The ab initio No Core Shell Model for Nuclear Structure and Reactions

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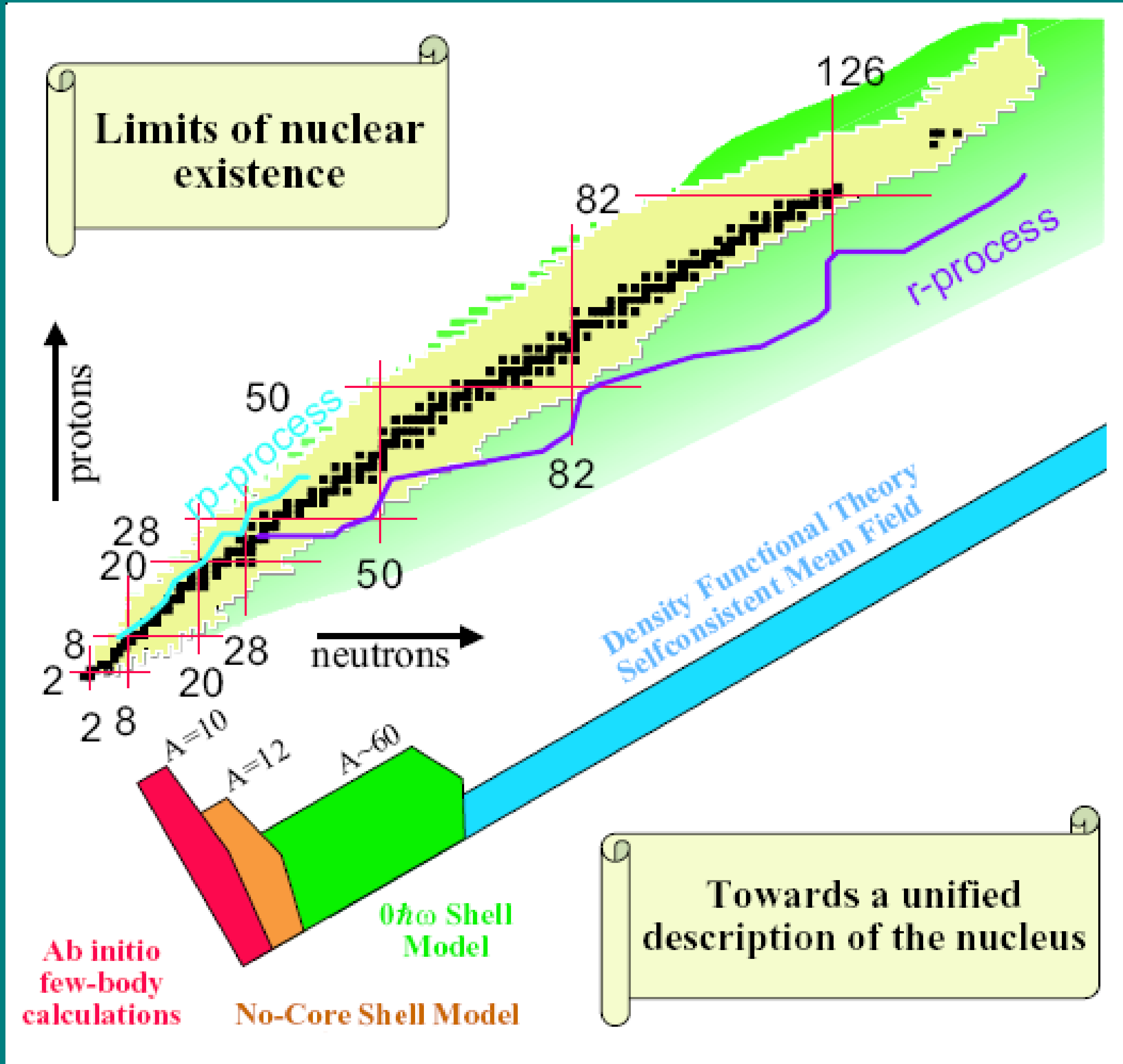
MICROSCOPIC NUCLEAR-STRUCTURE THEORY

1. Start with the bare interactions among the nucleons

2. Calculate nuclear properties using nuclear many-body theory



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

$$H \Psi = E \Psi$$

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

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

Some current shell-model references

1. B. A. Brown, "The Nuclear Shell Model towards the Drip Lines," *Progress in Particle and Nuclear Physics* **47**, 517 (2001)
2. 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)
3. I. Talmi, "Fifty Years of the Shell Model-The Quest for the Effective Interaction," *Advances in Nuclear Physics*, Vol. **27**, ed. J. W. Negele and E. Vogt (Plenum, NY, 2003)
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

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

Ref: P. Navrátil, J.P. Vary, B.R.B., PRC 62, 054311 (2000)

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

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

Two-body cluster approximation (a=2)

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

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

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 rewrite S(2) in terms of a new operator

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

Then the Hermitian effective operator in the P2 space can be expressed in the form

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

Analogously, any arbitrary operator can be written in the P_2 space

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

Exact solution for ω:

Let E_k and $|k\rangle$ be the eigensolutions

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

Let $|\alpha_P\rangle$ & $|\alpha_Q\rangle$ 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,...

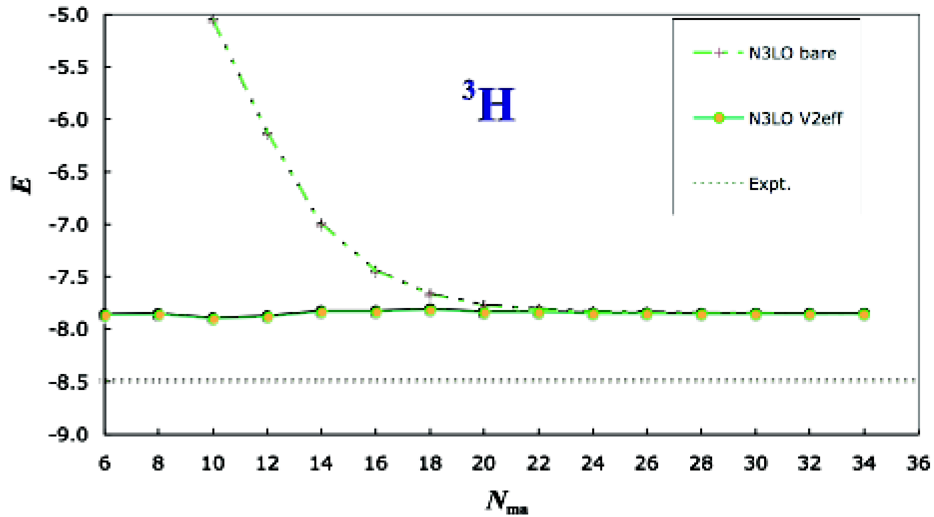
3. Calculate $\langle\alpha_Q^n|\omega|\alpha_P^n\rangle = \sum_{k\in K}\langle\alpha_Q|k_n\rangle\langle\tilde{k}_n|\alpha_P\rangle$

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

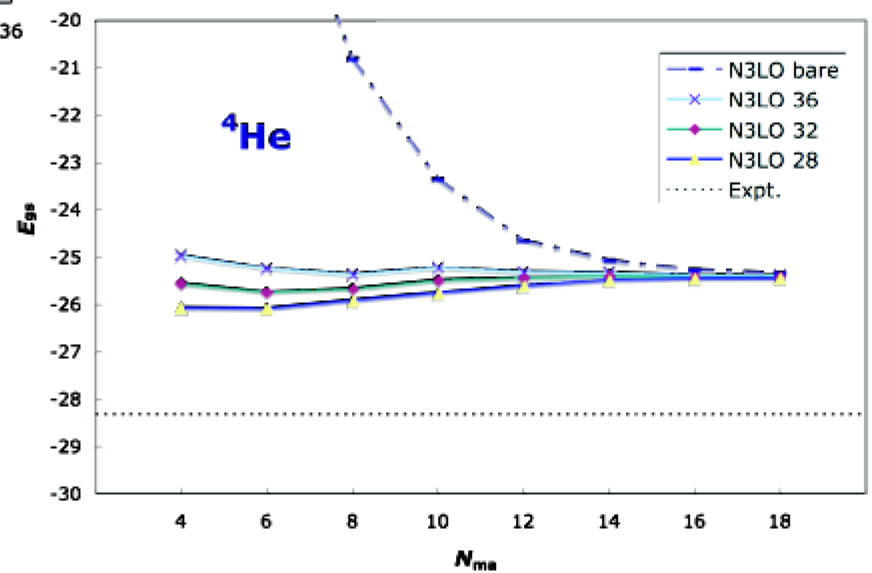
5. Diagonalize $\mathcal{H}_n^{\text{eff}}$ in the given model space, *i.e.*,
   $N_{max}\ \hbar\Omega$ = energy above the ground state

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



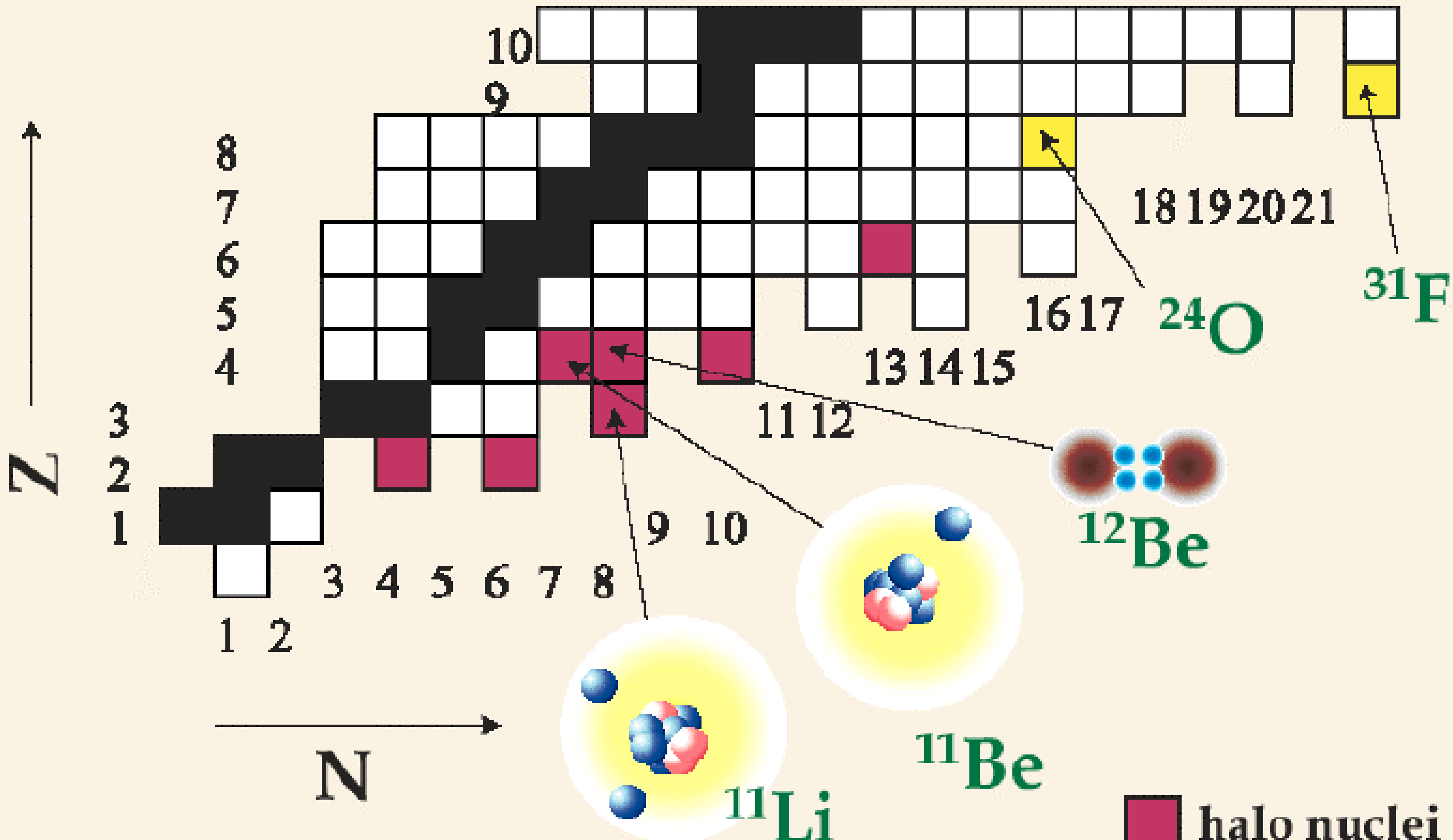
N^3LO NN	NCSM	FY	HH
^{3}H	7.852(5)	7.854	7.854
^{4}He	25.39(1)	25.37	25.38



