Overview of the Fall INT Program and Status Report on the No Core Shell Model

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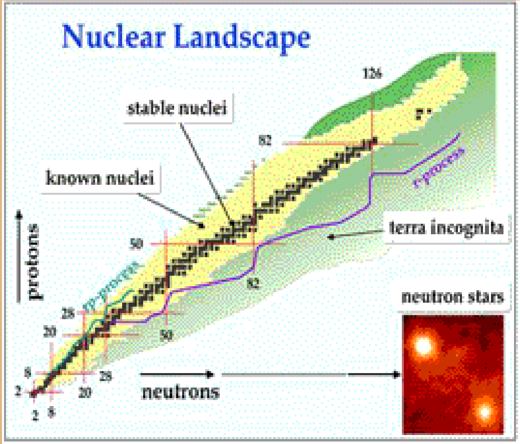
THE UNIVERSITY OF ARIZONA.

Arizona's First University.

INT Seattle

November 27, 2007



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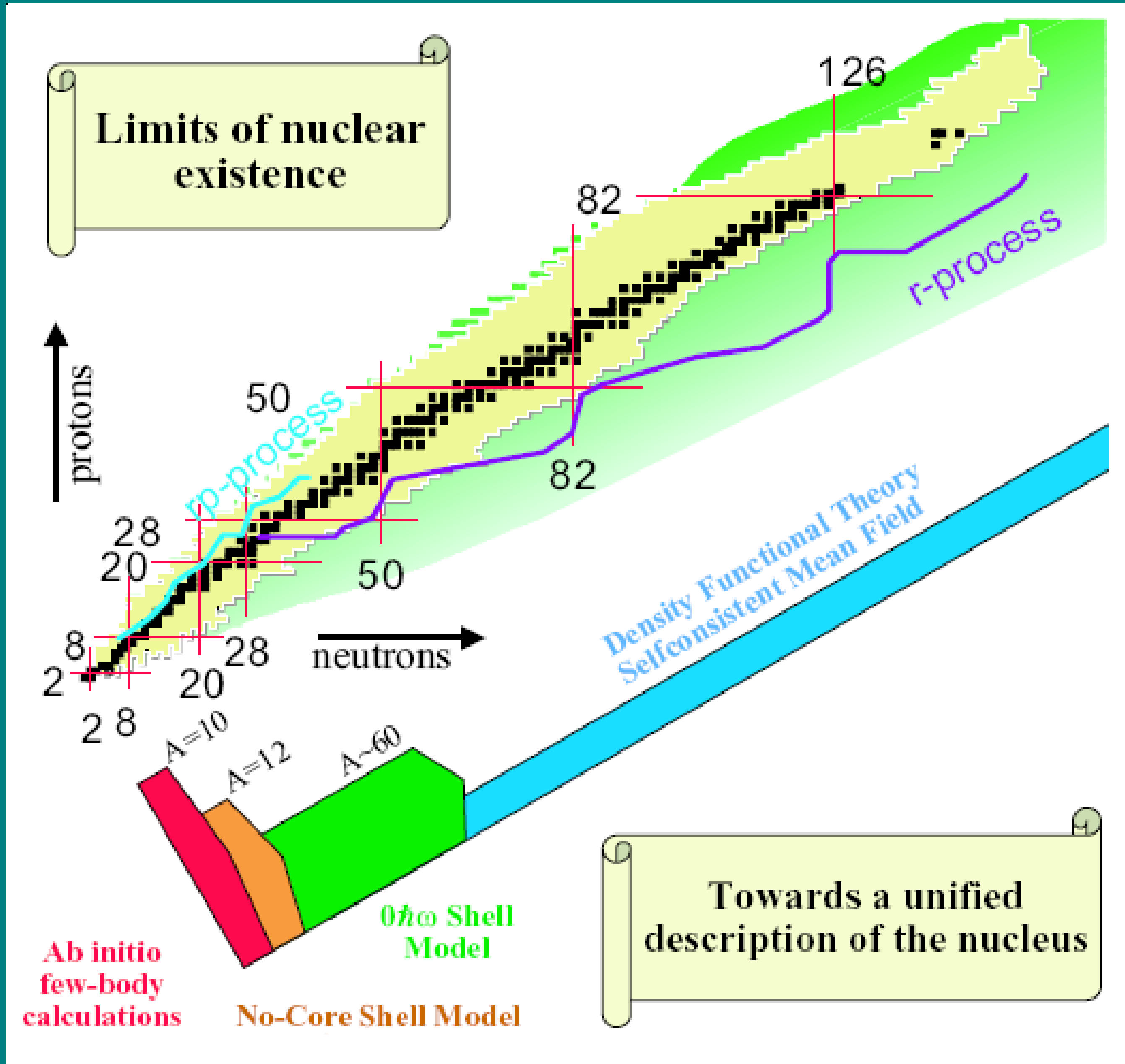
Nuclear Many-Body Approaches for the 21st Century

September 24 - November 30, 2007

The goal of our program is to bring together leading researchers in microscopic few-body and many-body theories to think and to discuss *outside the same old boxes* that have been used in the past, and to develop new ways and a new strategy to attack the nuclear many-body problem. Of particular interest is the determination of new ways to include many more correlations among the nucleons when calculations are performed in smaller or restricted model spaces, and especially how to accommodate special symmetries into the theory.

For example, we plan to bring together shell-model theorists with researchers doing symplectic and cluster calculations to look for ways to accommodate these into a more comprehensive theory, *i.e.*, how does collective rotational motion and clustering emerge in shell-model calculations. Theorists using group theory and cluster techniques will be brought into these discussions to study whether it is possible to to propose truncation schemes of the shell model based on symmetries and also to explore new methods to use group-theoretical techniques to model the nuclear many-body problem.

Another topic for extended discussion will be the role of the continuum in weakly-bound systems. This is of particular relevance in nuclei away from the stability line where all states are close to the neutron or proton separation threshold and effects of the continuum



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

Towards a unified description of the nucleus

The goal of nuclear 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 $\lesssim$ A $\lesssim$ 60
- Density Functional Theory calculations: A $\gtrsim$ 60

Workshop at the INT Fall-07 Program
on
New Approaches in Nuclear Many-Body Theory

October 15 - 19, 2007

Notice to all participants: The workshop is constructed so as to have only three 50 to 60 minute talks per day or two long talks and two short talks per day with much time for discussion. A speaker with 90 minutes is supposed to talk for 50 to 60 minutes and leave the remaining time for questions and discussion. If groups of participants want to organize their own discussion groups outside of the lectures and/or special seminars, please contact the organizers about making arrangements (e.g., space) for such events.

Monday, October 15, 2007

8:00-8:50:	Registration/Check-in/Finding Location in the INT
8:50-9:00:	Start of workshop: Opening comments by the organizers
9:00-10:30:	Achim Schwenk (TRIUMF): "Recent Developments in Two- and Three-Nucleon Interactions for Nuclear Structure"

http://www.int.washington.edu/PROGRAMS/07-3_wkshp.html

Topics for Study: Fall INT Program 2007

1. Forces among the nucleons

2. Many-body techniques for solving the A-nucleon problem

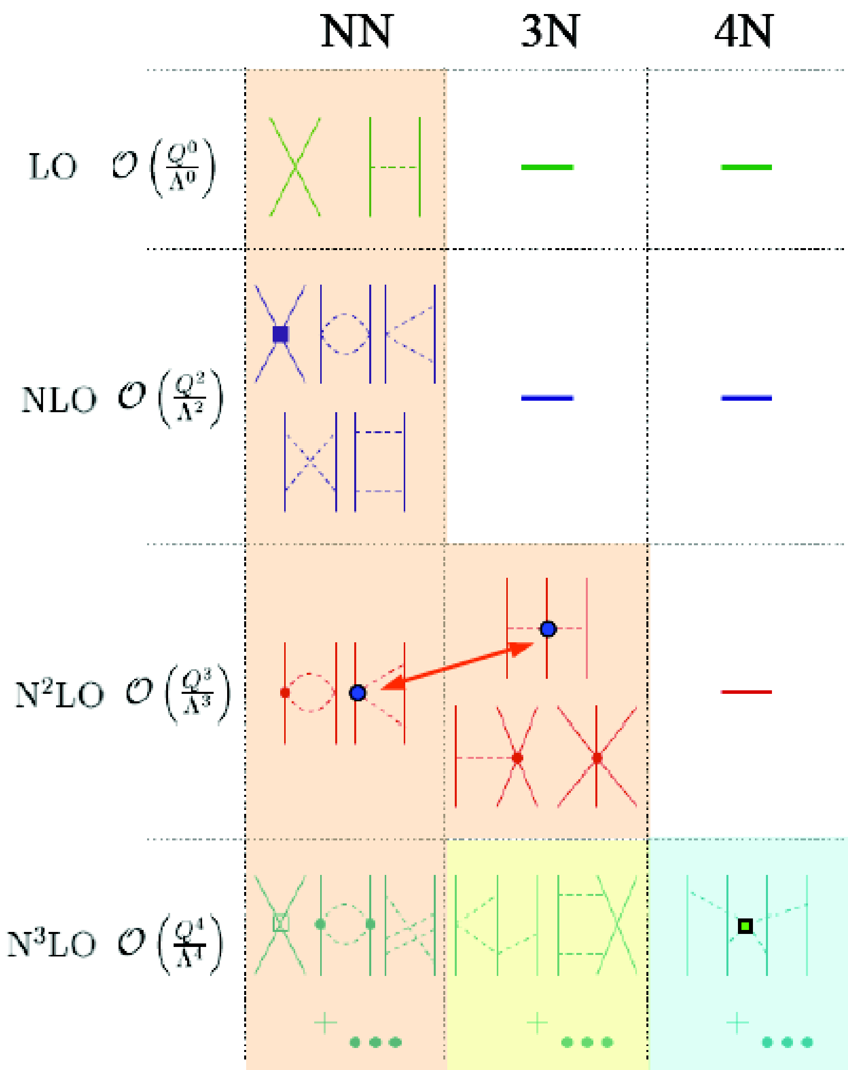
3. New methods/ Transformative ideas

I. Forces among nucleons

1. QCD ---> EFT ---> CPT --> Self-consistent nucleon interactions

Chiral effective field theory (EFT) for nuclear forces

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

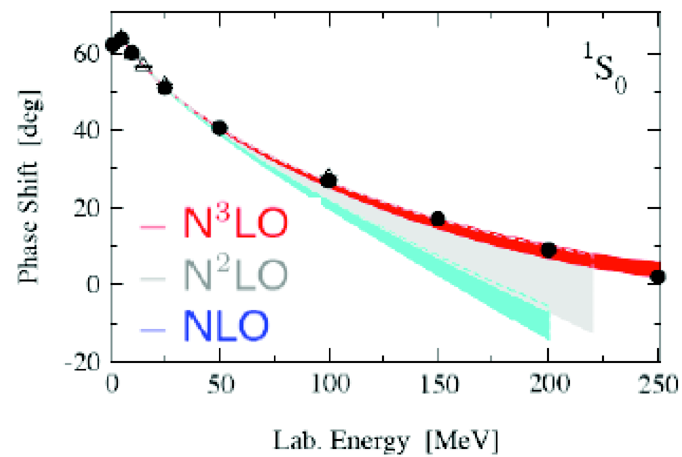


explains pheno hierarchy:
NN > 3N > 4N > …

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

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

theoretical error estimates



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

A. Schwenk

I. Forces among nucleons

1. QCD ---> EFT ---> CPT --> Self-consistent nucleon interactions

2. Need NN and NNN and perhaps NNNN interactions

	N^3LO	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. Navratil and E. Caurier, Phys. Rev. C 69, 014311 (2004)

