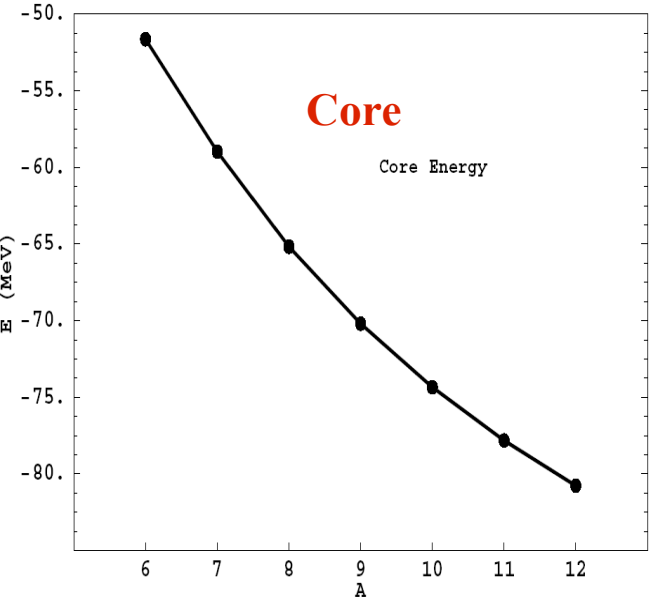
$V_1^{6,5}$: ^{5}He ^{5}Li

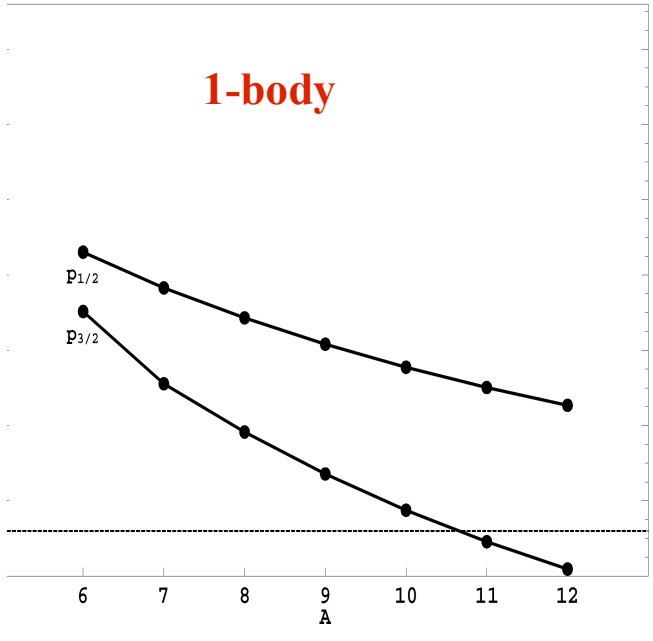
$V_2^{6,6}$: ^{6}He ^{6}Li ^{6}Be

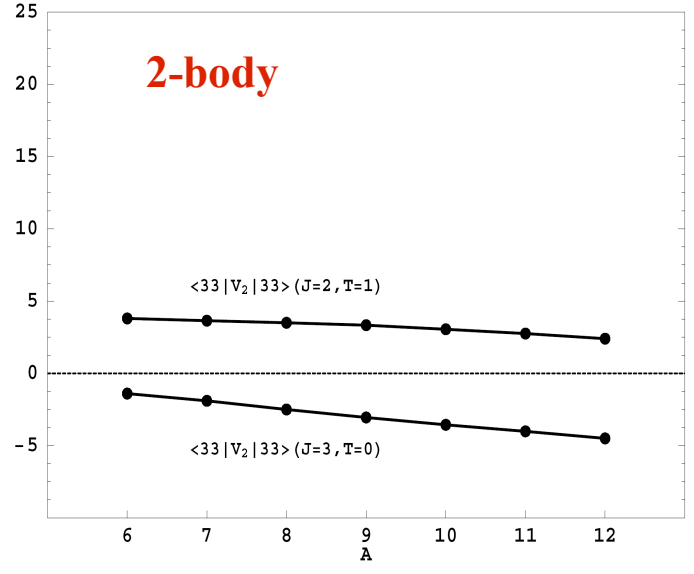
$N_{max} = 6$

With effective interaction for A !!!