- Short-range correlations ⇒ effective interaction
- Medium-range correlations ⇒ multi-$\hbar\Omega$ 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

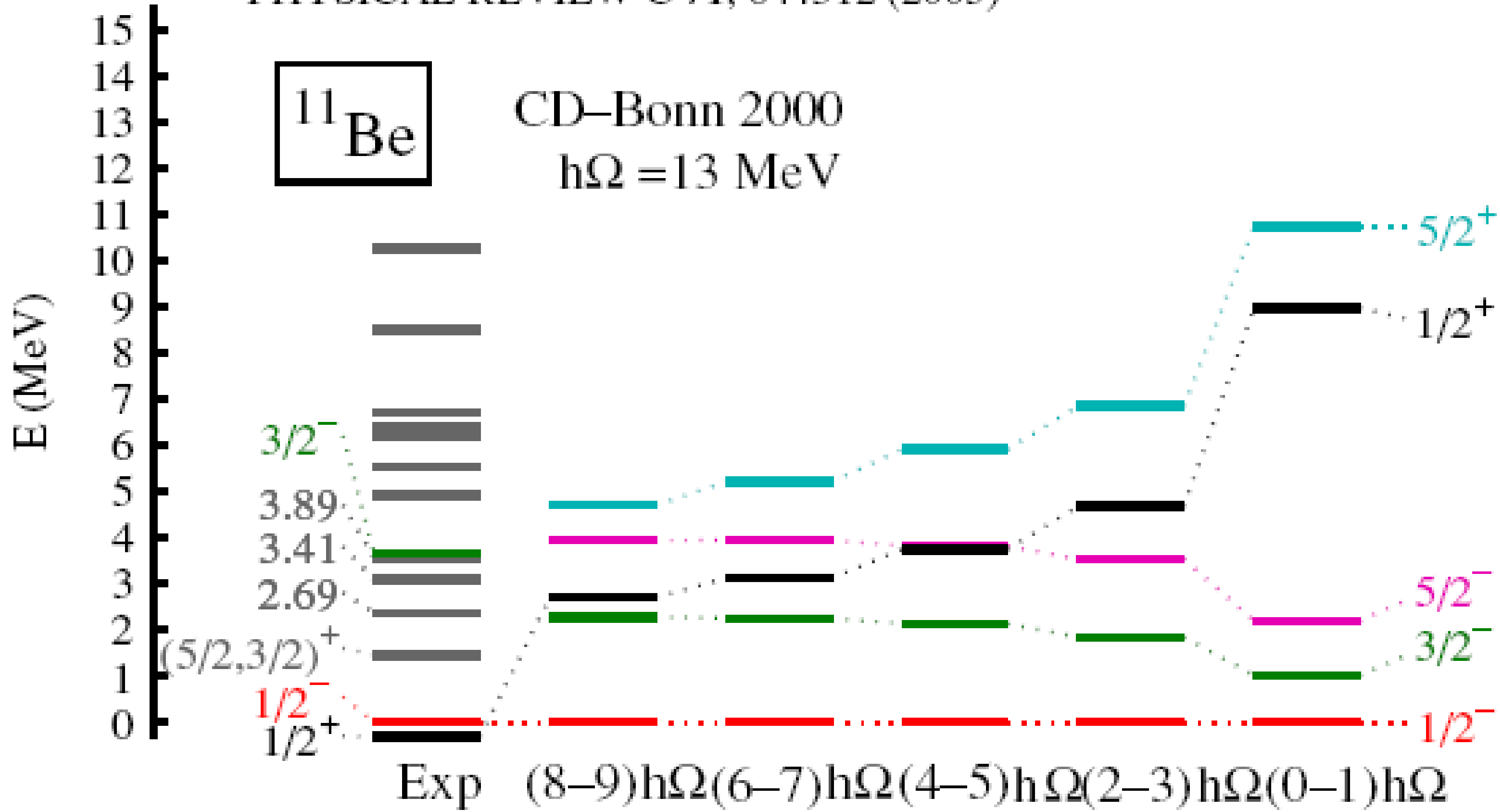
P. Navratil, INT Seminar, November 13, 2007, online

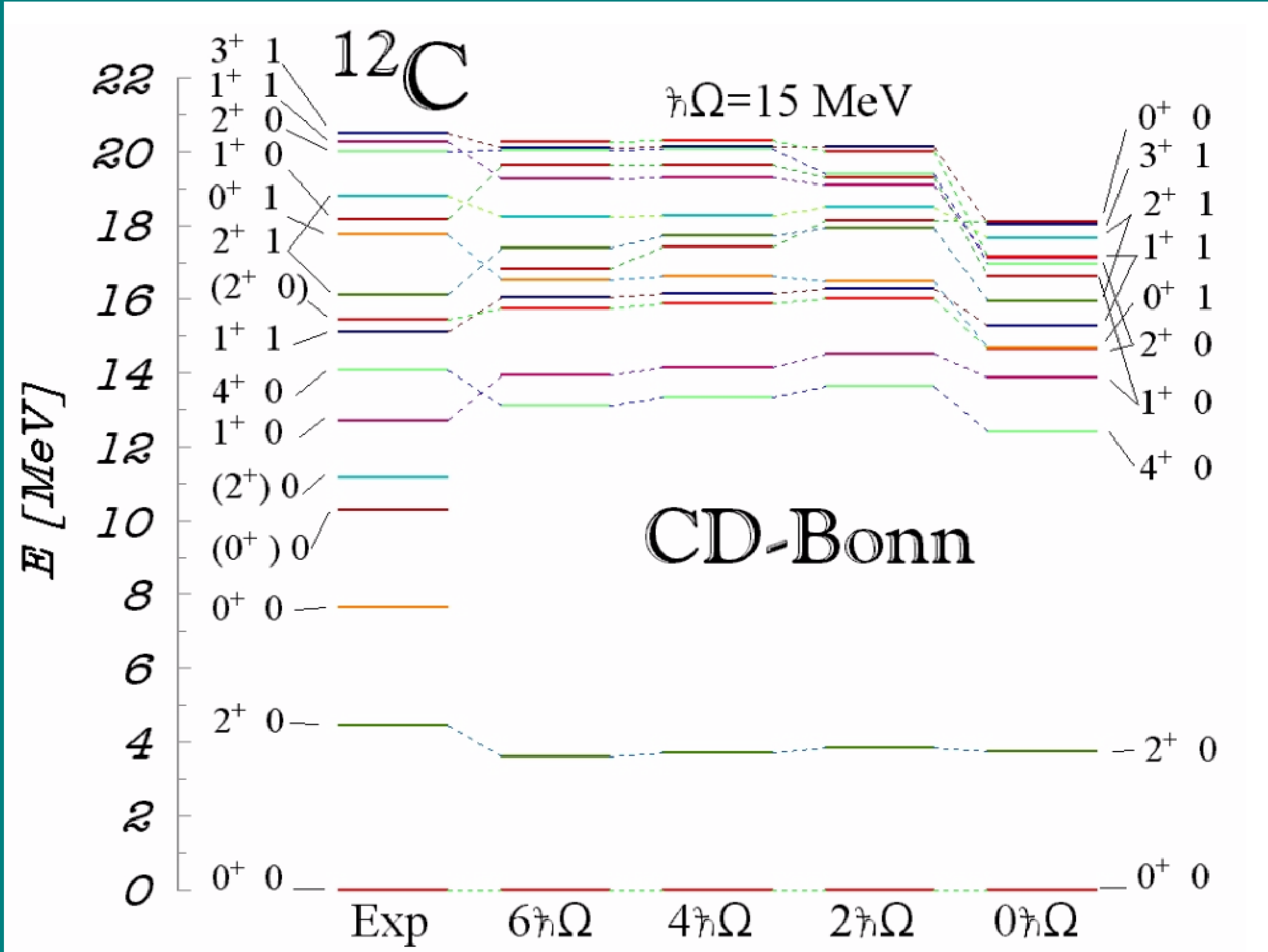
Light drip line nuclei



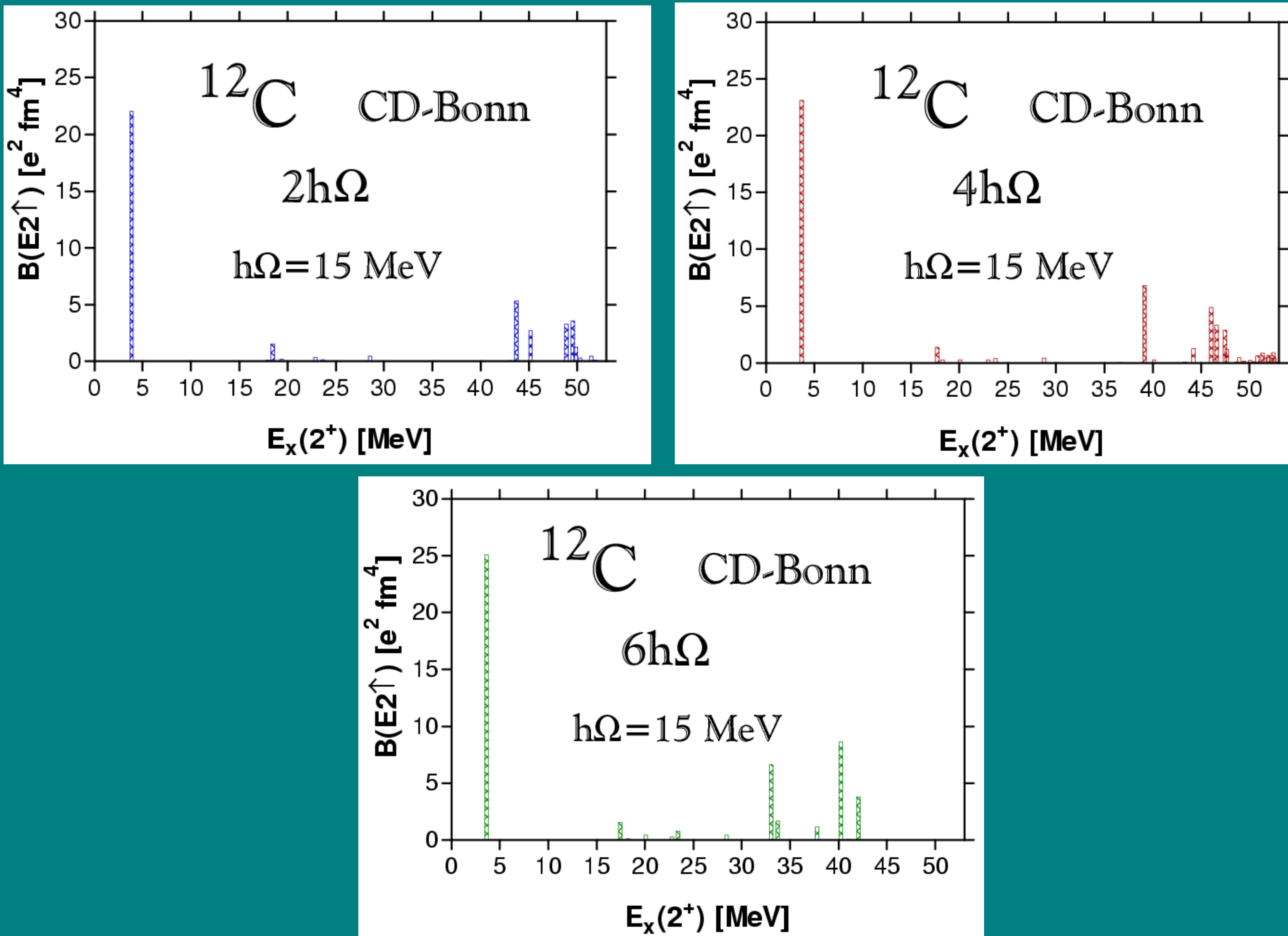
C. FORSSÉN, P. NAVRÁTIL, W. E. ORMAND, AND E. CAURIER