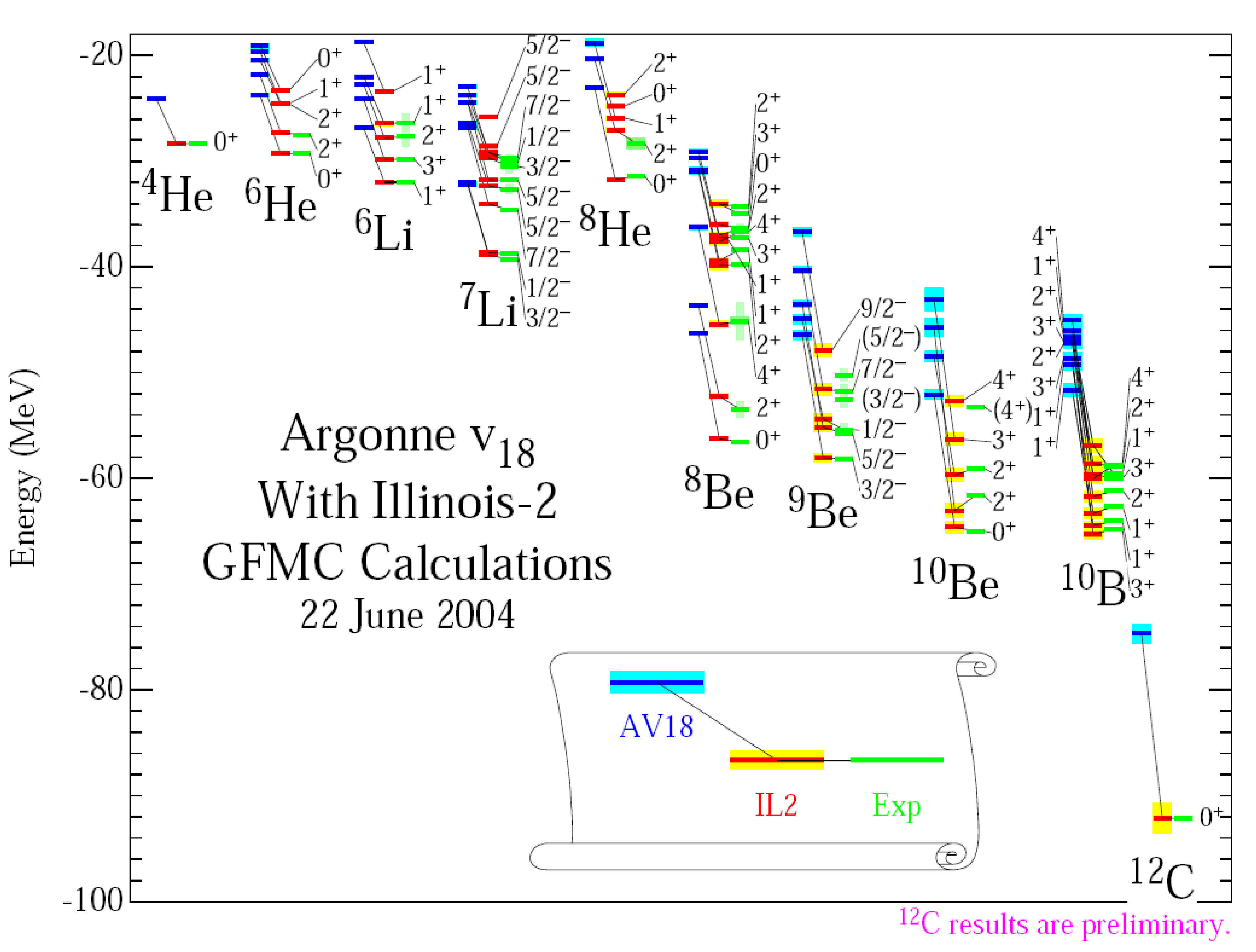
H. Kamada, *et al.*, Phys. Rev. C <u>64</u>, 044001 (2001)

PHYSICAL REVIEW C, VOLUME 64, 044001

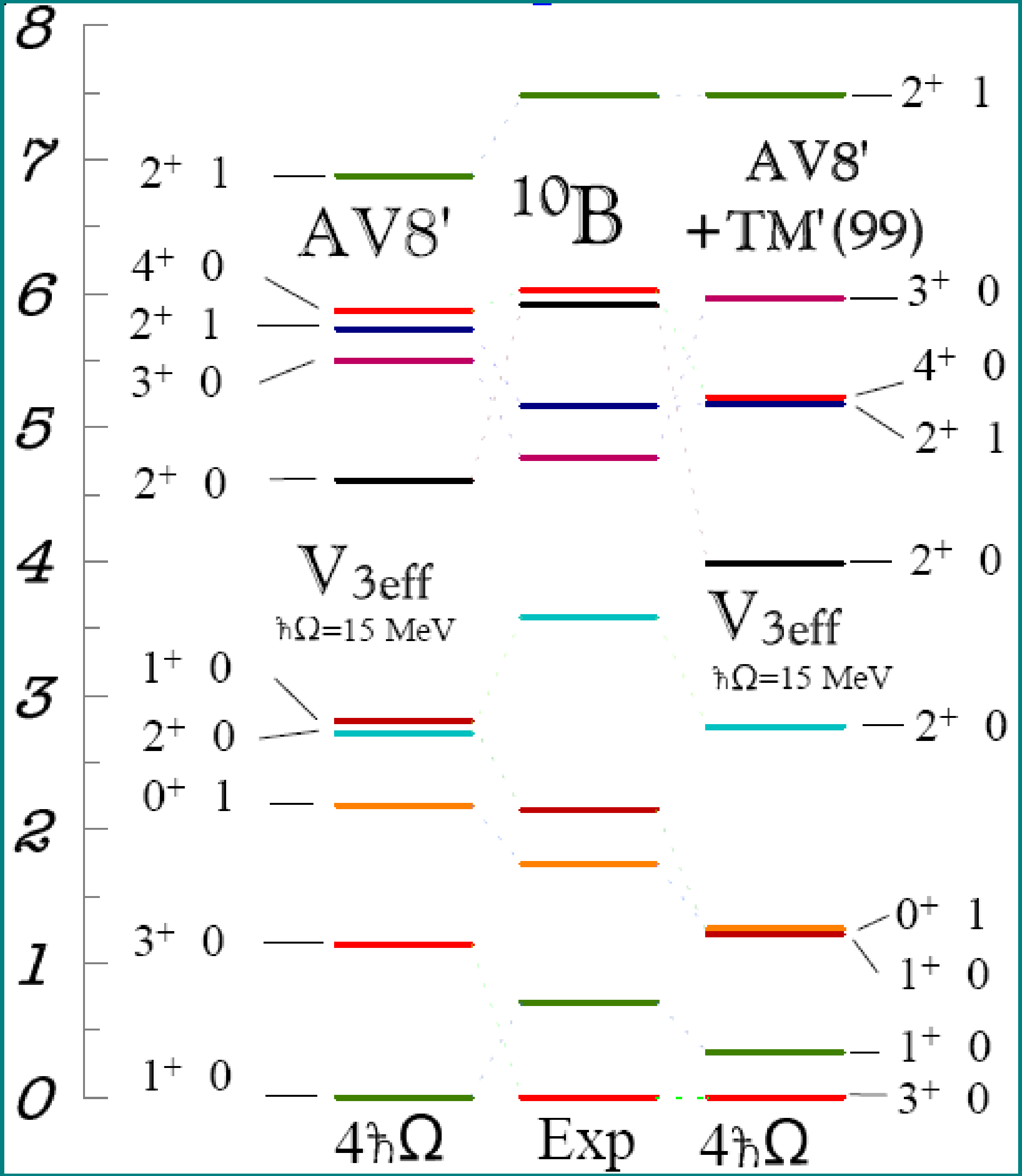
Benchmark test calculation of a four-nucleon bound state

In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic AV8′ *NN* interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.

$BE_{th} \approx 25.91$ MeV $\qquad$ $BE_{exp} \approx 28.296$ MeV



Argonne v18
With Illinois-2
GFMC Calculations
22 June 2004
Energy (MeV)
-20
-40
-60
-80
-100
4He
6He
6Li
7Li
8He
8Be
9Be
10Be
10B
12C
AV18
IL2
Exp
12C results are preliminary.



P. Navrátil and W. E. Ormand, Phys. Rev. C **68**, 034305 (2003)

I. Forces among nucleons

1. QCD ---> EFT ---> CPT --> Self-consistent nucleon interactions

2. Need NN and NNN and perhaps NNNN interactions

3. Which approach is best?
   a) Chiral Effective Field Theory
   b) Find NN interaction which minimizes the NNN interaction and then treat the NNN interaction perturbatively.

A. Schwenk

Tjon line

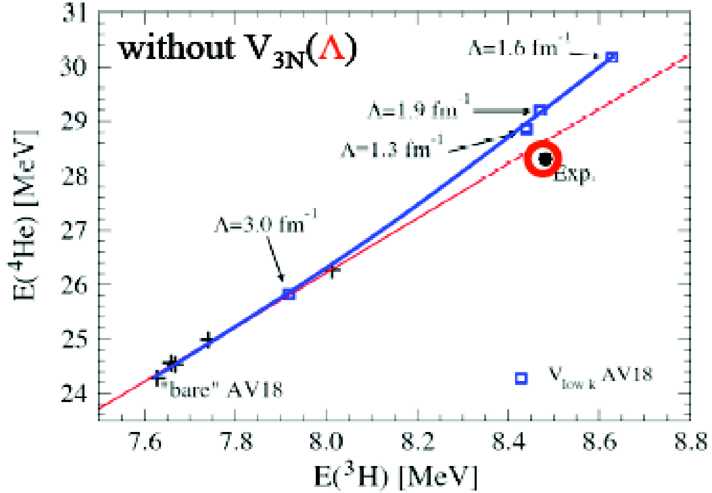
$V_{low\,k}(\Lambda)$ defines class of NN interactions with cutoff-independent low-energy NN observables

cutoff variation estimates errors due to neglected parts in $H(\Lambda)$

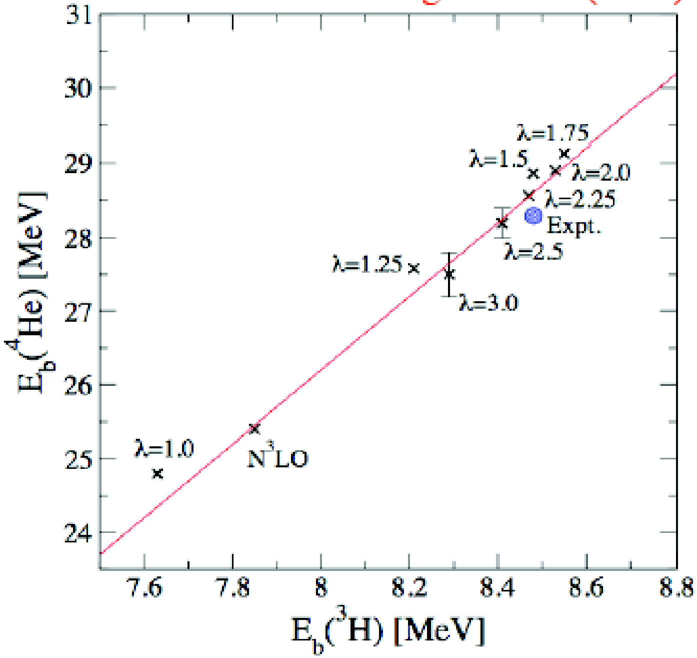
Cutoff dependence explains Tjon line, 3N required by renormalization

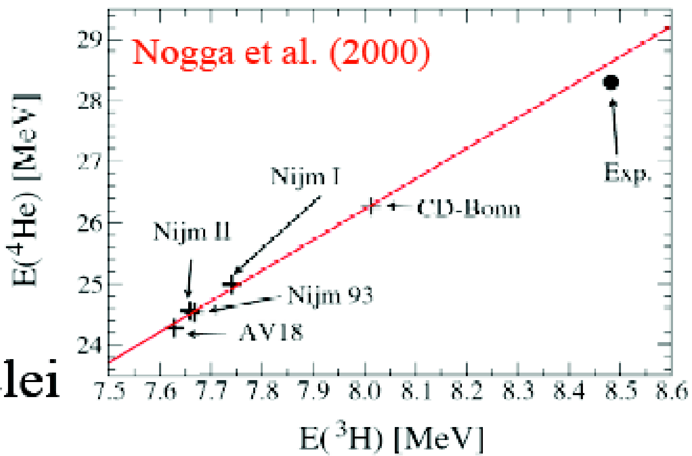
Experiment breaks from line ⇒ 3N

Nogga, Bogner, AS (2004)