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







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

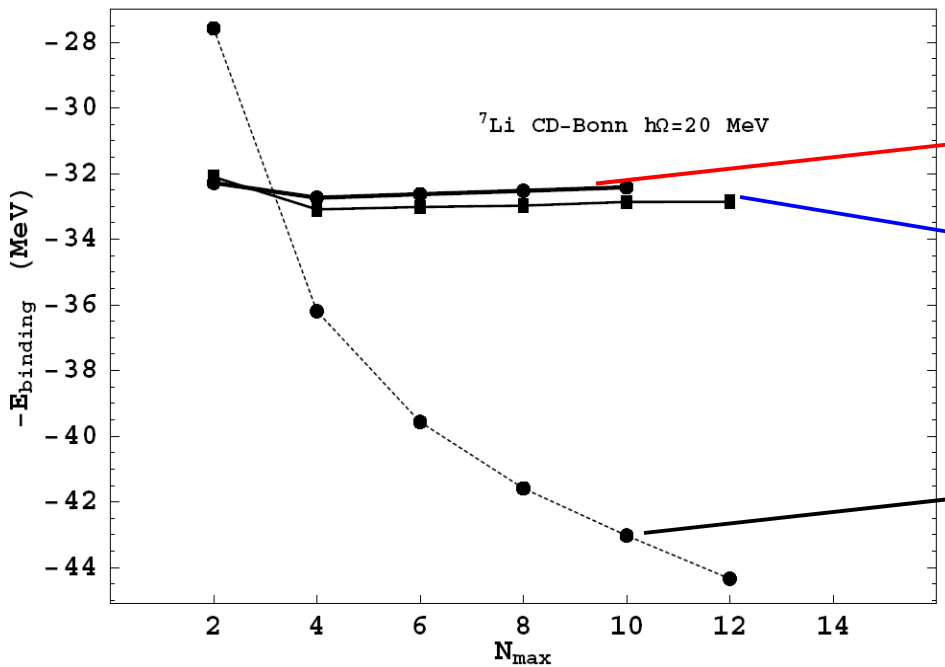
^{4}He

^{5}He ^{5}Li

^{6}He ^{6}Li ^{6}Be

With effective interaction for A=7 !!!