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

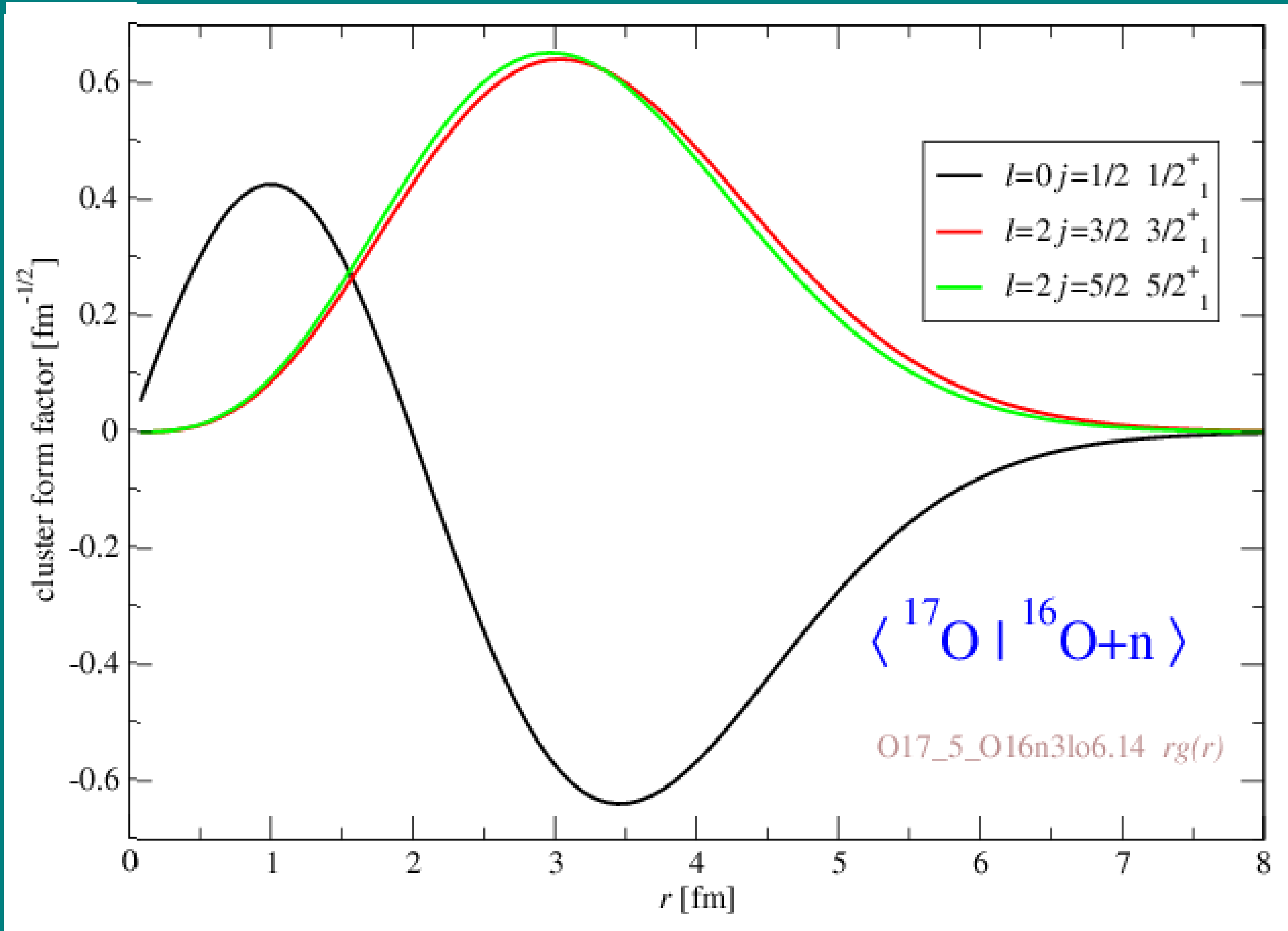




P. Navrátil, J. P. Vary and B. R. B., Phys. Rev. C 62, 054311 (2000)

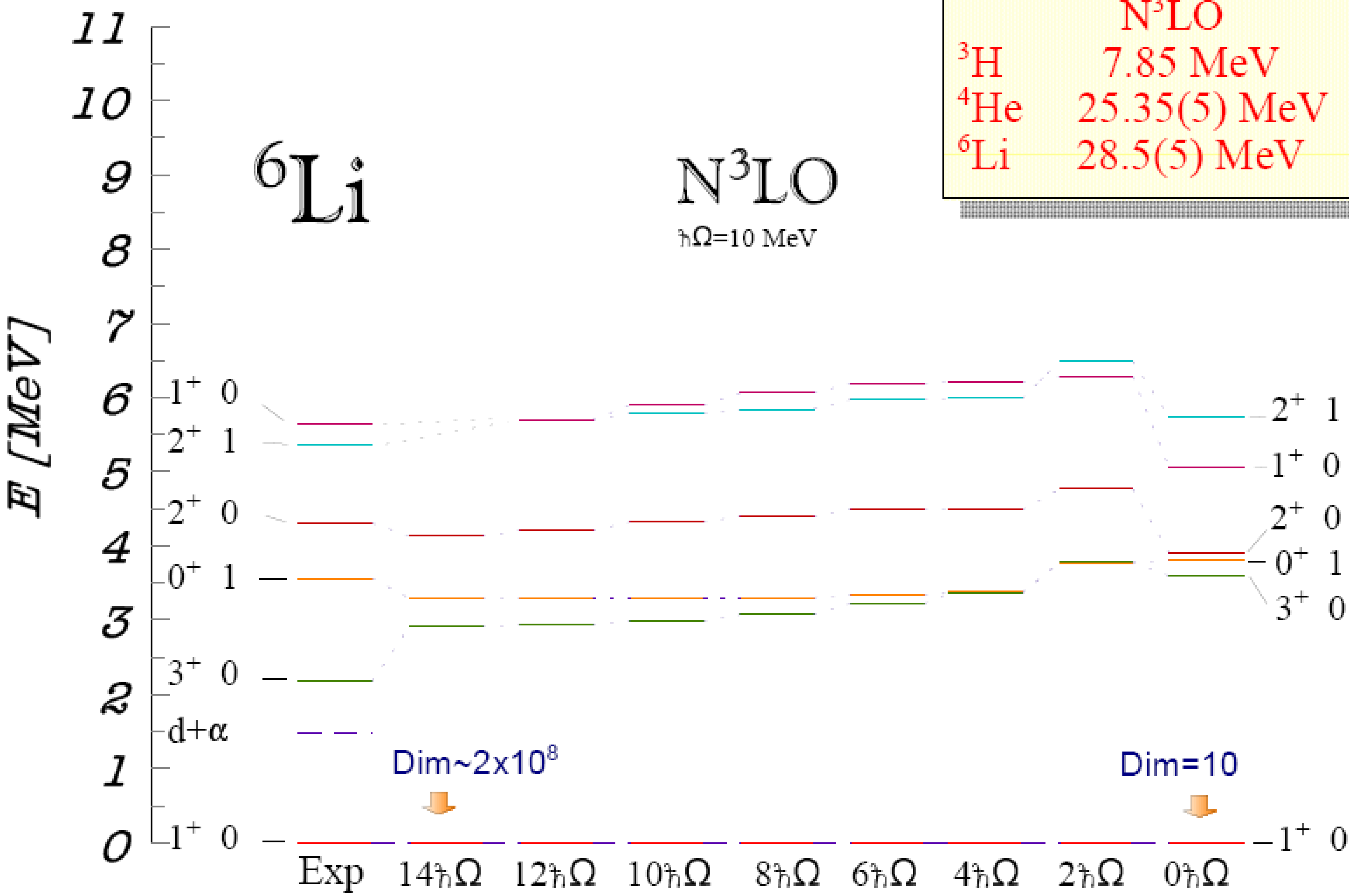


12C CD-Bonn
2hΩ
hΩ=15 MeV
4hΩ
hΩ=15 MeV
6hΩ
hΩ=15 MeV
B(E2↑) [e2 fm4]
Ex(2+) [MeV]



0.6
0.4
0.2
0
-0.2
-0.4
-0.6
cluster form factor [fm$^{-1/2}$]
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 $5/2^+_1$
$\langle {}^{17}O \mid {}^{16}O+n \rangle$
O17_5_O16n3lo6.14 $rg(r)$

P. Navratil



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

H. Kamada, *et al.*, Phys. Rev. C 64, 044001 (2001)

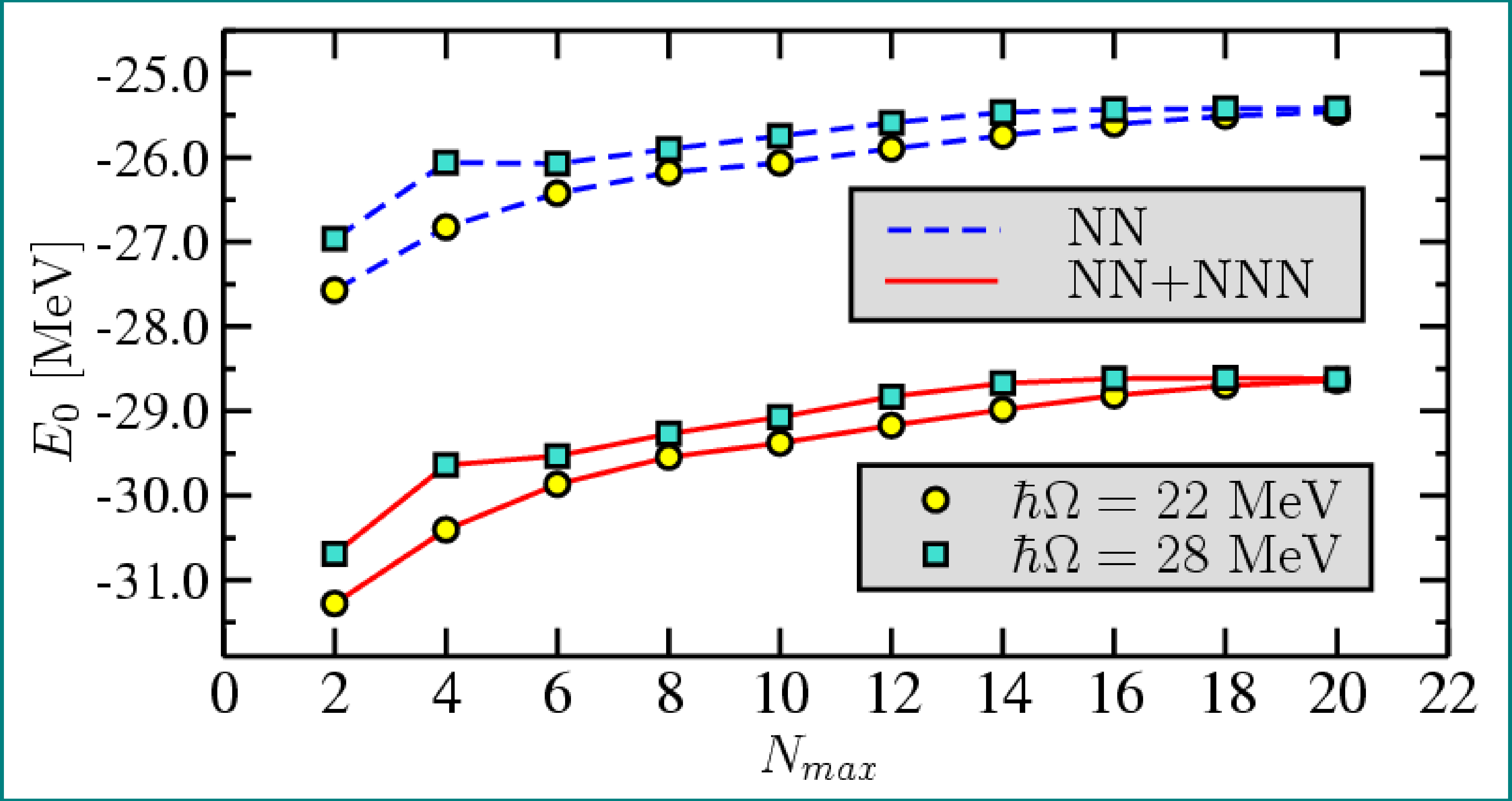
PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