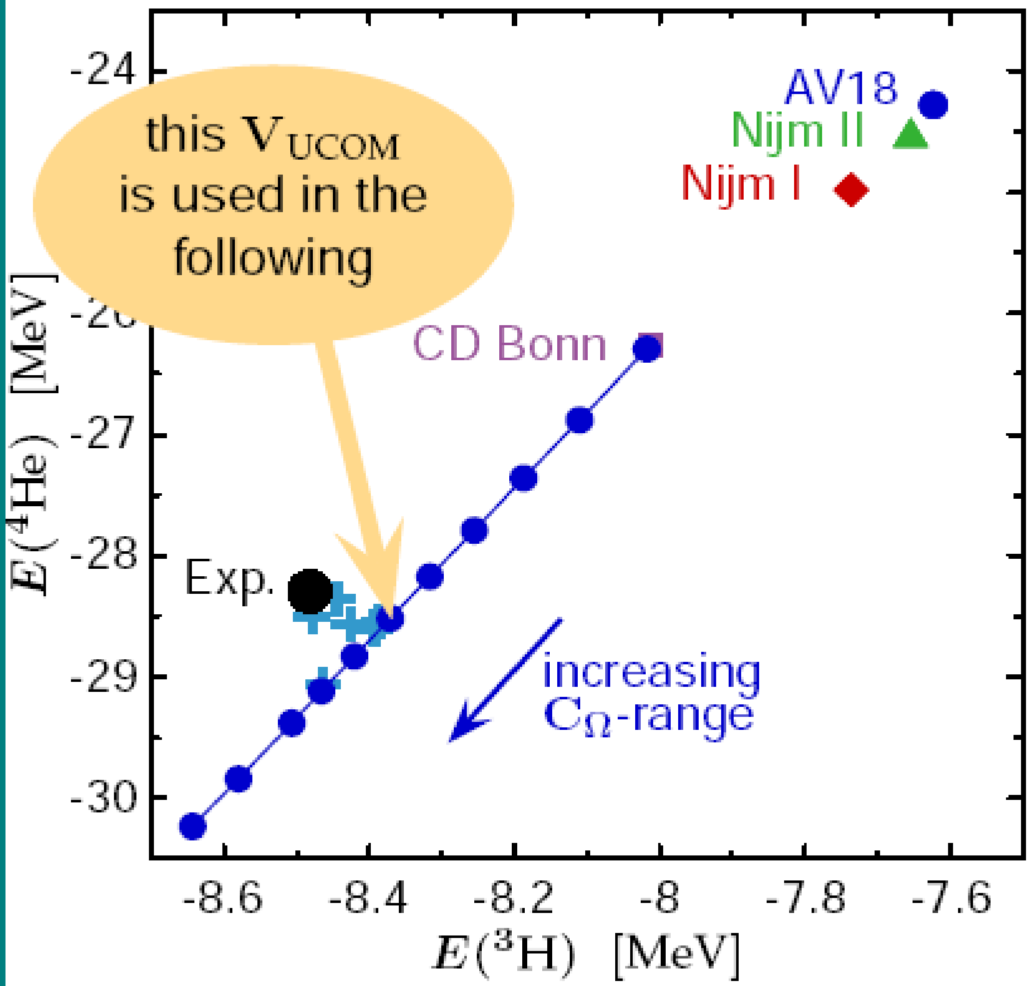
SRG interactions: Bogner et al. (2007)





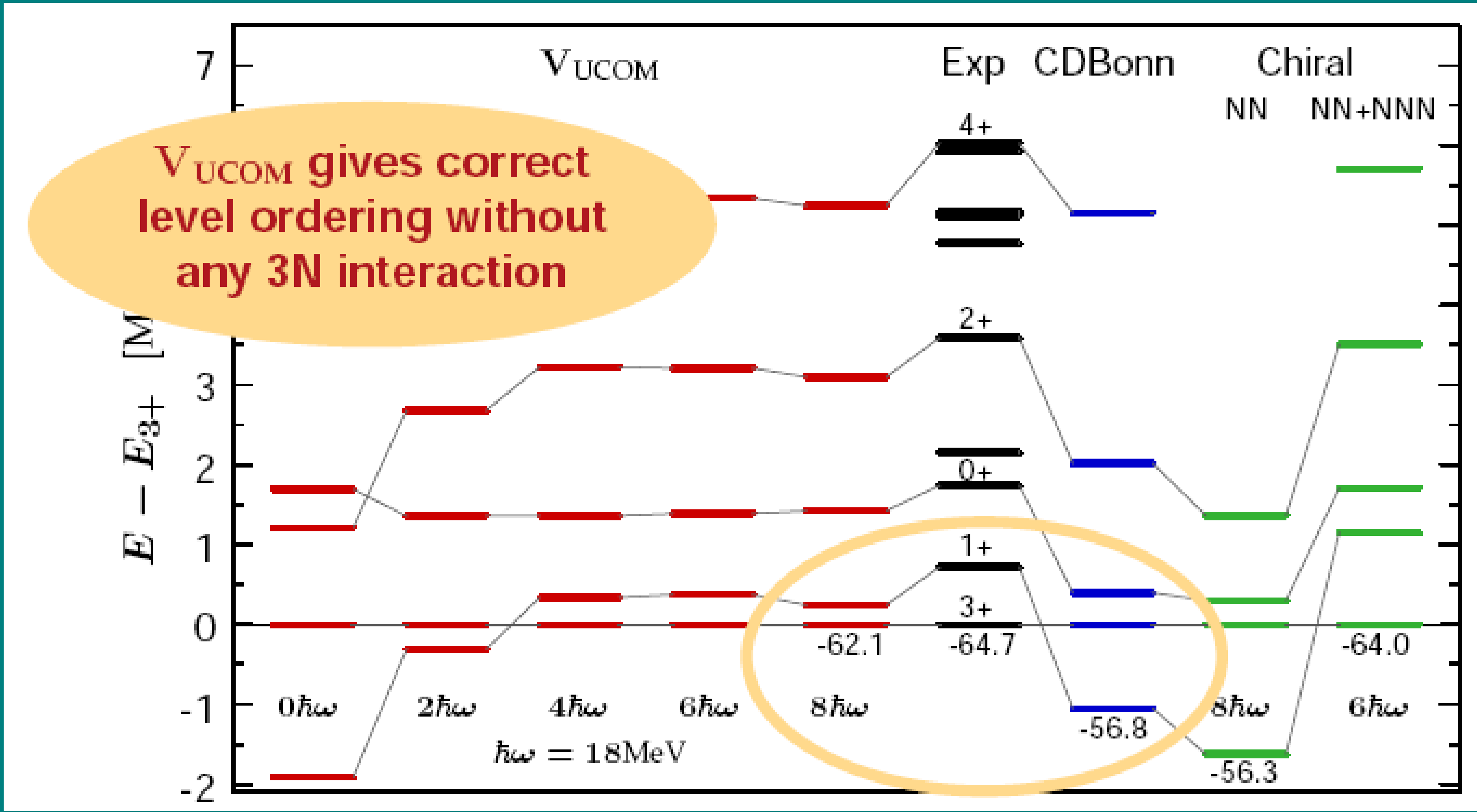
Tjon lines in p-shell nuclei

Bogner et al. (2007)



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions
- change of C_Ω-correlator range results in shift along Tjon-line

minimize net three-body force by choosing correlator with energies close to experimental value



V_UCOM
Exp
CDBonn
Chiral
NN
NN+NNN
V_UCOM gives correct level ordering without any 3N interaction
4+
2+
0+
1+
3+
-62.1
-64.7
-56.8
-56.3
-64.0
0ħω
2ħω
4ħω
6ħω
8ħω
8ħω
6ħω
ħω = 18MeV
7
3
2
1
0
-1
-2

I. Forces among nucleons

1. QCD ---> EFT ---> CPT --> Self-consistent nucleon interactions

2. Need NN and NNN and perhaps NNNN interactions

3. Which approach is best?

   a) Chiral Effective Field Theory

   b) Find NN interaction which minimizes the NNN interaction and then treat the NNN interaction perturbatively.

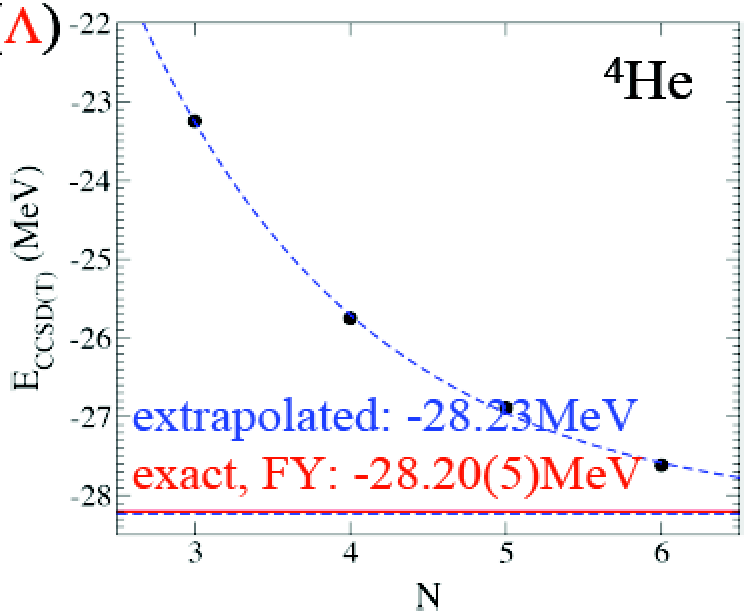
   c) Contract the NNN interaction into the nuclear medium as 0-, 1-, and 2-body density dependent parts + a small residual NNN force.

Towards 3N interactions in medium-mass nuclei

based on low-momentum $V_{\mathrm{low\,k}}(\Lambda) + V_{3N}(\Lambda)$

Hagen et al. (2007)

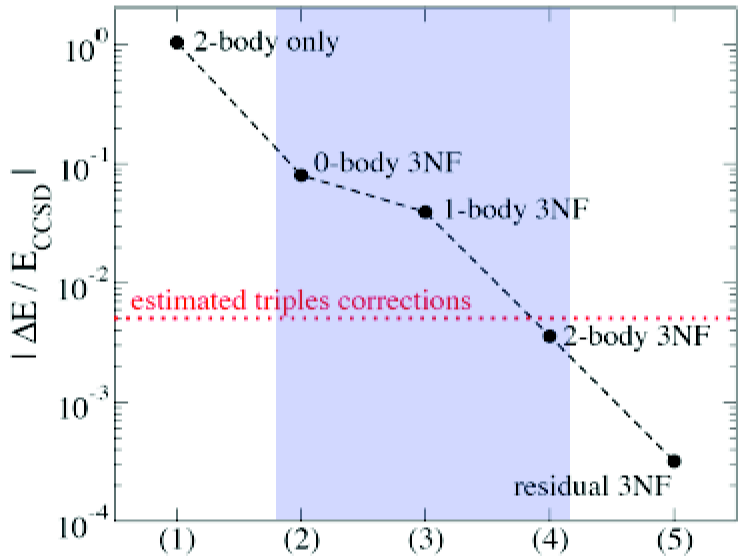
developed coupled-cluster theory with 3N interactions, first benchmark for ^{4}He



Results show that 0-, 1- and 2-body parts of 3N interaction dominate

residual 3N interaction can be neglected!
very promising

supports that monopole corrections for valence shell interactions due to 3N



I. Forces among nucleons

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3. Which approach is best?
   a) Chiral Effective Field Theory
   b) Find NN interaction which minimizes the NNN interaction and then treat the NNN interaction perturbatively.
   c) Contract the NNN interaction into the nuclear medium as 0-, 1-, and 2-body density dependent parts + a small residual NNN force.
   d) Other approaches: V_low-k, Similarity Renormalization Group (SRG), Unitary Correlation Operator Method (UCOM), INOY,...

II. Many-Body Techniques for Solving the A-Nucleon Problem

1. Light Nuclei: ab initio approaches: s- and p-shell nuclei
   Green Function Monte Carlo (GFMC) (R. Wiringa, et al.), No-Core Shell Model (NCSM), Faddeev-Yakubovsky, UCOM, V_low-k, SRG, ...
2. sd- and pf-shell nuclei:
   NCSM, extended NCSM, Standard Shell Model (SSM), Coupled Cluster (CC), Shell Model Monte Carlo (SMMC) (sign problem defeated?), Monte Carlo Shell Model (MCSM) (Otsuka, et al.) ...
3. Heavier Nuclei:
   Density Functional Theory (DFT) (G. Bertsch et al., SciDAC project UNEDF), CC, Monte Carlo approaches, ...