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



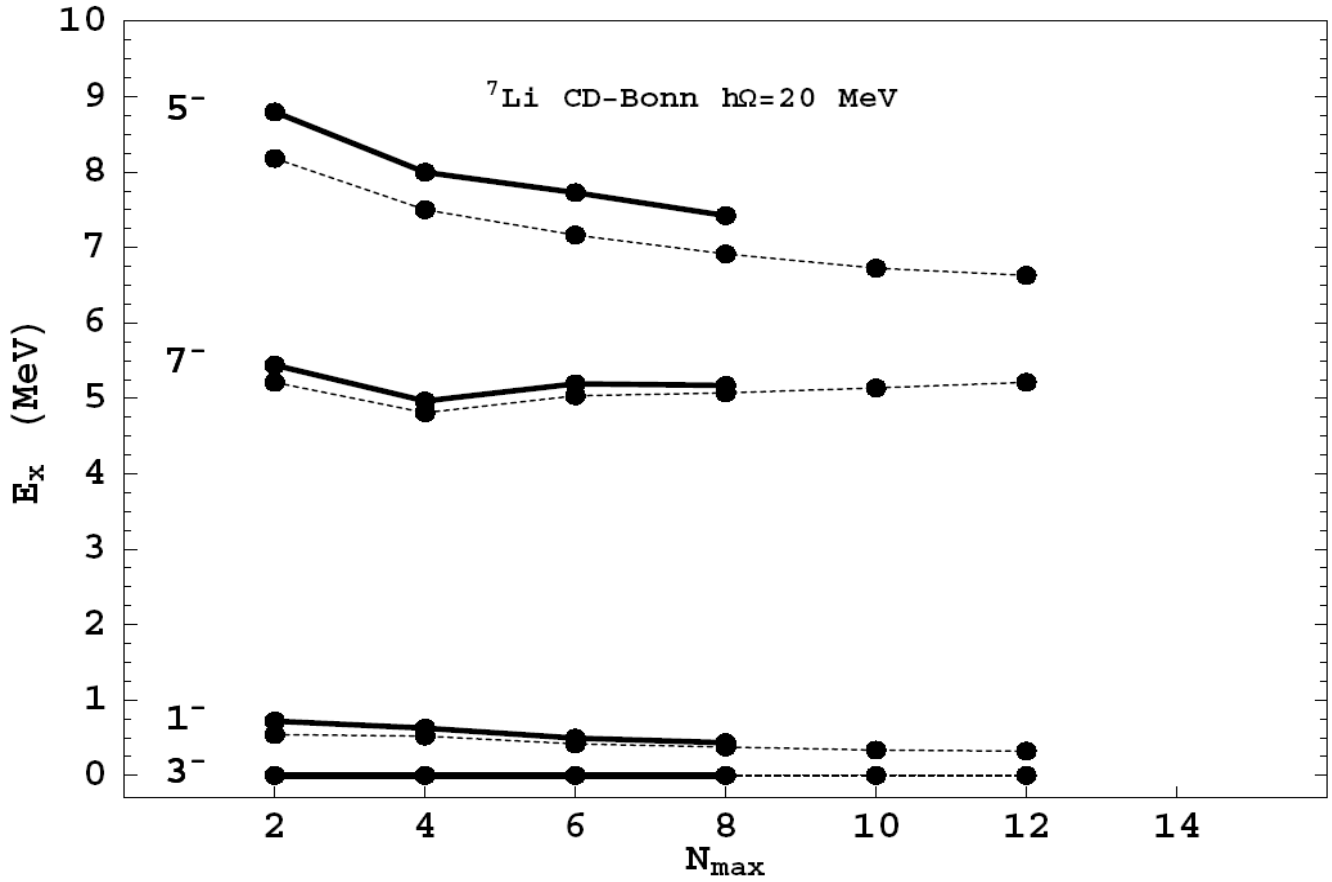
Exact NCSM

SSM with A-dependent core

SSM with inert core

2-body Valence Cluster approximation for A=7

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



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

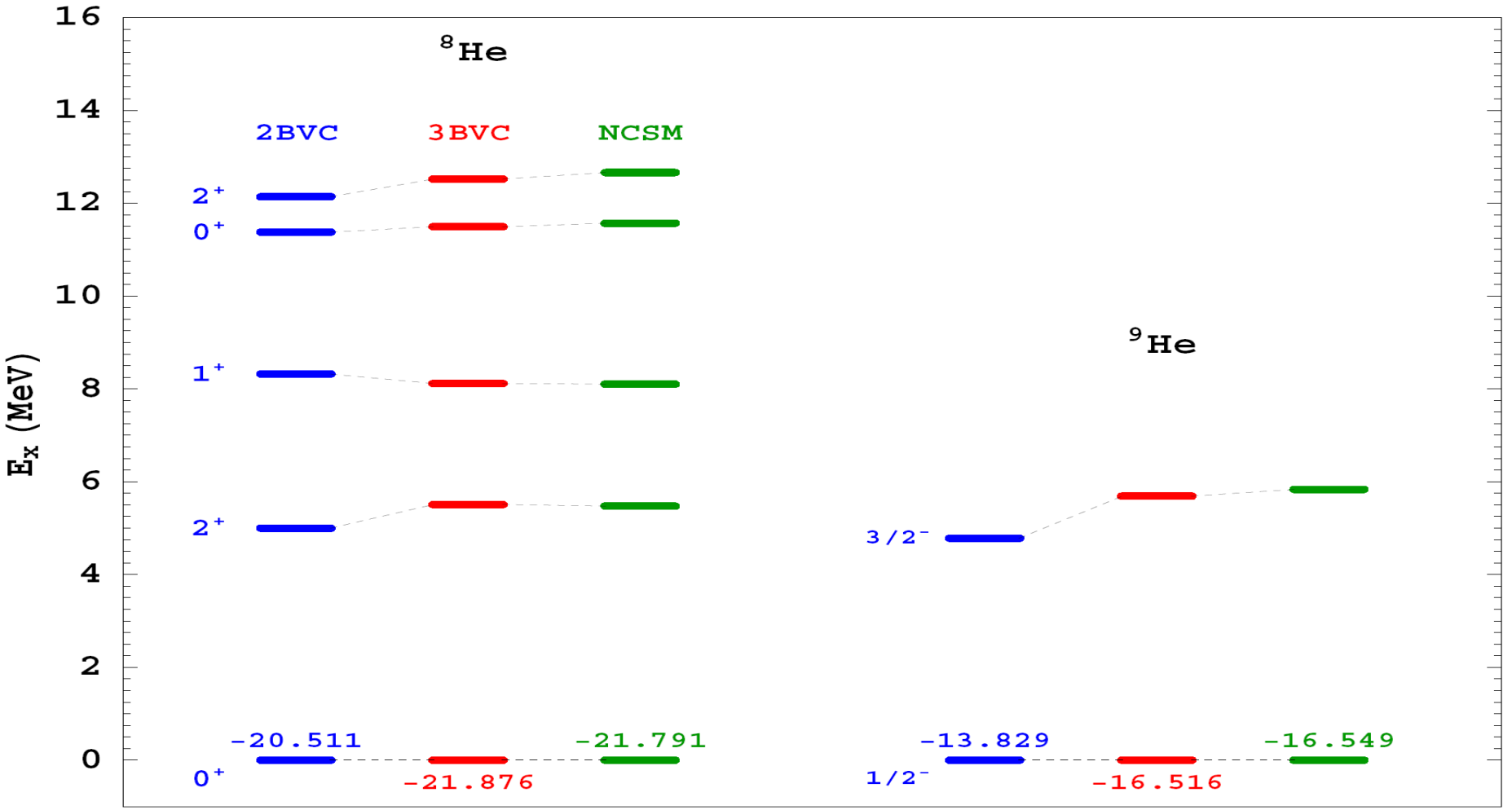
With effective interaction for A !!!