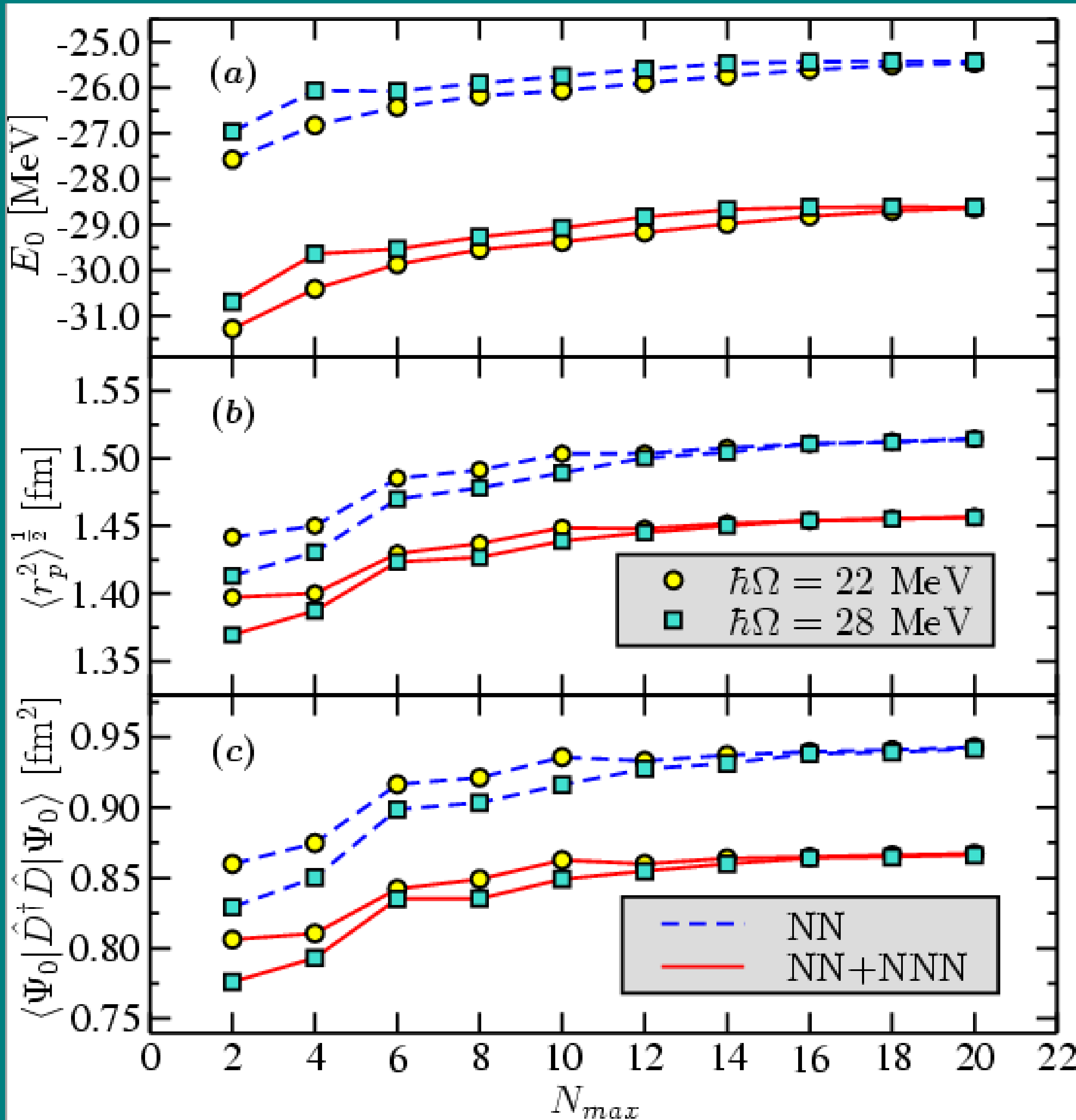
In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's 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

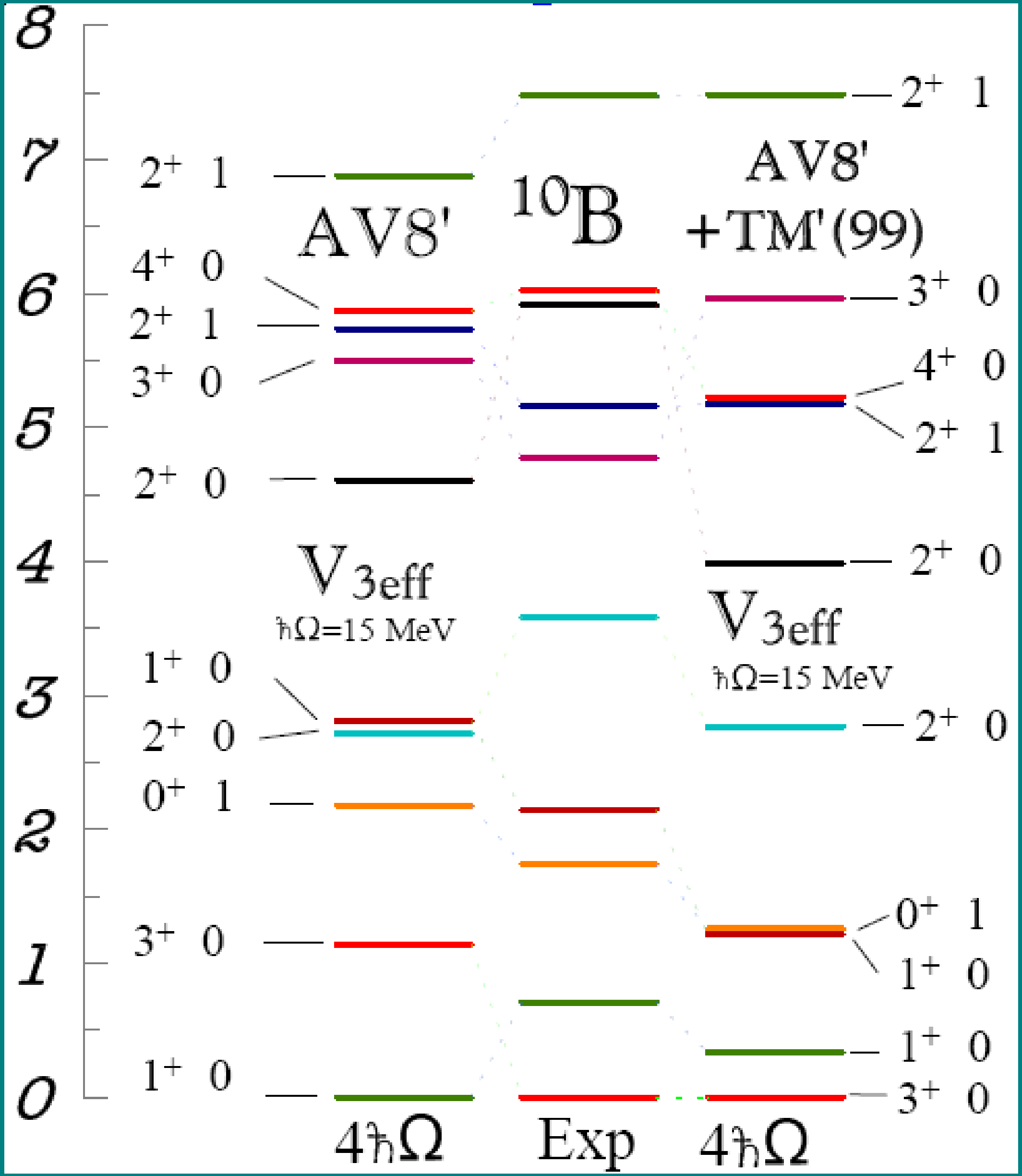
$BE_{exp} \approx 28.296$ MeV



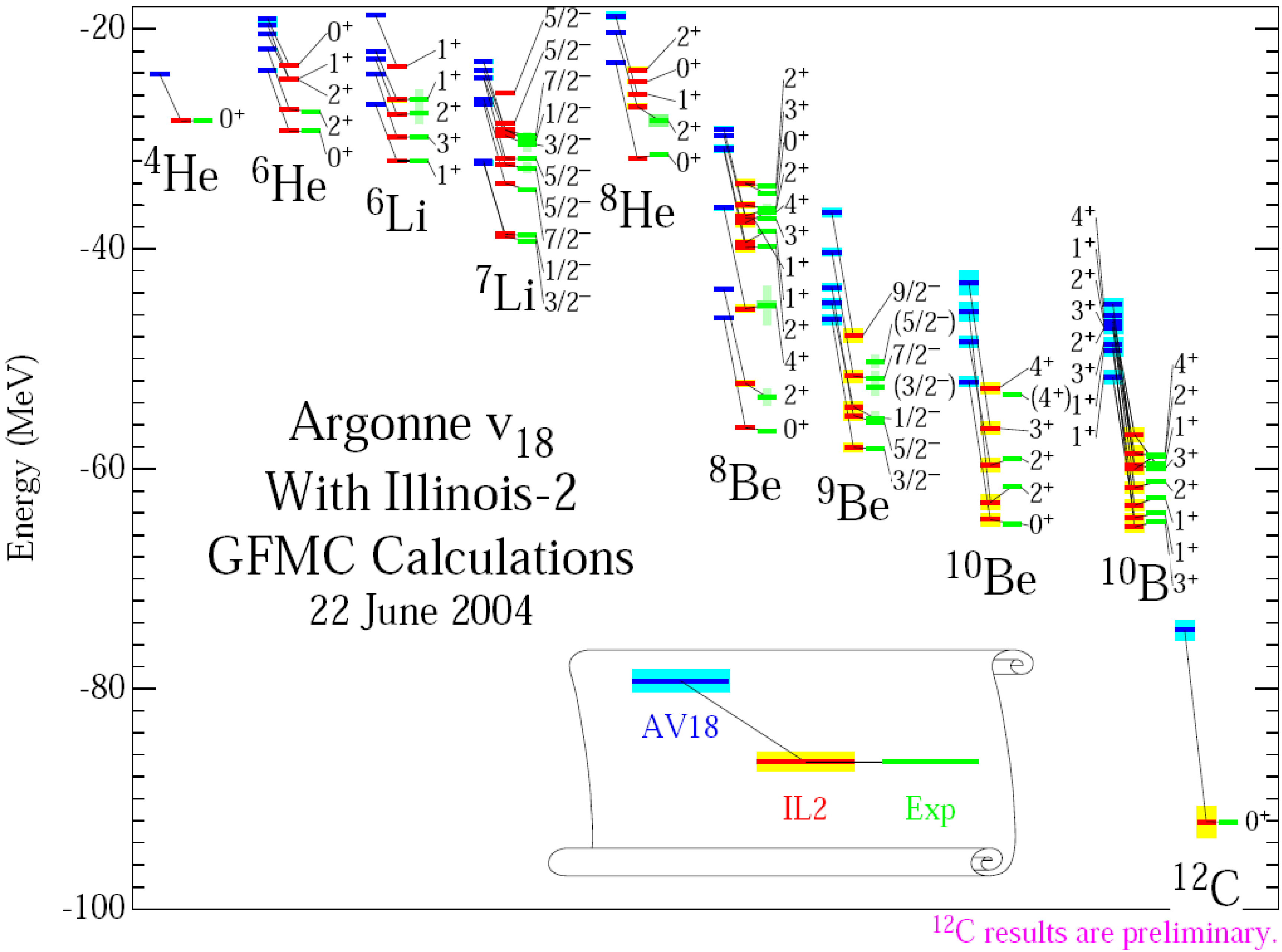
Results for 4He: S. Quaglioni and P. Navratil, arXiv:0704.1336


(a)
(b)
(c)
E_0 [MeV]
-25.0
-26.0
-27.0
-28.0
-29.0
-30.0
-31.0
$\langle r_p^2 \rangle^{\frac{1}{2}}$ [fm]
1.55
1.50
1.45
1.40
1.35
$\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle$ [fm^2]
0.95
0.90
0.85
0.80
0.75
$\hbar\Omega = 22$ MeV
$\hbar\Omega = 28$ MeV
NN
NN+NNN
0
2
4
6
8
10
12
14
16
18
20
22
N_{max}

4He



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


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.