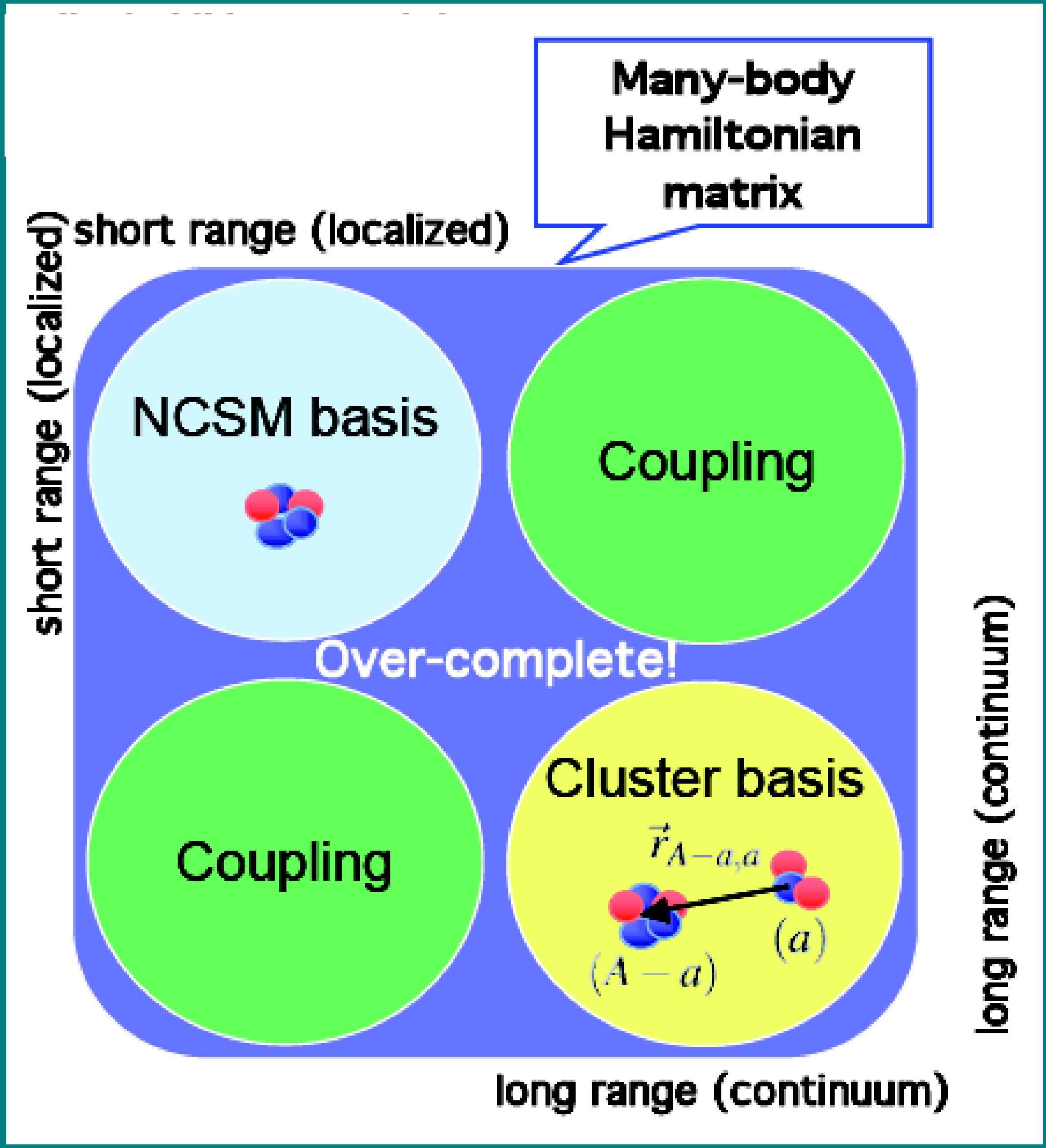
III. New Methods/Transformative Ideas (???)

1. “sof t” NN inte ractions plus weak NNN interactions

2. Coupled Cluster calculations with NNN interactions

3. Universal Nuclear Energy Density Functional

4. Building more correlations into smaller model space:
   a) Fermionic Molecular Dynamics Approach (T. Neff, et al.)
   b) Extensions of the NCSM:
      i) Projected NCSM/SSM (this talk)
      ii) Symplectic (3,R) NCSM (J. Draayer, et al.)
      iii) Importance Truncated NCSM (Navratil and Roth)
      iv) NCSM + Resonating Group Method (Navratil & Quaglioni)



P. Navratil and S. Quaglioni, INT seminars fall 2007

Status Report on the NCSM

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', A V18
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 $V_{ij} \rightarrow V_{ij}^{effective}$
- In general, V_{ij}^{eff} is an A-body interaction
- We want to make an a-body cluster approximation

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

$$a < A$$

Two-body cluster approximation (a=2)

$$\mathcal{H} \approx \mathcal{H}^{(I)} + \mathcal{H}^{(2)}$$

$$H_2^{\Omega} = \underbrace{H_{0_2} + H_2^{CM}}_{h_1+h_2} + V_{12} = \frac{\vec{p}^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}^{\,2} + H_2^{CM} + V(\sqrt{2}\vec{r}) - \frac{m\Omega^2}{A}\vec{r}^{\,2}$$

Carry out a unitary transformation on H_2^{Ω}

$$\mathcal{H}_2 = e^{-S^{(2)}} H_2^{\Omega} e^{S^{(2)}} \quad \text{where } S^{(2)} \text{ is anti Hermitian}$$

$S^{(2)}$ is determined from the decoupling condition

$$Q_2 e^{-S^{(2)}} H_2^{\Omega} e^{S^{(2)}} P_2 = 0$$

P_2 = model space, Q_2 = excluded space, $P_2 + Q_2 = 1$

$$\text{with the restrictions} \quad P_2 S^{(2)} P_2 = Q_2 S^{(2)} Q_2 = 0$$

Two-body cluster approximation (a=2)

It is convenient to write $S^{(2)}$ in terms of another operator "ω" as

$$S^{(2)} = \mathrm{arctanh}(\omega - \omega^\dagger) \quad \text{with} \quad Q_2 \omega P_2 = \omega$$

Then the Hermitian effective operator in the P_2 space can be expressed in the form

$$\mathcal{H}_{\mathrm{eff}}^{(2)} = P_2 \mathcal{H}_2 P_2 = \frac{P_2 + P_2 \omega^\dagger Q_2}{\sqrt{P_2 + \omega^\dagger \omega}} H_2^{\Omega} \frac{P_2 + Q_2 \omega P_2}{\sqrt{P_2 + \omega^\dagger \omega}}$$

Analogously, <u>any</u> <u>arbitrary</u> operator can be written in the P_2 space as

$$\mathcal{O}_{\mathrm{eff}}^{(2)} = P_2 \mathcal{O}_2 P_2 = \frac{P_2 + P_2 \omega^\dagger Q_2}{\sqrt{P_2 + \omega^\dagger \omega}} O \frac{P_2 + Q_2 \omega P_2}{\sqrt{P_2 + \omega^\dagger \omega}}$$

Exact solution for ω:

Let E_k and $|k\rangle$ be the eigensolutions of H_2^{Ω},

$$H_2^{\Omega}|k\rangle = E_k|k\rangle$$

Let $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ be HO states belonging to the model space P and the excluded space Q, respectively. Then ω is given by:

$$\langle\alpha_Q|k\rangle = \sum_{\alpha_P}\langle\alpha_Q|\omega|\alpha_P\rangle\langle\alpha_P|k\rangle$$

or

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in K}\langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle$$

NCSM ROAD MAP

1. Choose a NN interaction (or NN + NNN interactions)

2. Solve $H_n^\Omega |k_n\rangle = E_n |k_n\rangle$ for E_n and $|k_n\rangle$ with n=2,3,...

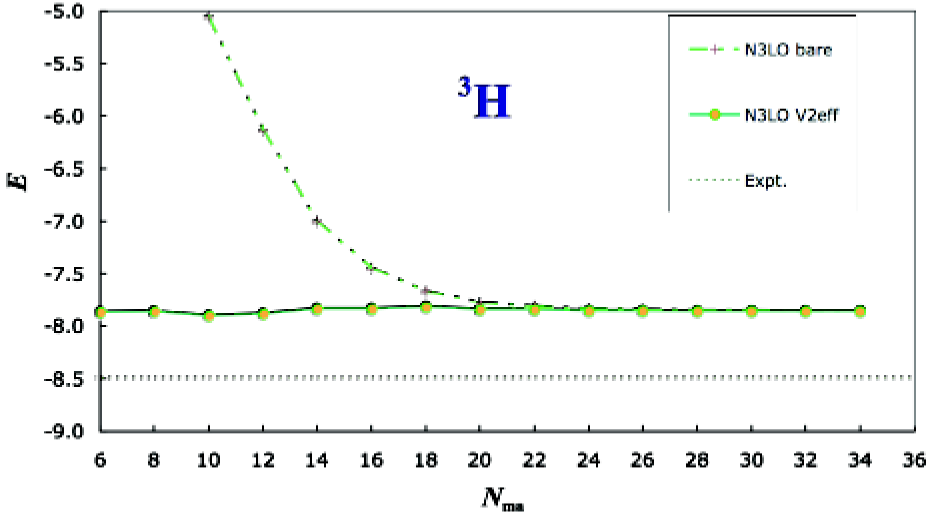
3. Calculate $\langle \alpha_Q^n | \omega | \alpha_P^n \rangle = \sum_{k \in K} \langle \alpha_Q | k_n \rangle \langle \tilde{k}_n | \alpha_P \rangle$

4. Determine $\mathcal{H}_n^{eff}$ and $\mathcal{O}_n^{eff}$ in the given model space

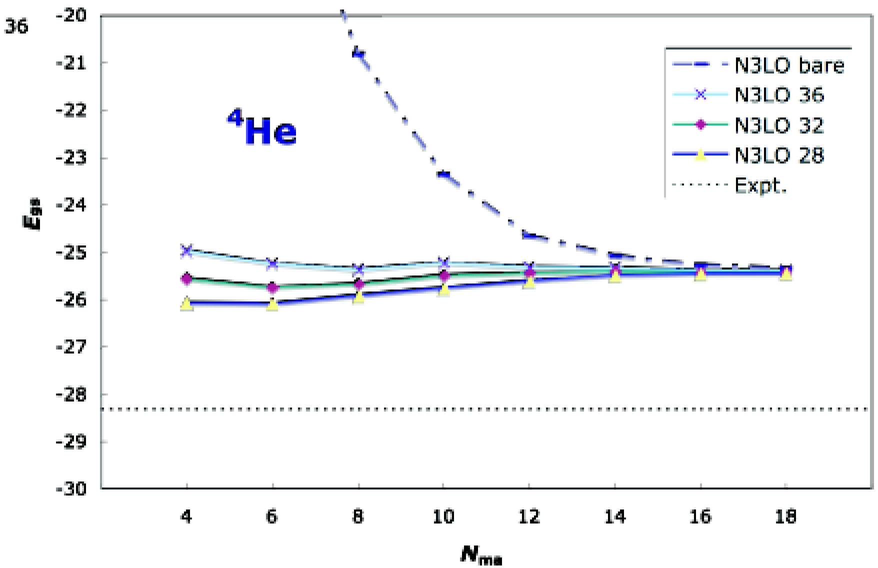
5. Diagonalize $\mathcal{H}_n^{eff}$ in the given model space, *i.e.*,
   $N_{max}\hbar\Omega$ = energy above the ground state

6. To check convergence of results repeat calculations
   for: *i)* increasing N_{max} and/or cluster level
   ii) several values of $\hbar\Omega$