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

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

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

3-body Valence Cluster approximation for A>6



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

3) negligible role of 4-body and higher-order interactions for identical nucleons

COLLABORATORS

Alexander Lisetskiy, U. of Arizona
Michael Kruse, U. of Arizona
Ionel Stetcu, LANL
Petr Navratil, LLNL
James Vary, Iowa State U.

From 4hΩ NCSM to sd CSM for ^{18}F

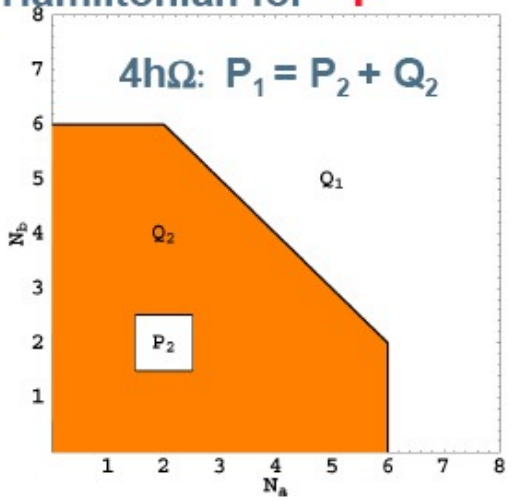
Petr Navrátil, Michael Thoresen, and Bruce R. Barrett, Phys. Rev. C 55, R573 (1997)

Step 2: Projection of 18-body 4hΩ Hamiltonian onto 0hΩ 2-body Hamiltonian for ^{18}F

$$H_{eff}([sd]^2) = \sum_k |k,N_{max}=4,A=18> E_k(A=18) \overline{<k,N_{max}=4,A=18)|}$$

$$|k,N_{max}=4,A=18> = U_{k,kp2}|k_{p2}[0h\Omega,18]> + U_{k,kq2}|k_{q2}[2+4h\Omega,18]>$$

$\dim(P_1) = 6\,706\,870 \qquad \dim(P_2)=28 \qquad \dim(Q_2) = 6\,706\,842$



$$H_{\rm diag} = U H U^\dagger$$

$E_k(A=18)$ $\quad$ $H(N_{max}=4,A=18)$

$$U = \begin{pmatrix} U_{PP} & U_{PQ} \\ U_{QP} & U_{QQ} \end{pmatrix}$$

$$H_{\rm eff} = \frac{U_p^\dagger}{\sqrt{U_p^\dagger U_p}} H^p_{\rm diag} \frac{U_p}{\sqrt{U_p^\dagger U_p}}.$$

$$H_{eff} = H_{eff}(1b) + H_{eff}(2b) + H_{eff}(3b) + H_{eff}(4b) + \ldots$$