Exact solution for ω: 3-body cluster level

Let E_k and $|k\rangle$ be the eigensolutions

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

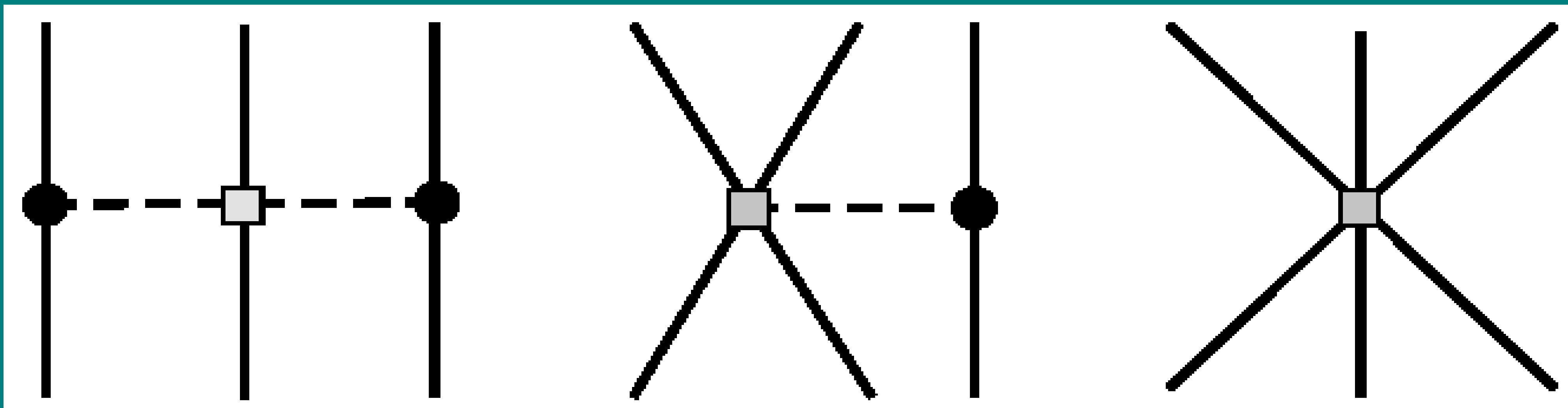
Let $|\alpha_P\rangle$ & $|\alpha_Q\rangle$ be HO states belonging to the model space P and the excluded space Q,
respectively. Then ω is given by:

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

or

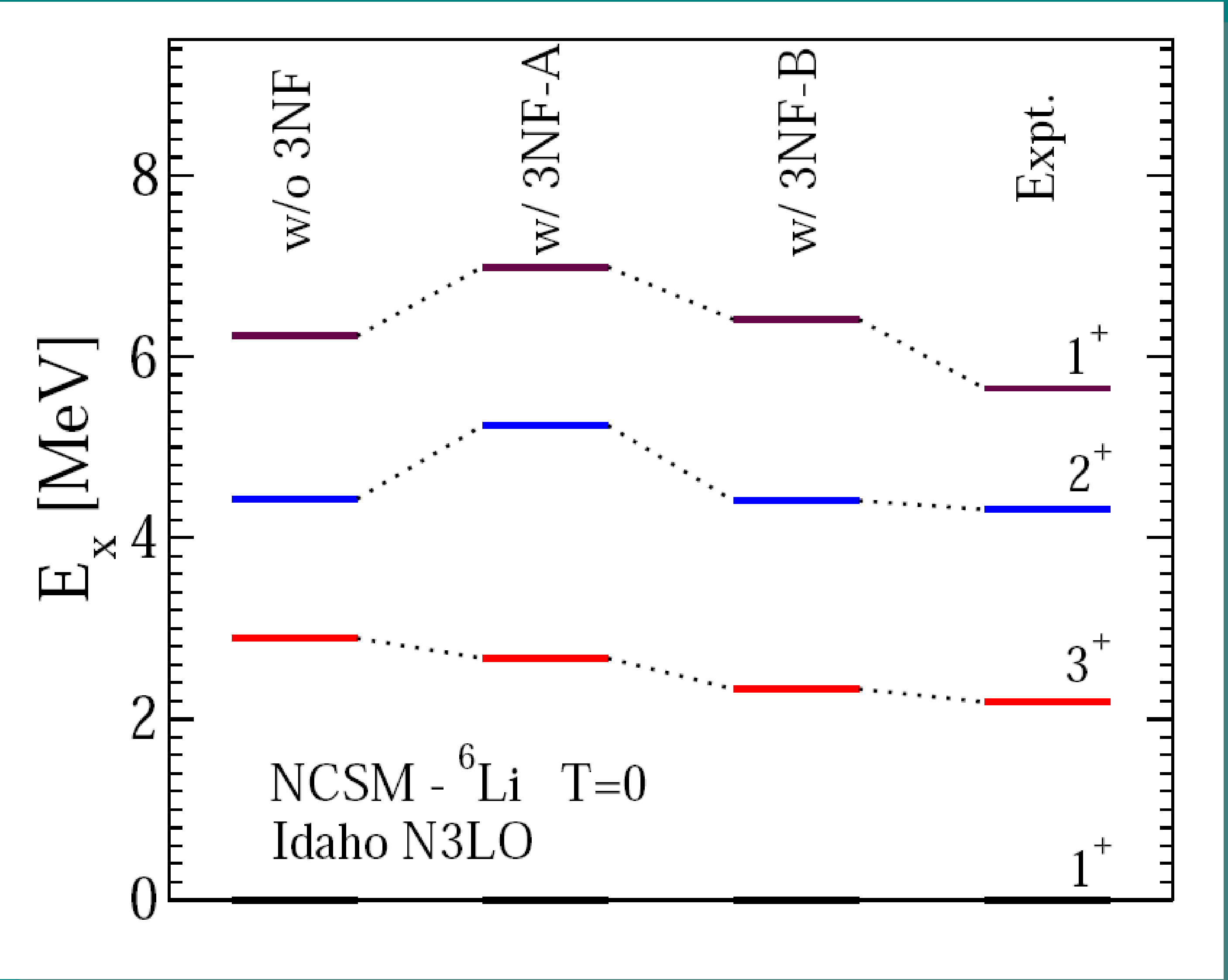
$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in K}\langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle$$

Topology of the leading chiral 3NF

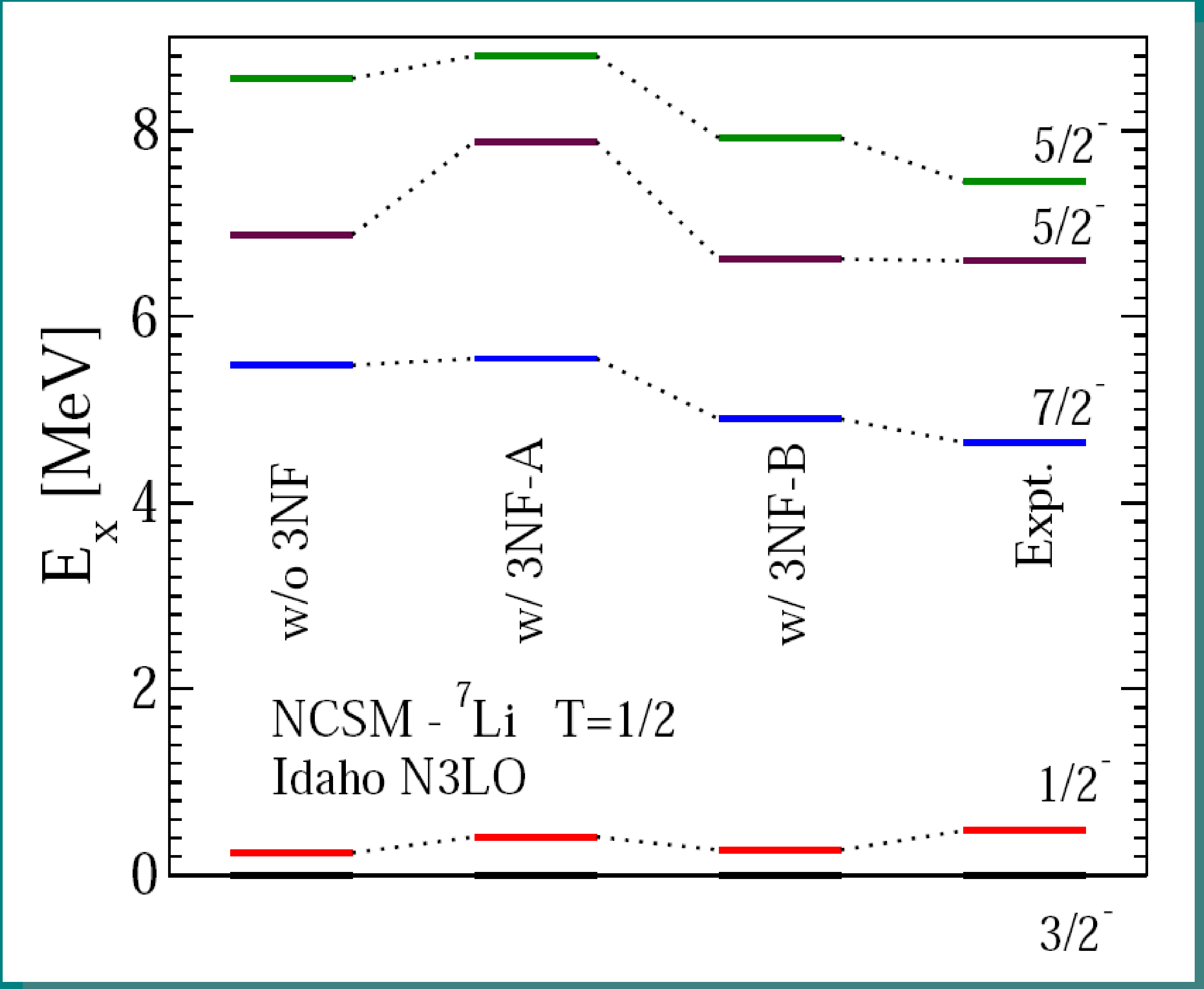


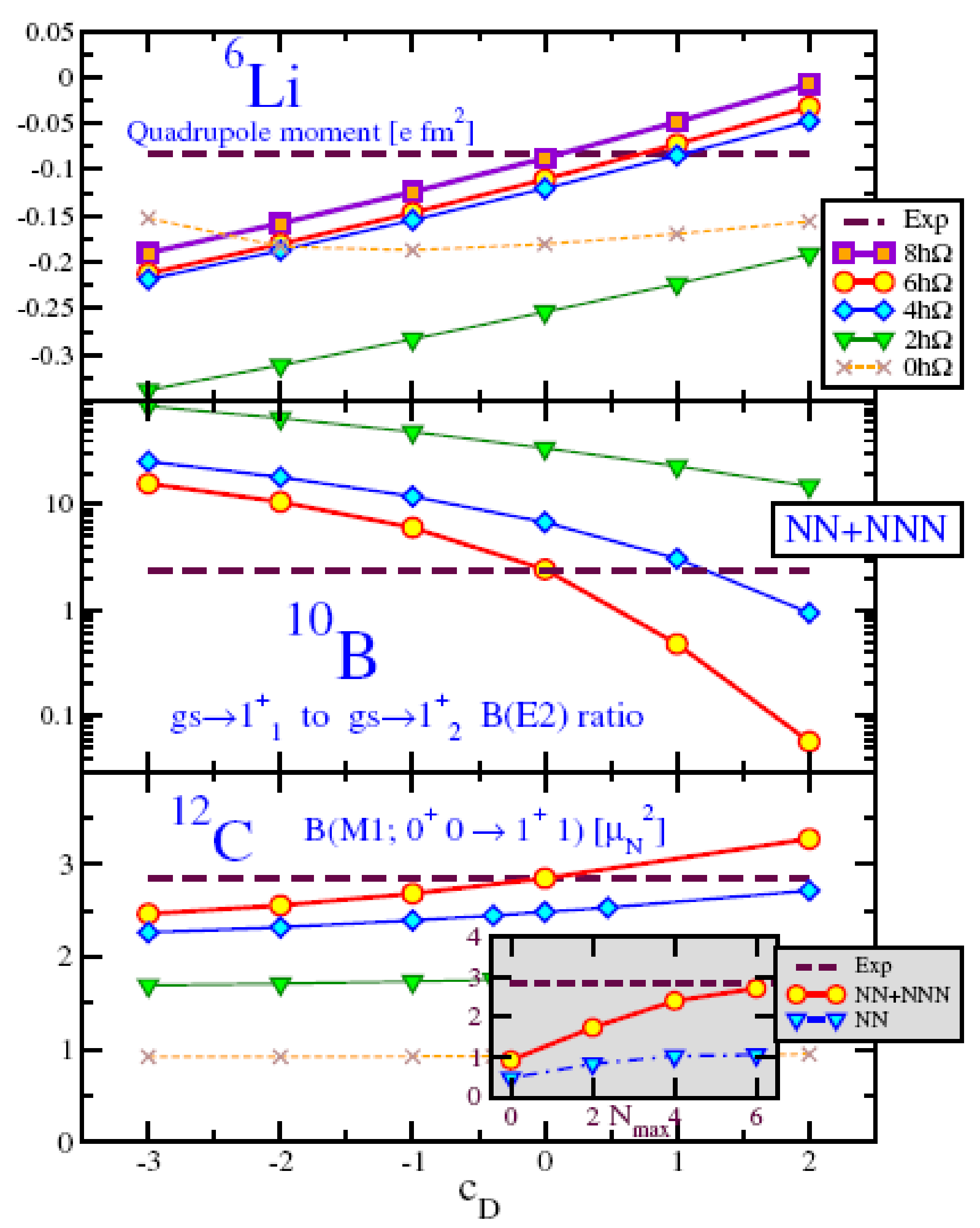
2π-exchange part (c-terms) | 1π-exchange/contact part (D-term) | Pure contact part (E-term)