- NCSM convergence test
  - Comparison to other methods

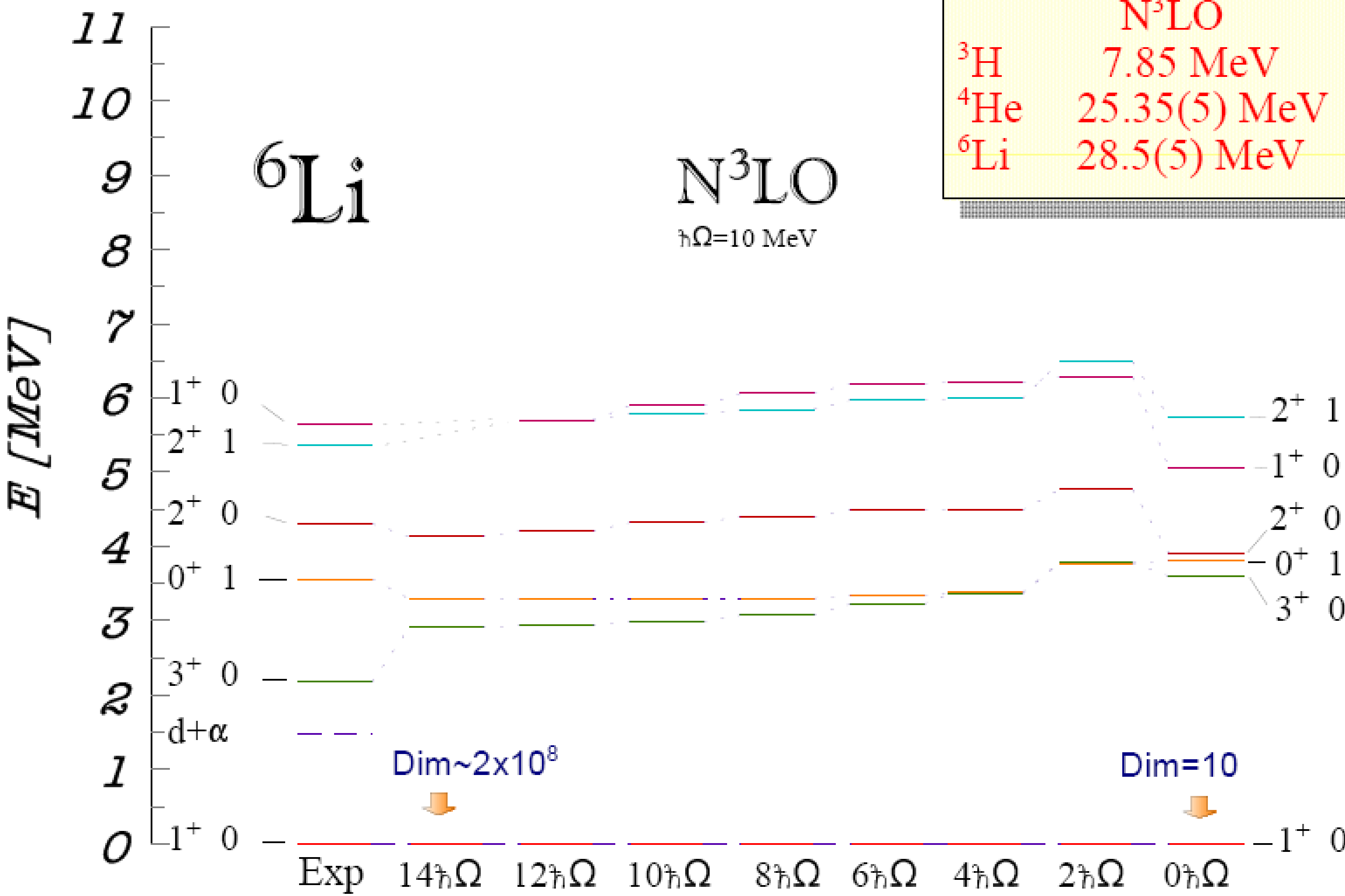


N^3LO NN	NCSM	FY	HH
^3H	7.852(5)	7.854	7.854
^4He	25.39(1)	25.37	25.38



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

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



	N^{3}LO	Exp
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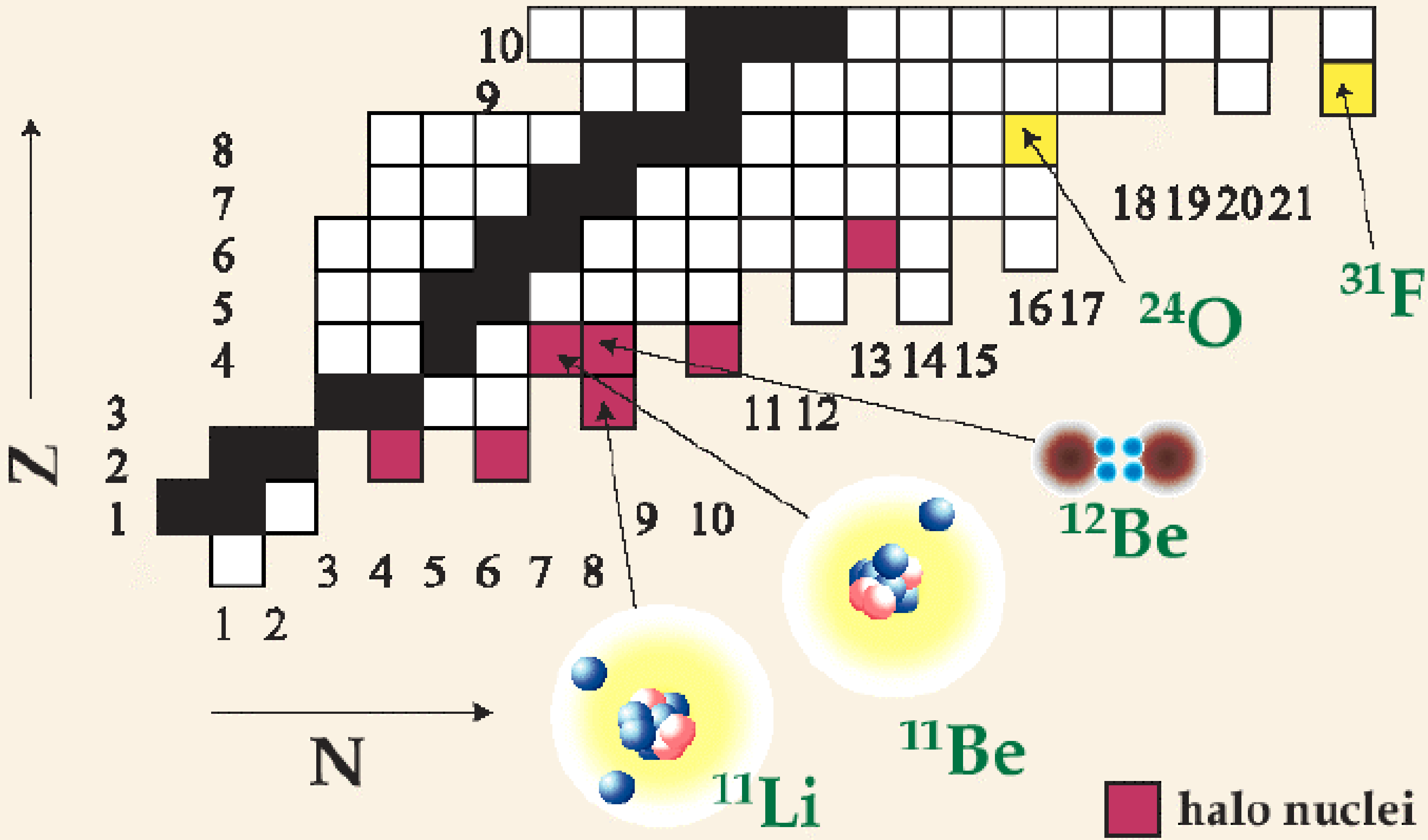
^{6}Li	28.5(5) MeV	31.99 MeV

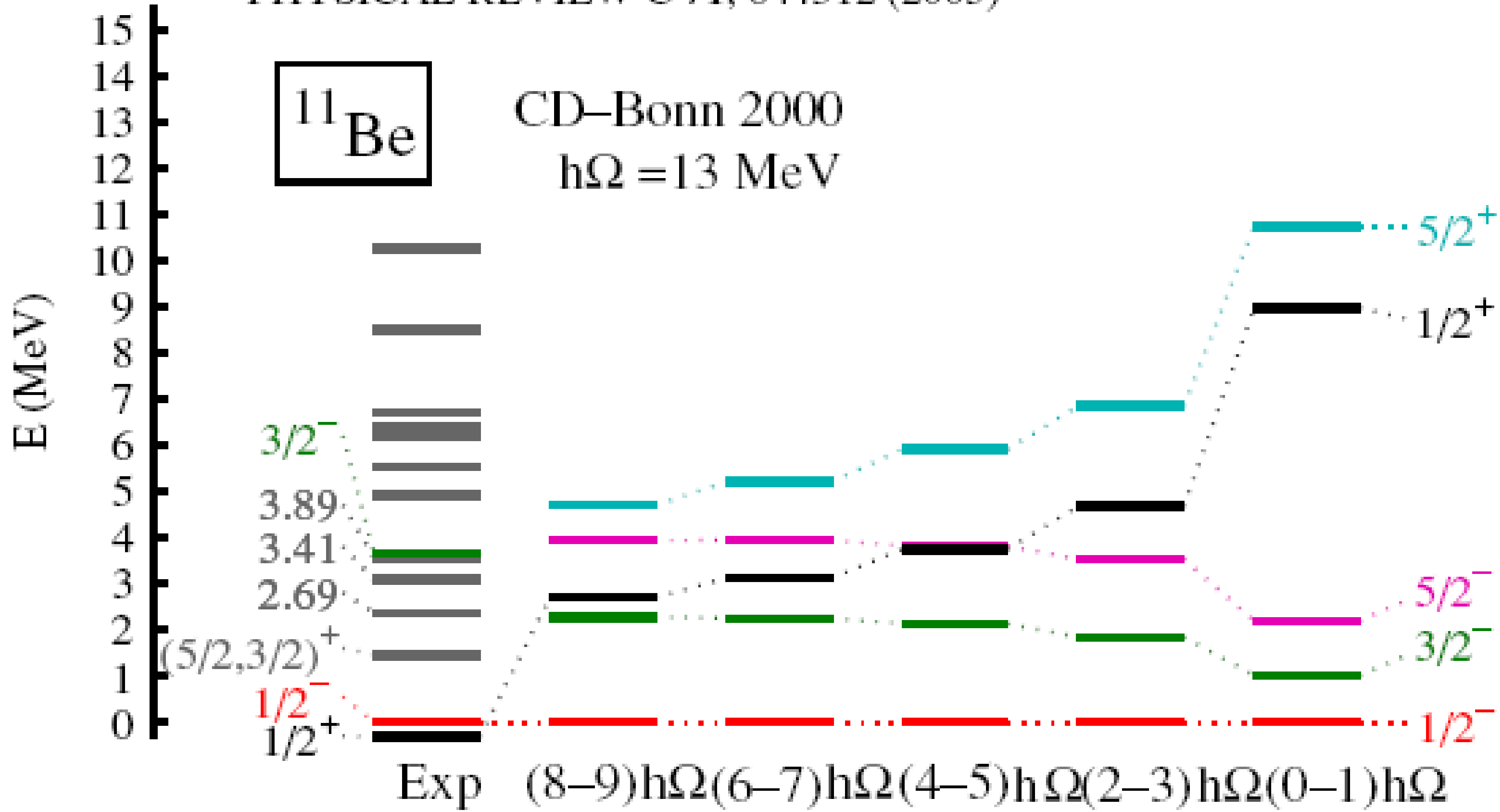
P. Navrátil and E. Caurier, Phys. Rev. C **69**, 014311 (2004)

Light drip line nuclei



C. FORSSÉN, P. NAVRÁTIL, W. E. ORMAND, AND E. CAURIER

PHYSICAL REVIEW C **71**, 044312 (2005)



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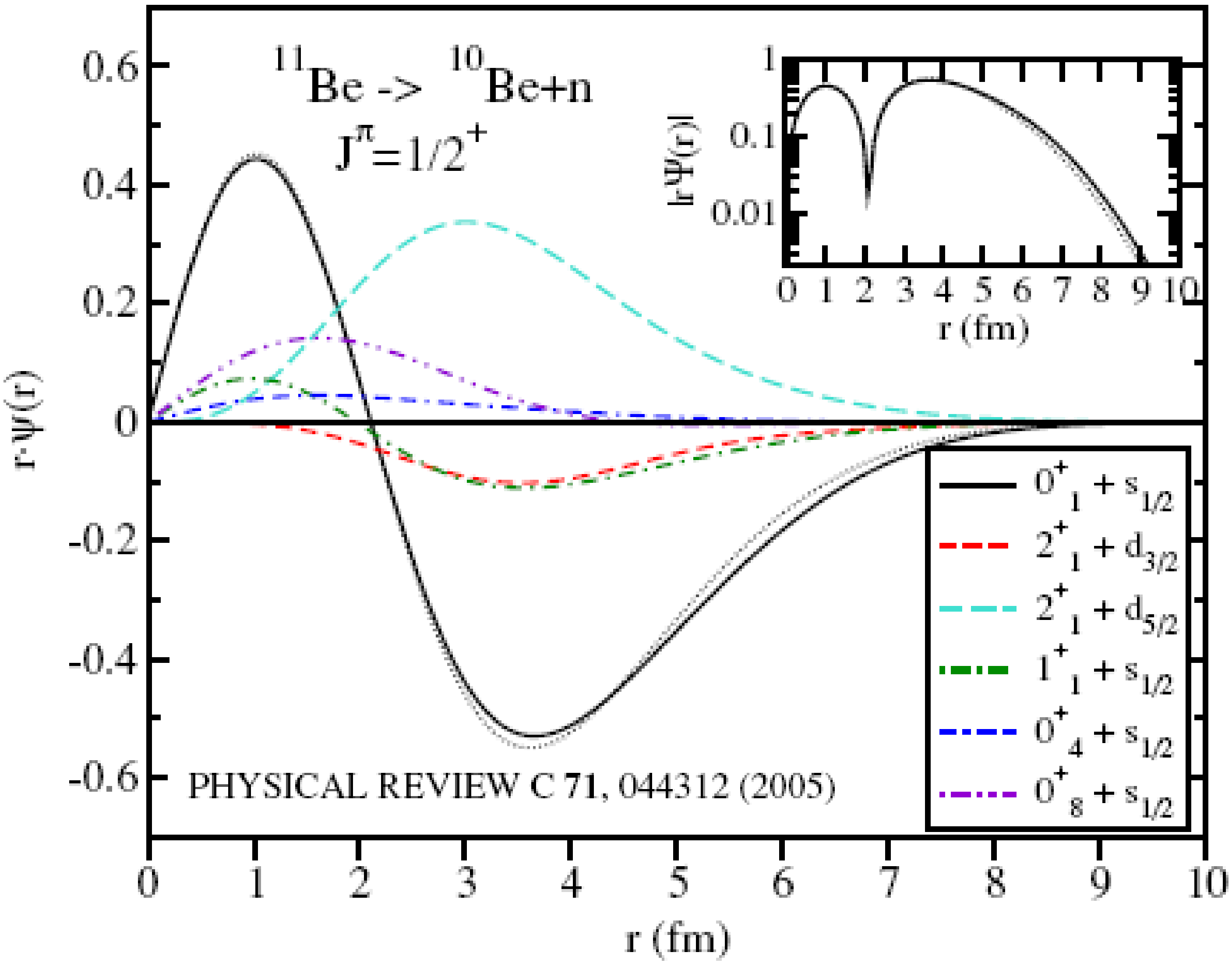
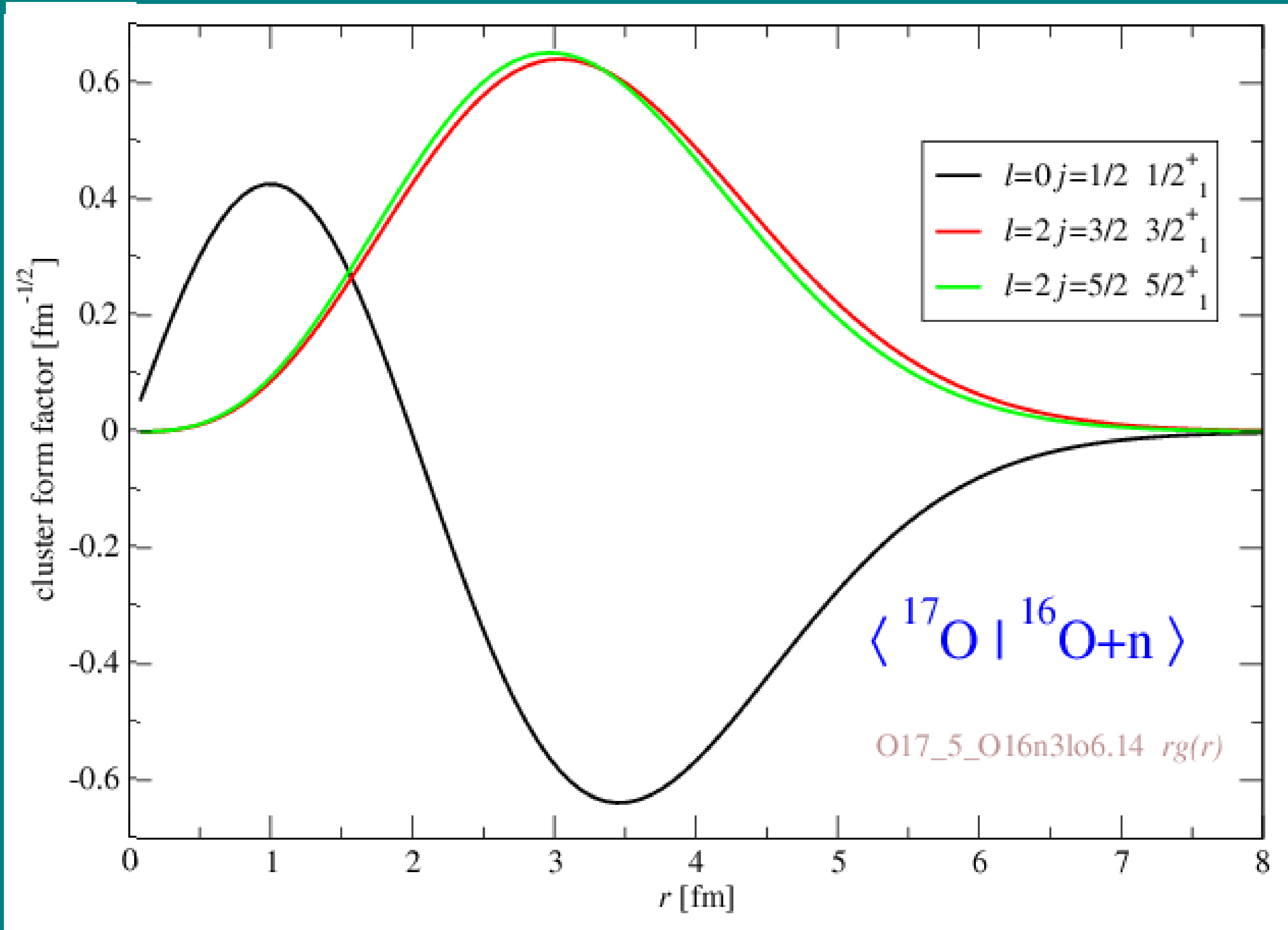


PHYSICAL REVIEW C 71, 044312 (2005)



cluster form factor [fm^-1/2]
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
1
2
3
4
5
6
7
8
r [fm]
l=0 j=1/2 1/2+1
l=2 j=3/2 3/2+1
l=2 j=5/2 5/2+1
⟨ 17O | 16O+n ⟩
O17_5_O16n3lo6.14 rg(r)

P. Navratil

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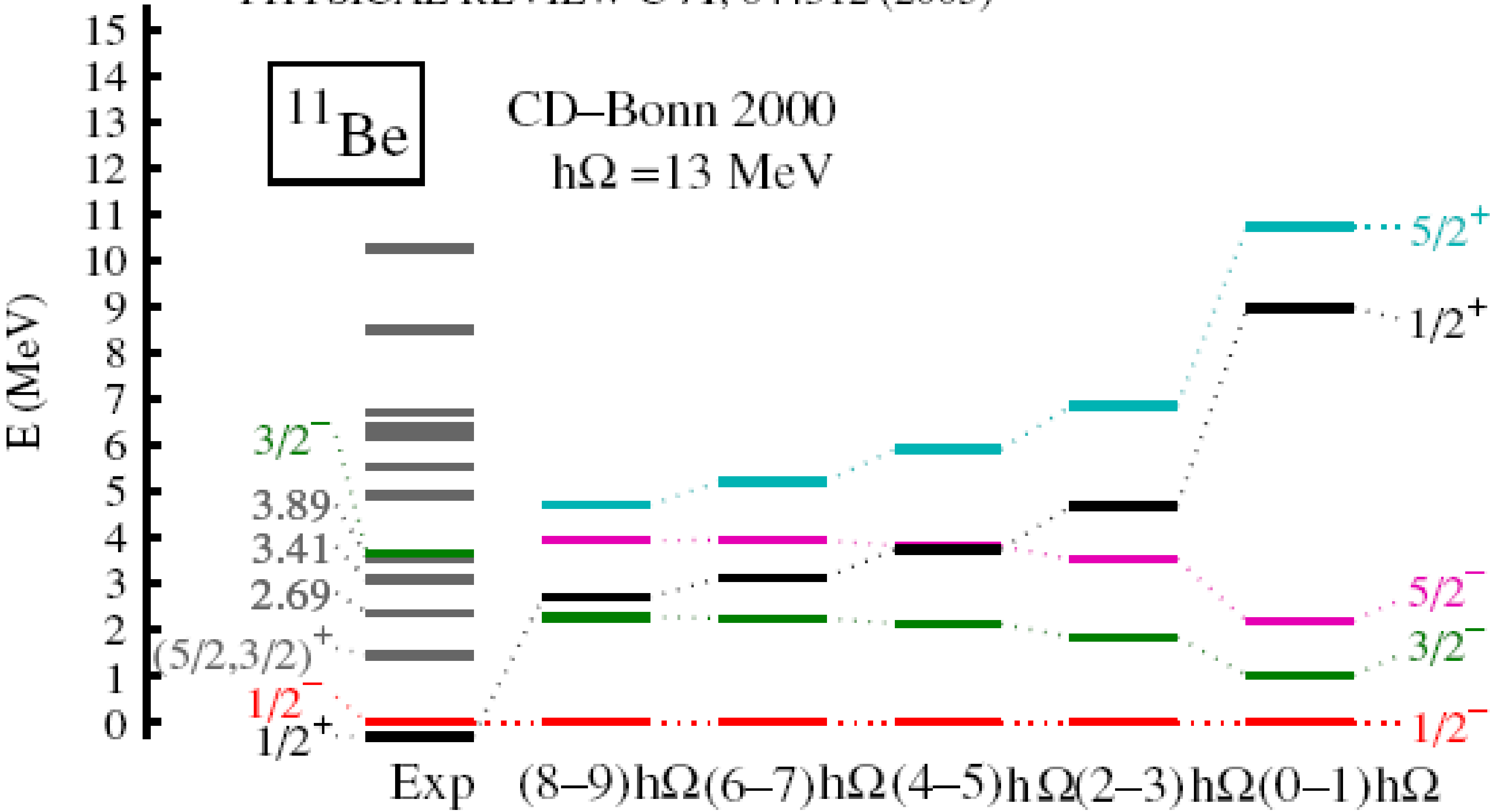
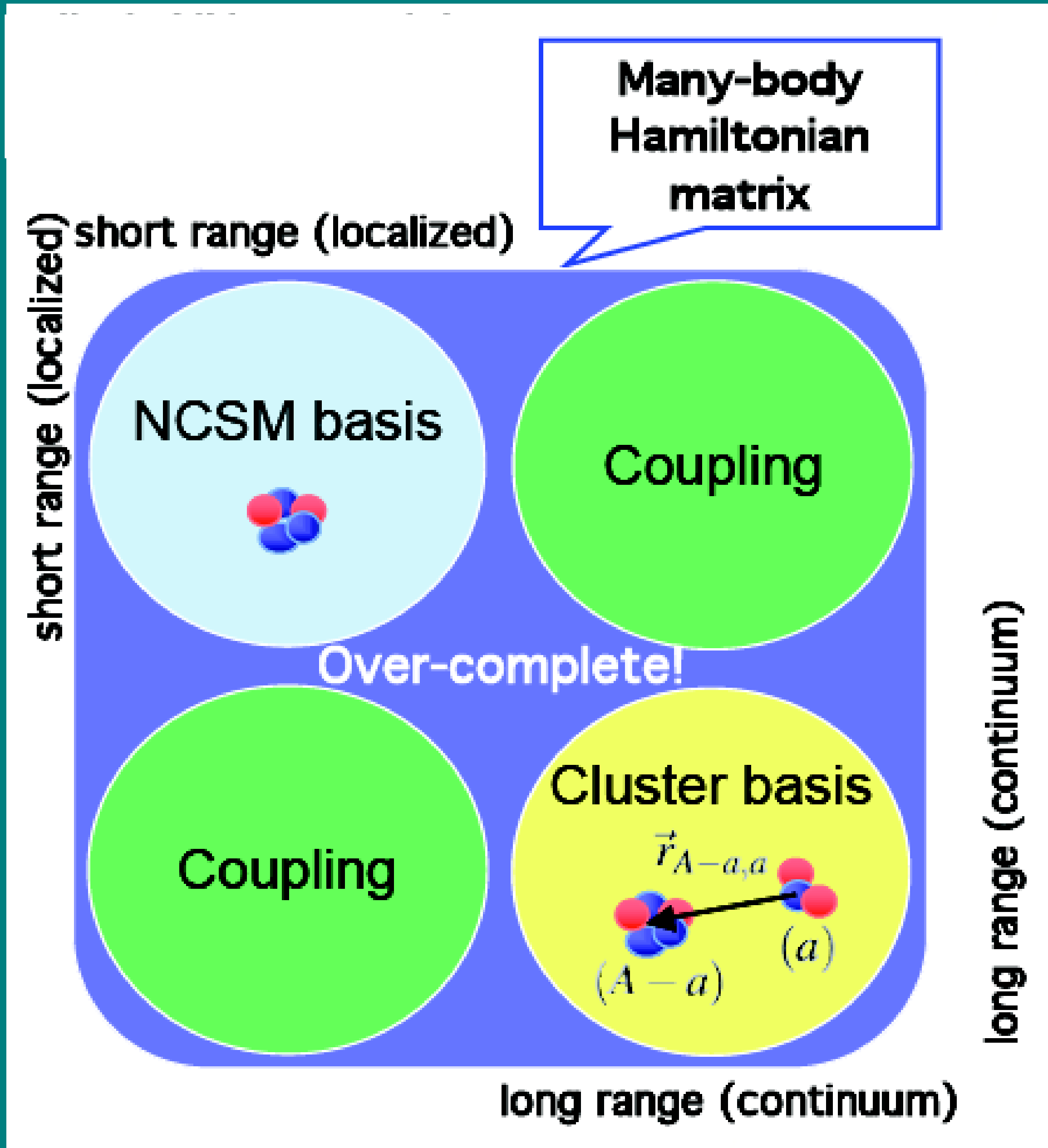
PHYSICAL REVIEW C **71**, 044312 (2005)