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



A. Nogga, et al., Phys. Rev. C 73, 064002 (2006)

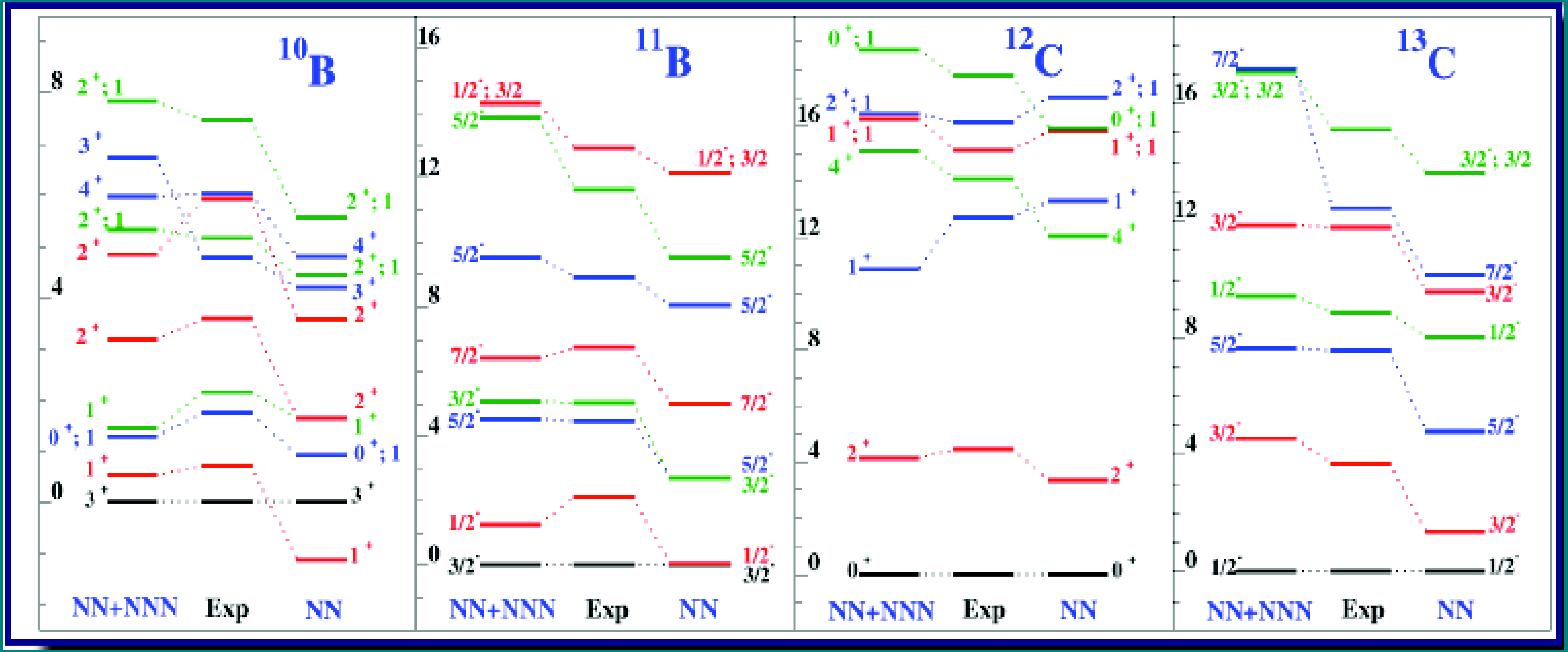




P. Navratil, et al. PRL 99, 042501 (2007)

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

N3LO Interaction: D.R. Entem, et al., Phys. Rev. C 86, 041001 (2007)



H. Kamada, *et al.*, Phys. Rev. C 64, 044011 (2001)

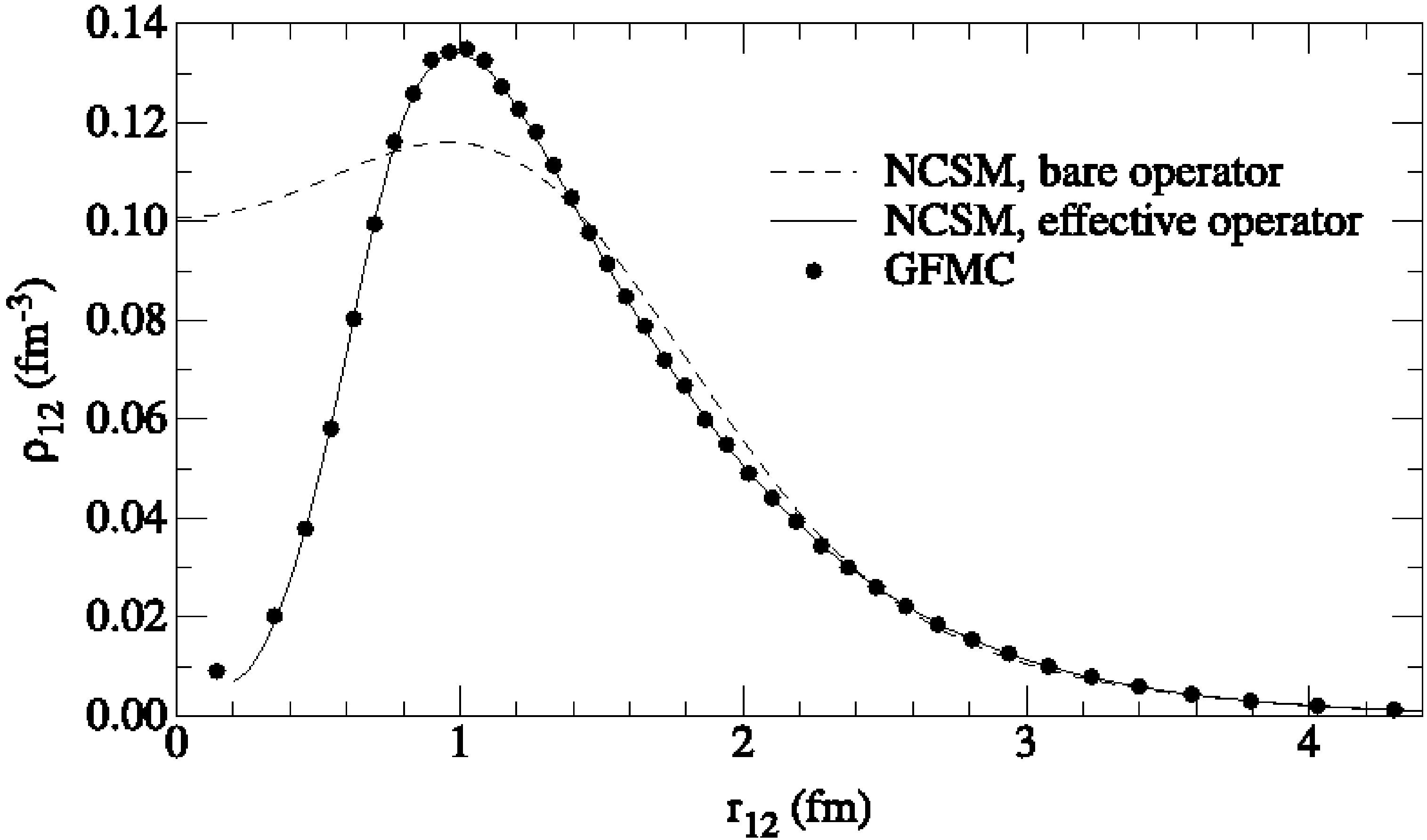


Figure 2. *NCSM and GFMC NN pair density in ^4He.*

Renormalization of other physical operators

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

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

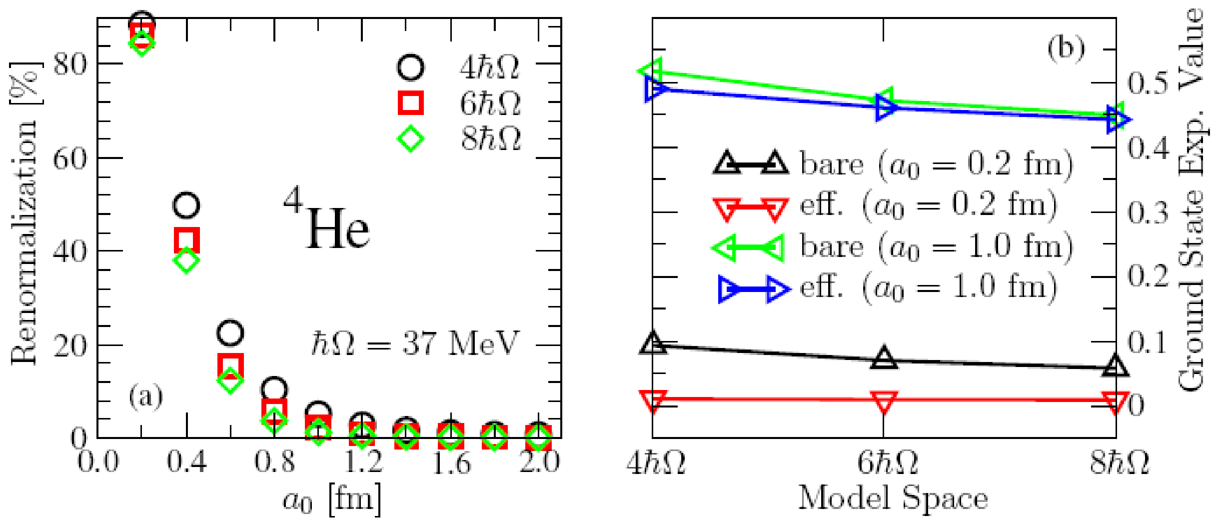
Nucleus	Observable	Model Space	Bare operator	Effective operator
^{2}H	Q_0	$4\hbar\Omega$	0.179	0.270
^{6}Li	$B(E2, 1^+0 \to 3^+0)$	$2\hbar\Omega$	2.647	2.784
^{6}Li	$B(E2, 1^+0 \to 3^+0)$	$10\hbar\Omega$	10.221	-
^{6}Li	$B(E2, 2^+0 \to 1^+0)$	$2\hbar\Omega$	2.183	2.269
^{6}Li	$B(E2, 2^+0 \to 1^+0)$	$10\hbar\Omega$	4.502	-
^{10}C	$B(E2, 2_1^+0 \to 0^+0)$	$4\hbar\Omega$	3.05	3.08
^{12}C	$B(E2, 2_1^+0 \to 0^+0)$	$4\hbar\Omega$	4.03	4.05
^{4}He	$\langle g.s.\vert T_{rel}\vert g.s.\rangle$	$8\hbar\Omega$	71.48	154.51

Stetcu, Barrett, Navratil, Vary, Phys. Rev. C 71, 044325 (2005)

- small model space: expect larger renormalization
- large variation with the model space
- three-body forces: might be important, but not the issue

- $a \to A$ for fixed model space;
- $P \to \infty$ for fixed cluster.