P. Navratil and S. Quaglioni, INT seminars fall 2007

From 4hΩ NCSM to sd CSM for ^{18}F

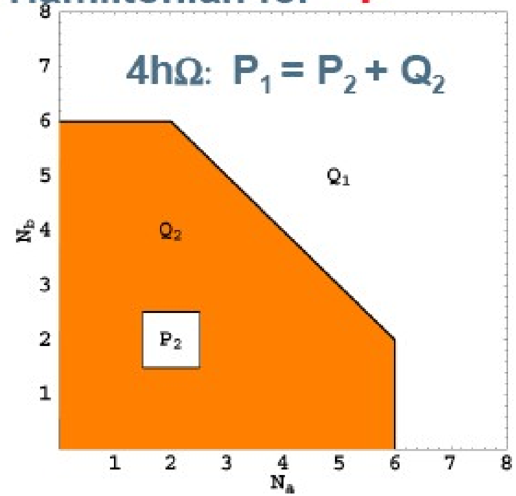
Petr Navrátil, Michael Thoresen, and Bruce R. Barrett, Phys. Rev. C 55, R573 (1997)

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

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

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

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



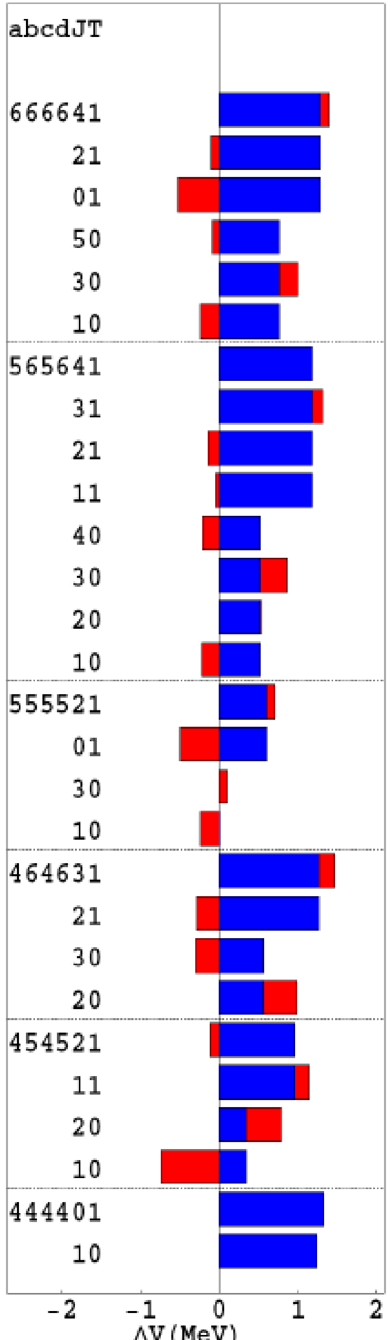
$$H_{\rm diag} = U H U^\dagger$$

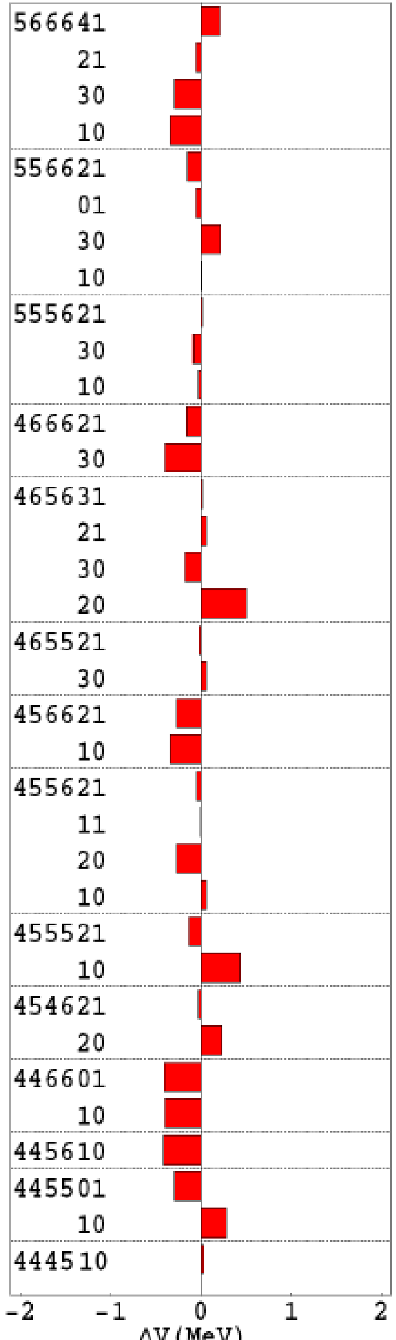
$E_k(A=18)$ $H(N_{max}=4,A=18)$

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

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

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





Comparison of 4AV18SD & sd-part of 4AV18

$\Delta V(abcd;JT) =$

$V_{eff}(4AV18SD) - V(4AV18) - \Delta V_{mon}(55,T=0)$

$\Delta V(abcd;JT) =$

$\Delta V_{mon}(ab,T) + \Delta V_{res}(abcd;JT) - \Delta V_{mon}(55,T=0)$

Next steps

Testing different methods to derive interactions directly: 4AV18SD is exact mapping of the 4AV18

Testing 4AV18SD interaction for other sd-shell nuclei

4 - $s_{1/2}$ 5 - $d_{3/2}$ 6 - $d_{5/2}$

Exact solution for ω: 3-body cluster level

Let E_k and $|k\rangle$ be the eigensolutions of H_3^{Ω},

$$H_3^{\Omega}\,|k\rangle = E_k\,|k\rangle$$

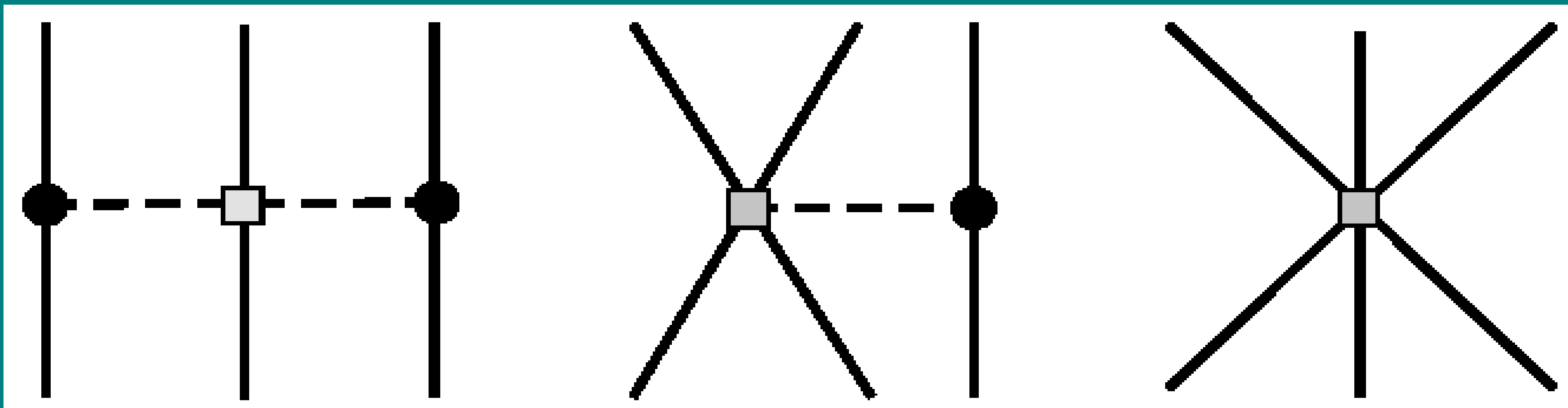
Let $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ be HO states belonging to the model space P and the excluded space Q, respectively. Then ω is given by:

$$\langle\alpha_Q|k\rangle = \sum_{\alpha_P}\langle\alpha_Q|\omega|\alpha_P\rangle\langle\alpha_P|k\rangle$$

or

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in K}\langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle$$

Topology of the leading chiral 3NF

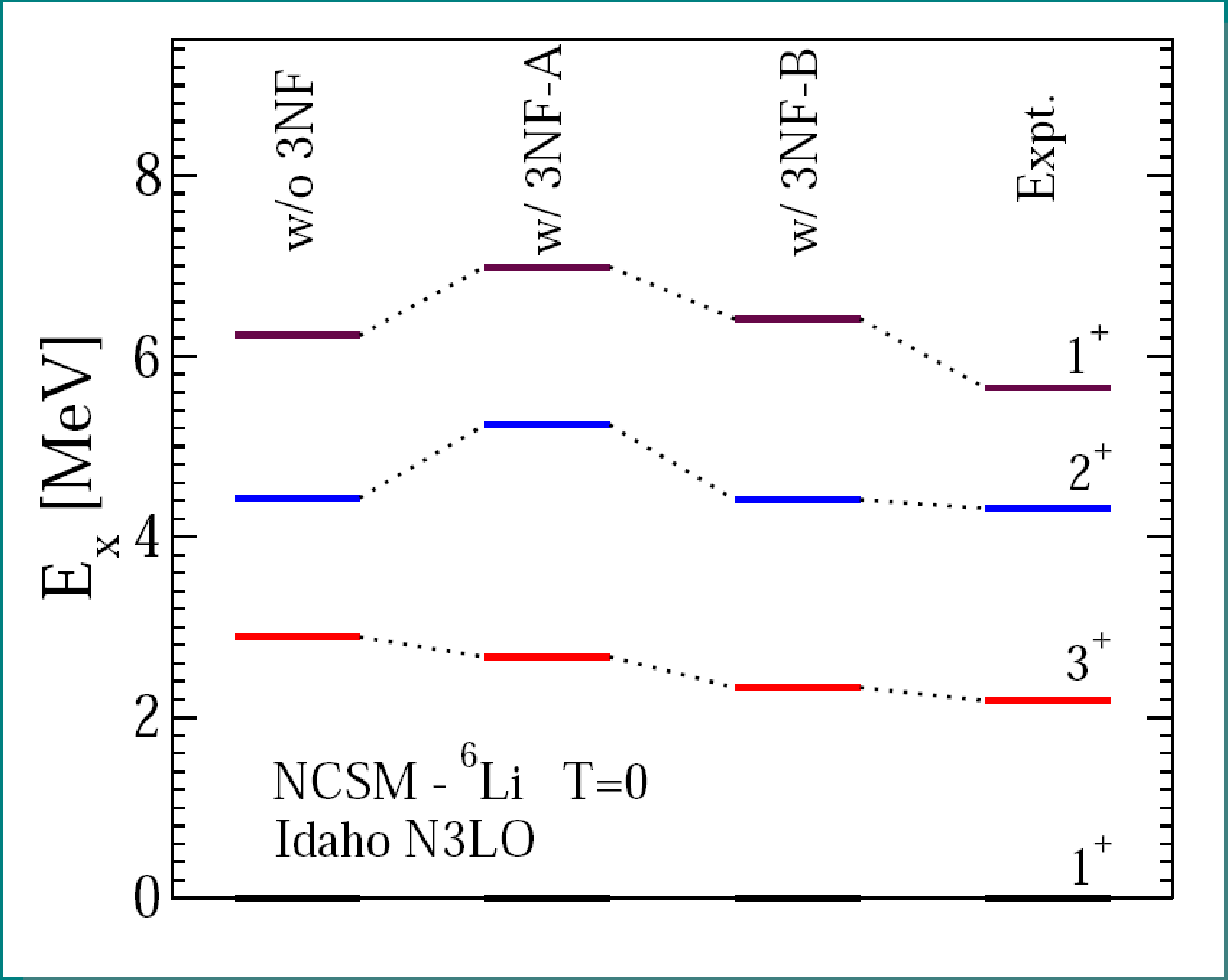


2π-exchange part
(c-terms)