Range dependence

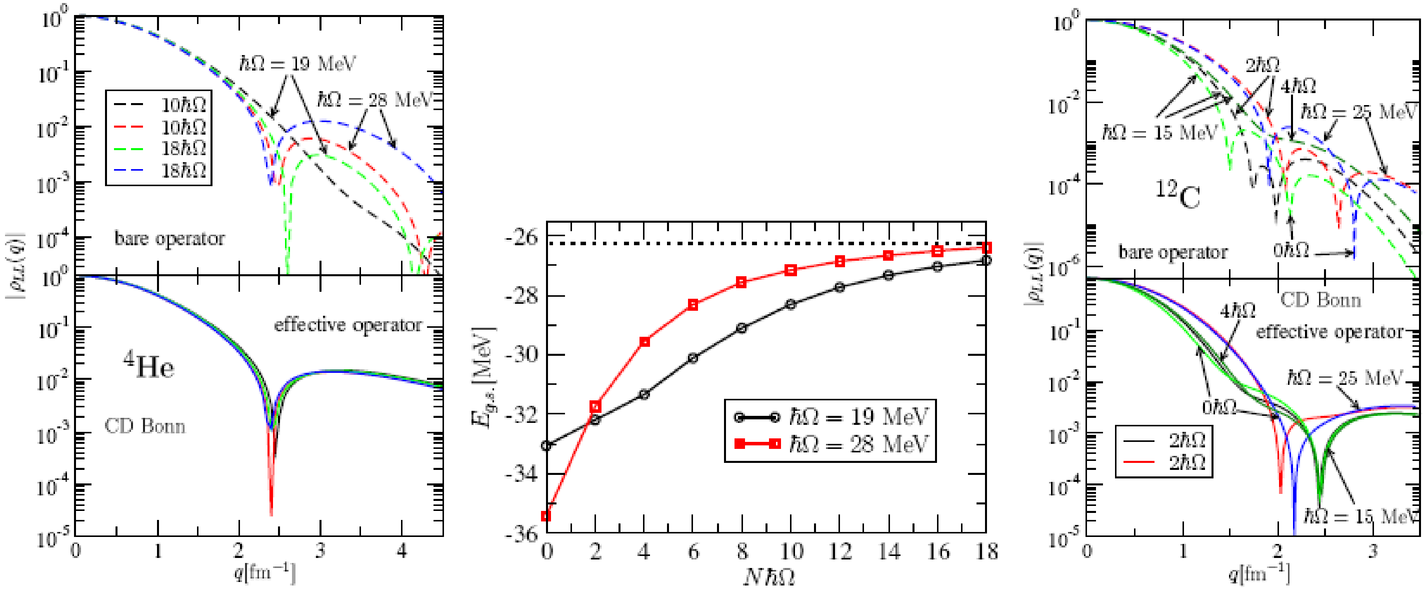


$$O \sim \exp\left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{a_0^2}\right]$$

Stetcu, Barrett, Navratil, Vary, Phys. Rev. C **71**, 044325 (2005)

Longitudinal-longitudinal distribution function

$$\rho_{LL}(q) = \frac{1}{4Z}\sum_{j\neq i}(1+\tau_z(i))(1+\tau_z(j))\langle g.s.|j_0(q|\vec{r_i}-\vec{r_j}|)|g.s.\rangle$$

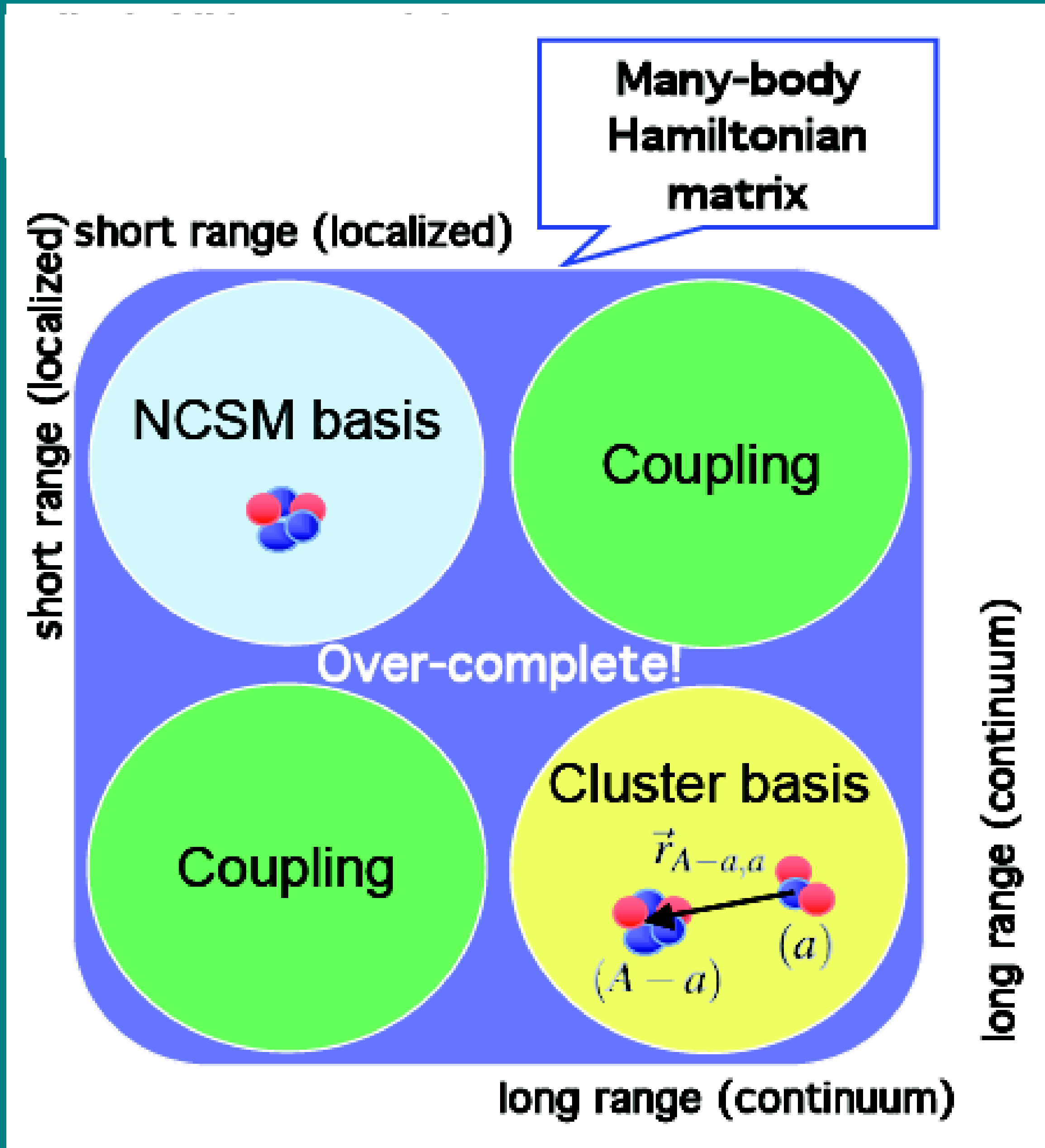


Stetcu, Barrett, Navratil, Vary, nucl-th/0601076

Model space independence at high momentum transfer: good renormalization at the two-body cluster level

SOME REMAINING CHALLENGES

1. Understanding the fundamental interactions among the nucleons in terms of QCD, e.g., NN, NNN, ...
2. Determination of the mean field (the monopole effect).
3. Microscopic calculations of medium- to heavy-mass nuclei:
   a.) How to use the advances for light nuclei to develop techniques for heavier nuclei.
   b.) Building in more correlations among the nucleons in small model spaces, e.g., effective interactions for heavier nuclei.
4. Extensions of these microscopic advances for nuclear structure to nuclear reactions.



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

COLLABORATORS

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Petr Navratil, Lawrence Livermore National Laboratory
James P. Vary, Iowa State University

$$\mathcal{H} = X H X^{-1}$$

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle$$

$$\mathcal{H}(P+Q)|\Psi\rangle = E|\Psi\rangle$$

$$Q|\Psi\rangle = \frac{1}{E-QHQ} QHP|\Psi\rangle$$

$$H_{eff} = \underline{PHP} + PHQ\frac{1}{E-QHQ}QHP$$

$\Rightarrow$ Decoupling condition : $QHP = 0$

Example: Consider the transformation

$$\mathcal{H} = e^{-\omega} H e^{\omega} \text{ with } \omega = Q\omega P$$

then $\mathcal{H} = (1-\omega) H (1+\omega)$, $\omega^2 = \omega^3 = \cdots = 0$

$$Q\mathcal{H}P = 0 = Q(1-\omega)H(1+\omega)P$$
$$= QHP - Q\omega HP + QH\omega P - Q\omega H\omega P$$

And

$$H_{eff} \equiv P\mathcal{H}P = PHP + PH\omega$$

Alternate form for H_{eff} using $Q\omega P = \omega$

$Q\omega P = \omega \Rightarrow$

$$Q\omega P|K\rangle = \omega|K\rangle \equiv Q|K\rangle$$

where $|K\rangle$ is a solution of $H|K\rangle = E|K\rangle$

$$H(P+Q)|K\rangle = E|K\rangle$$

$$H(P+Q\omega P)|K\rangle = E|K\rangle$$

① $P\,H(P+Q\omega P)|K\rangle = E\,P|K\rangle$ → projected state ⇒ not orthogonal

② $(P\omega^{+}Q)\,H(P+Q\omega P)|K\rangle = E\,(P\omega^{+}Q)|K\rangle$

$1+2 \Rightarrow (P+P\omega^{+}Q)\,H(P+Q\omega P)|K\rangle = E(P+P\omega^{+}Q)|K\rangle$

Orthogonal states are given by

$|\Phi\rangle = \sqrt{P+P\omega^{+}Q}\;|K\rangle$ so that

(← $Q\omega P|K\rangle$)

$$\underbrace{\frac{1}{\sqrt{P+P\omega^{+}Q}}(P+P\omega^{+}Q)\,H\,(P+Q\omega P)\frac{1}{\sqrt{P+P\omega^{+}Q\omega P}}}_{H_{eff}}|\Phi\rangle = E|\Phi\rangle$$

Exact solution for matrix elements of ω, i.e., $\langle \alpha_Q | \omega | \alpha_P \rangle$

$$H|K\rangle = E_K|K\rangle$$

E_K is one of the eigen-energies that we want to reproduce. Subset $\underline{\underline{K}}$ of full eigenspace.

$|\alpha_P\rangle$ = basis state in P space

$|\alpha_Q\rangle$ = basis state in Q space

As seen earlier $Q\omega P = \omega \Rightarrow$

$Q\omega P|K\rangle = \omega|K\rangle = Q|K\rangle$ so that

$$\langle \alpha_Q | Q\omega P | K\rangle = \langle \alpha_Q | Q | K\rangle$$

($P = \sum_{\alpha_P} |\alpha_P\rangle\langle\alpha_P|$; $\langle \alpha_Q | Q | K\rangle$: Component of K in the Q space.)

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

Dimension "<u>d</u>" of K and the model space are the <u>same</u>. **Have "d" such equations.**

Invert the $d \times d$ $\langle \alpha_P | K\rangle$ matrix. $\Rightarrow$

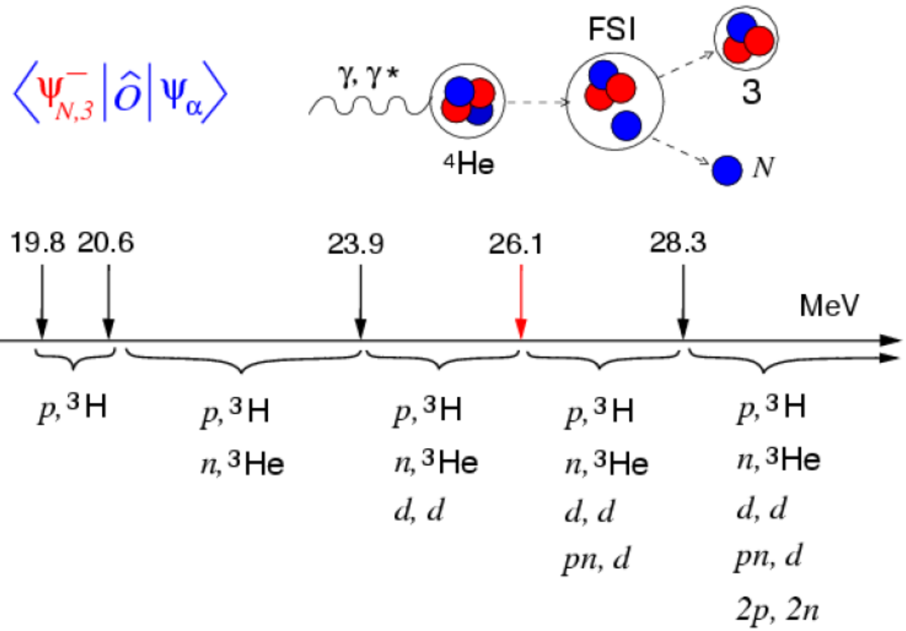
$$\langle \alpha_Q | \omega | \alpha_P\rangle = \sum_{K \in \mathcal{K}} \langle \alpha_Q | K\rangle \overbrace{\langle K | \alpha_P\rangle}^{\text{"inverse"}}$$

Microscopic approach to nuclear reactions

Where is the challenge?