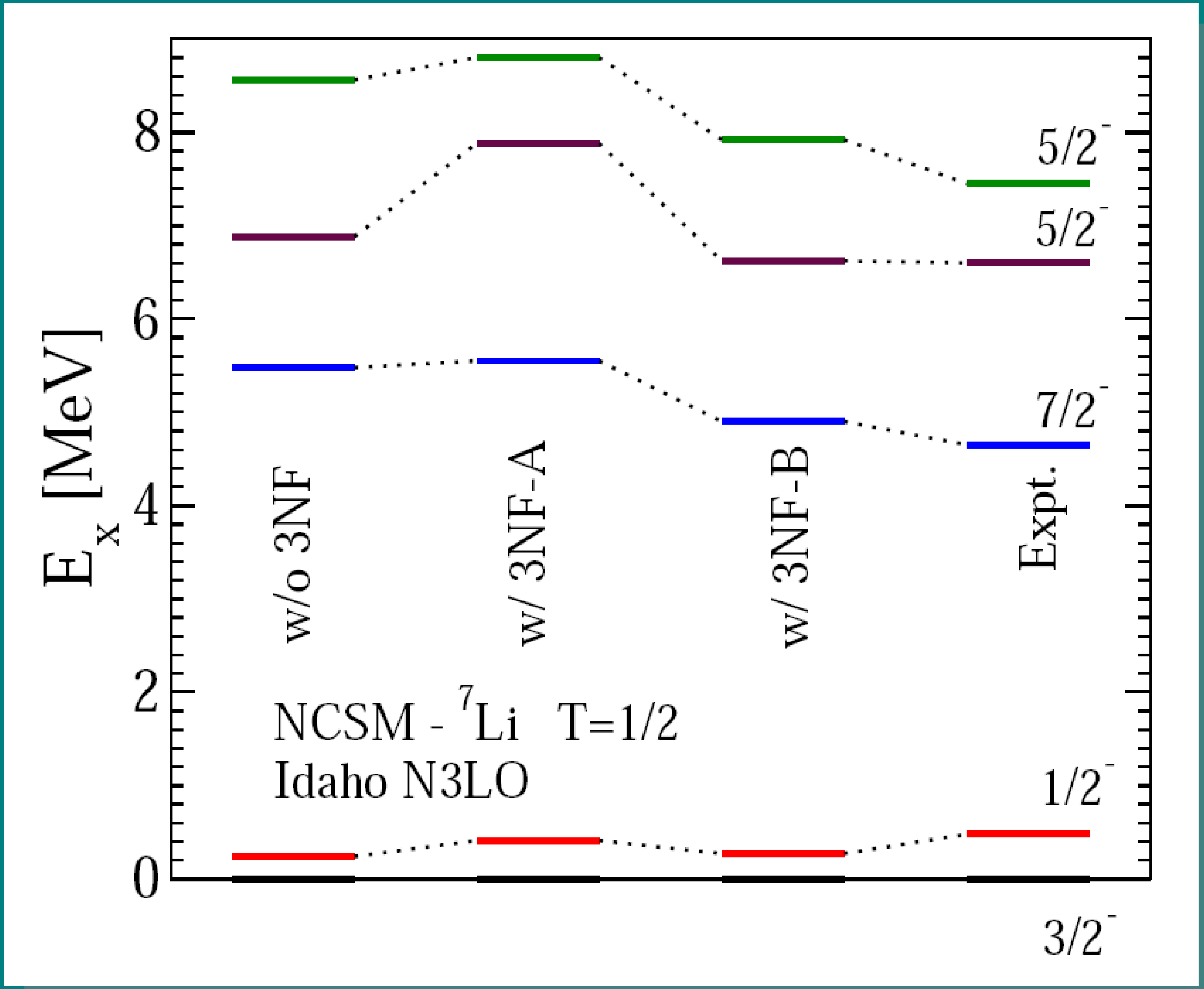
1π-exchange/contact
part (D-term)

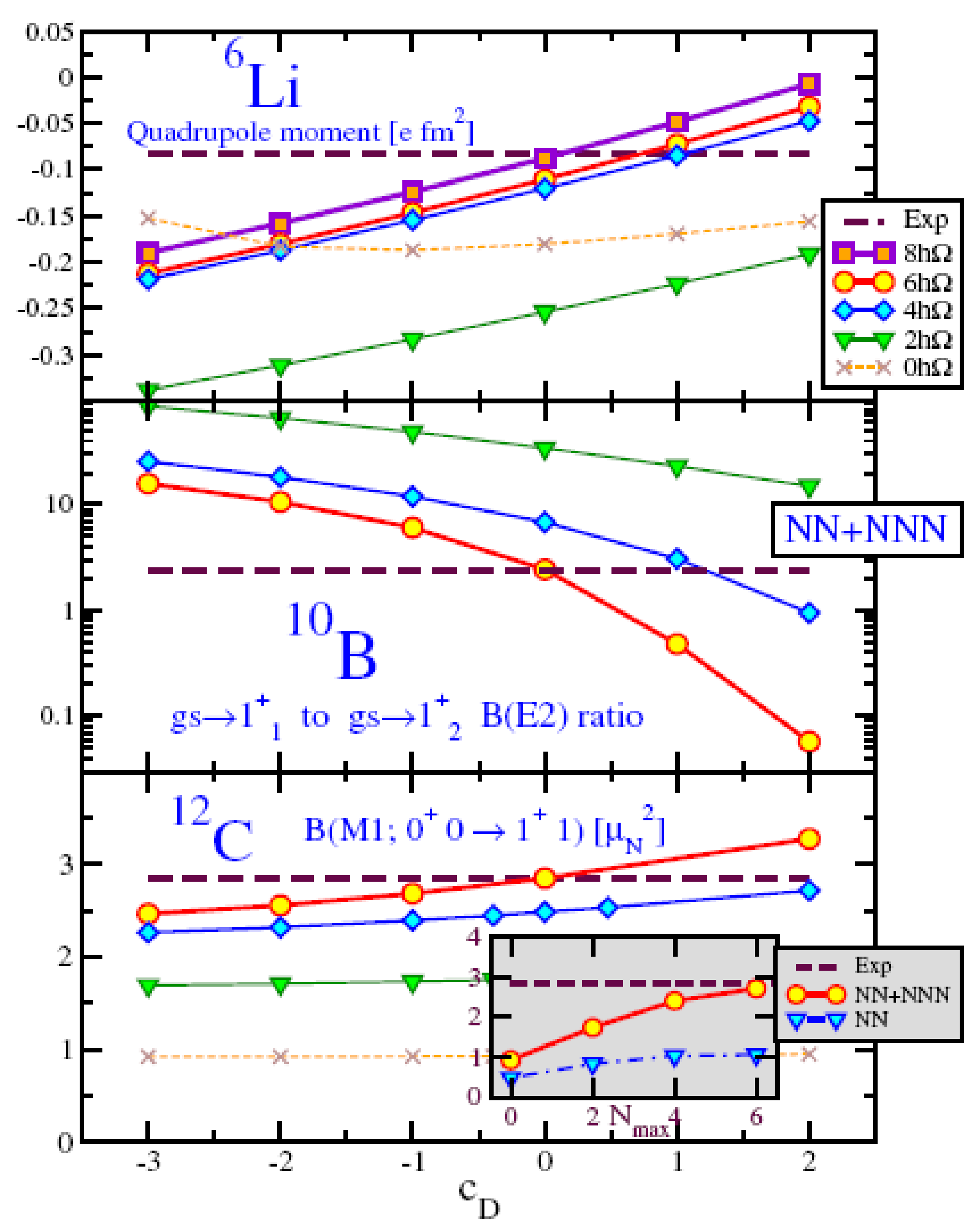
Pure contact part
(E-term)

A. Nogga, *et al.*, NPA 737, 236 (2004)



A. Nogga, *et al.*, nucl-th/0511082 (2005)





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P. Navratil, et al., Phys. Rev. Letters 99, 042501 (2007)

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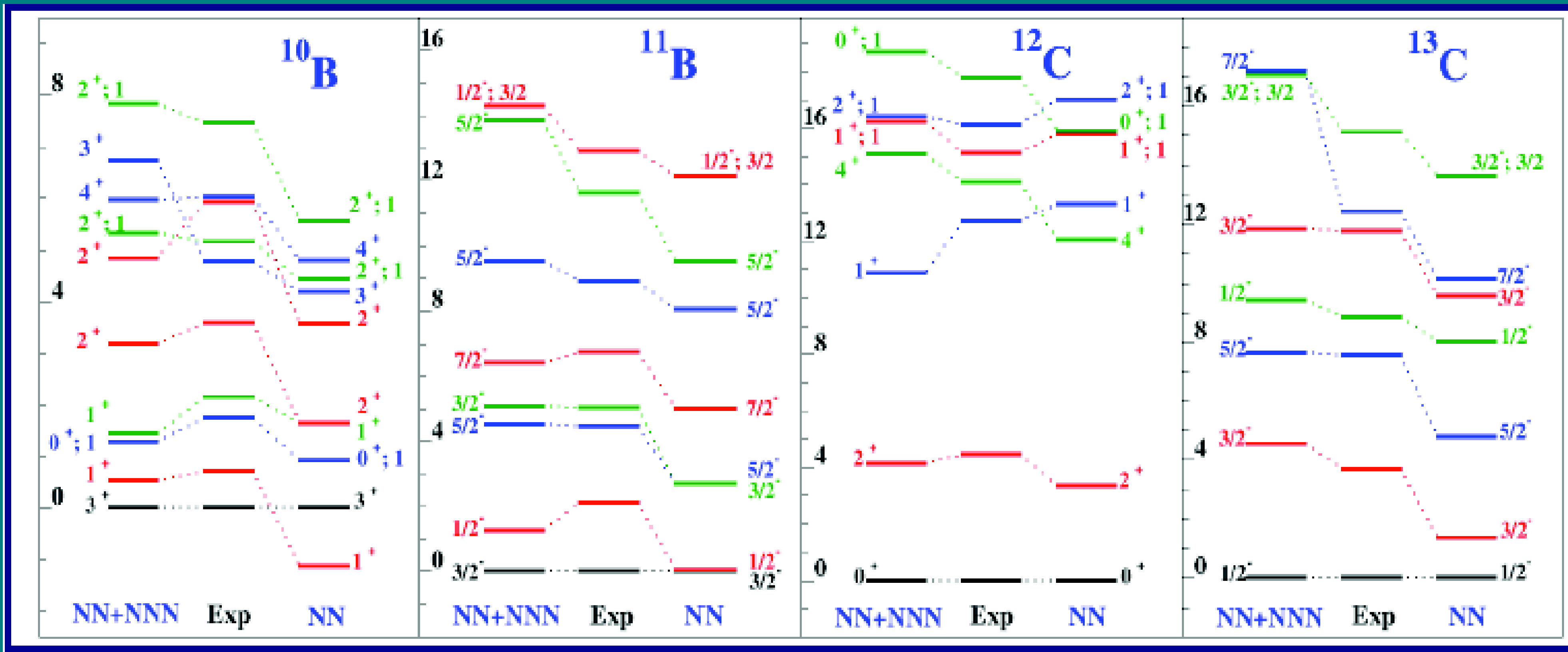

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