Full and consistent treatment of the FSI also beyond the 3-body breakup threshold

Channels up to the π−production threshold



Lorentz integral transform 101

Efros, Leidemann, Orlandini, Phys. Lett. B338, 130 (1994).

$$R(E) = \sum_{\nu} |\langle \psi_0 | O | \psi_\nu \rangle|^2 \delta(E - E_\nu)$$

LIT approach: calculate the transform of $R(E)$ and then invert:

$$\Phi[R](\sigma) = \int R(E) K(\sigma, E) dE$$

Lorentz kernel:

$$K(\sigma, E) = \frac{1}{(E - \sigma_R)^2 + \sigma_I^2}$$

$$\Phi[R](\sigma) = \langle \phi | \phi \rangle$$

$$(H - \sigma_R - i\sigma_I)|\phi\rangle = O|\psi_0\rangle$$

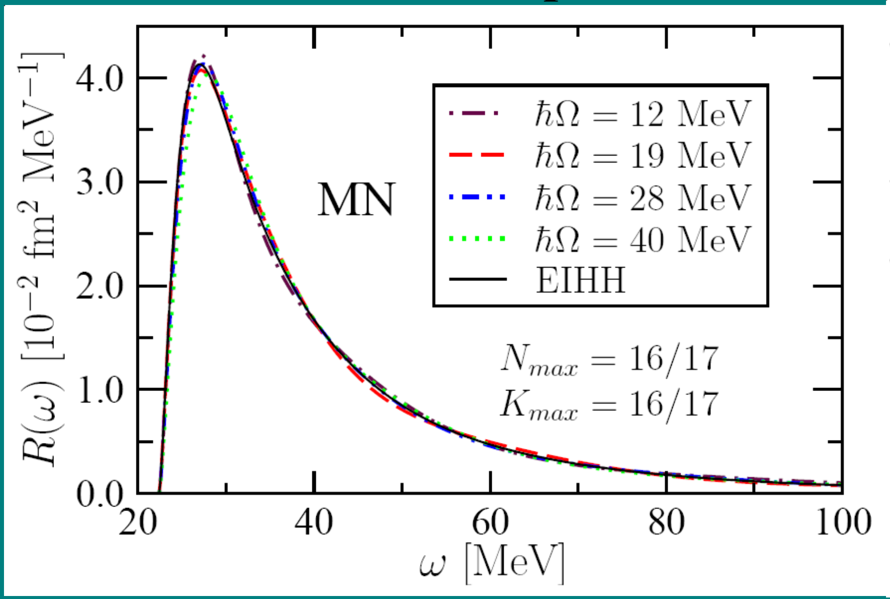
Summary

4

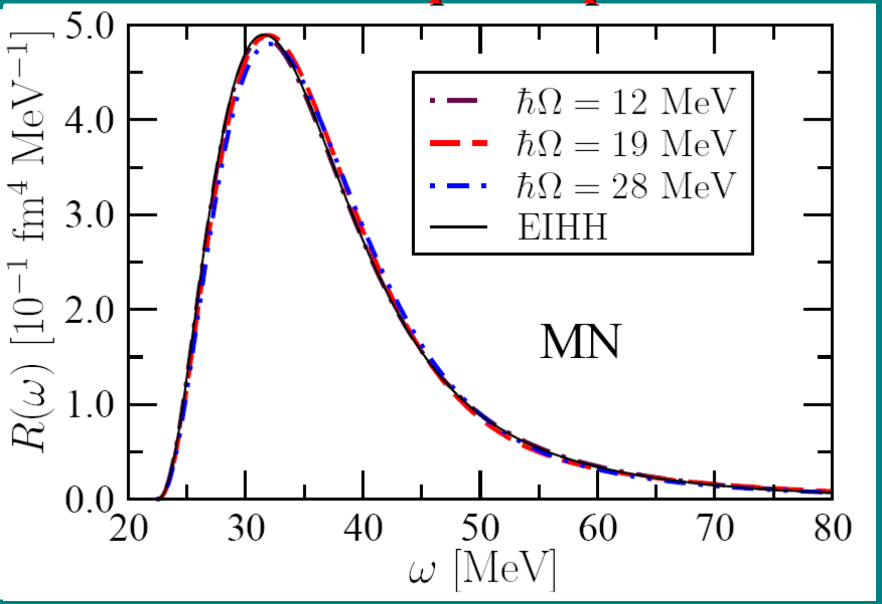
ground-state properties

	E_0 [MeV]	$M_0(\hat{D})$ [fm^2]	$M_0(\hat{Q})$ [fm^4]
EIHH	$-30.779(1)$	$0.7883(1)$	$8.54(1)$
NCSM	$-30.80(5)$	$0.786(6)$	$8.56(14)$

isovector dipole



isoscalar quadrupole



Conclusions

Test calculation of the 4He response functions to the isovector dipole and isoscalar quadrupole excitations by means of the LIT method with both NCSM and EIHH

1. benchmarking calculation with a semirealistic NN interaction: the NCSM is able to obtain results equivalent to the EIHH

2. opens the door for possible LIT investigations of heavier nuclei

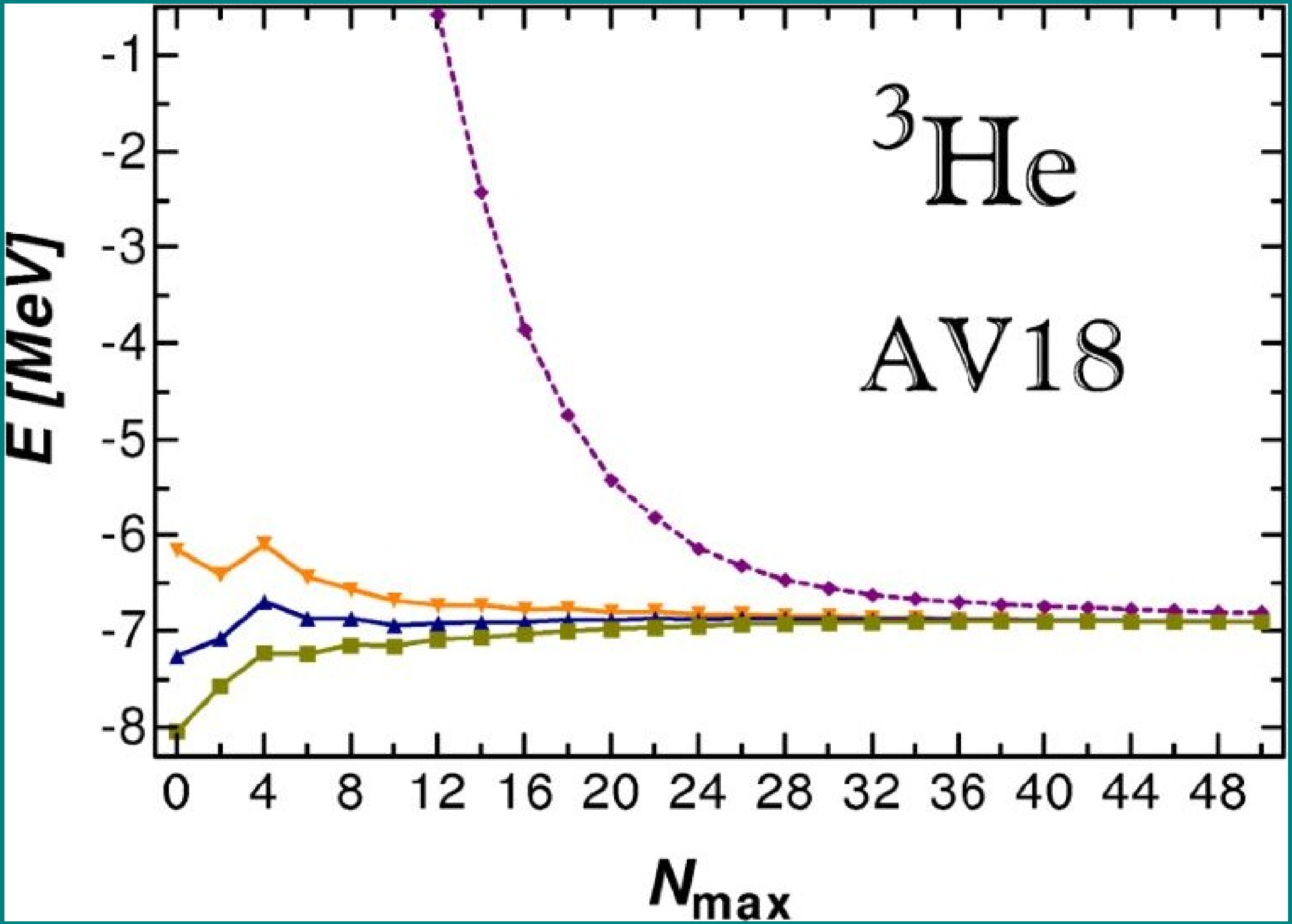
3. however: a more substantial numerical effort will be necessary!!

CONCLUSIONS

1. The NCSM formalism can be used to compare and analyze different theoretical approaches/models for 3N interactions

2. Sufficiently short-ranged physical operators yield accurate results even in very small model spaces.

3. EIHH and NCSM approaches yield the same results for LIT calculations of inclusive cross sections for light nuclei --> can use the NCSM for taking LIT calculations to heavier nuclei.



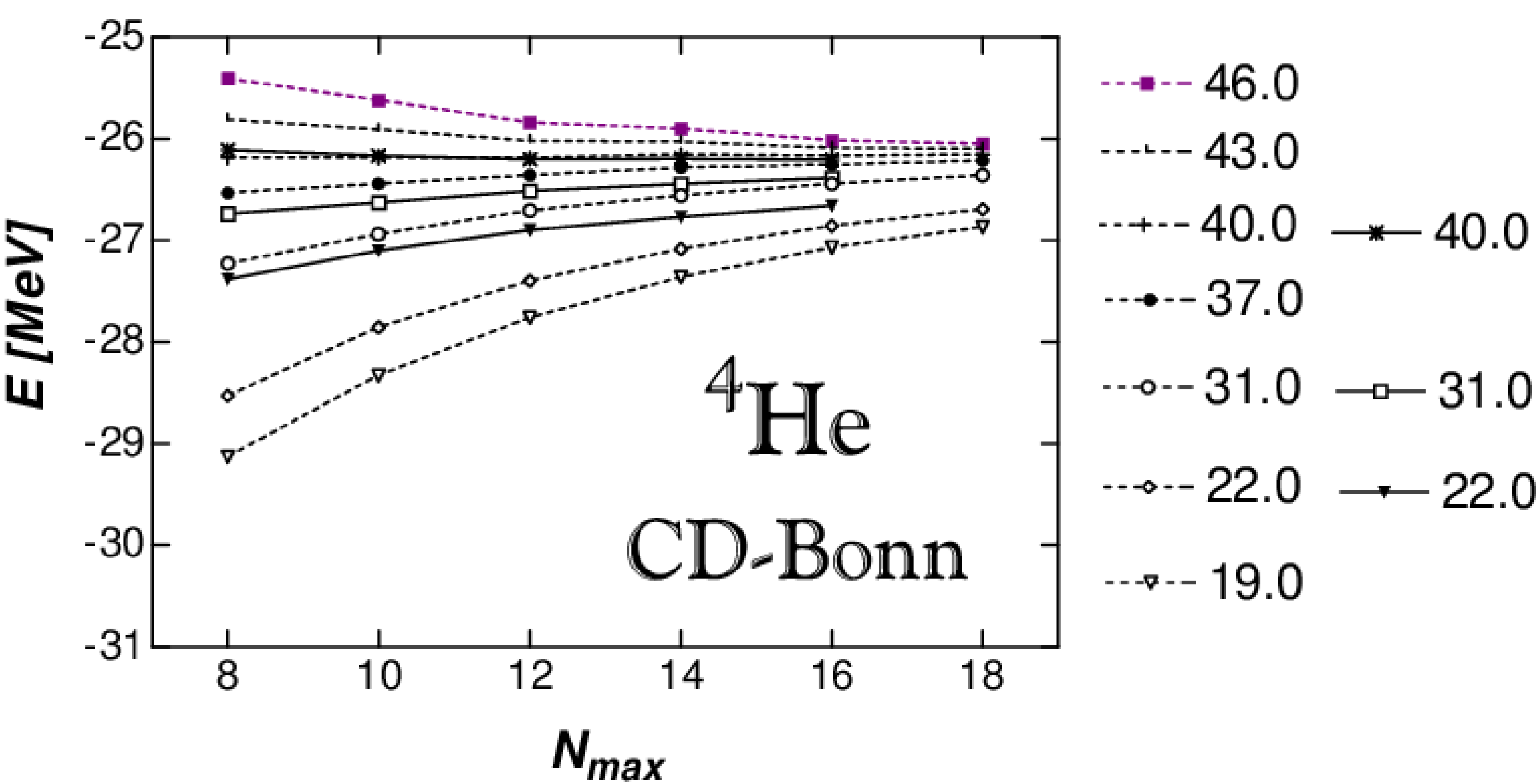
bare

$\hbar\Omega = 32$

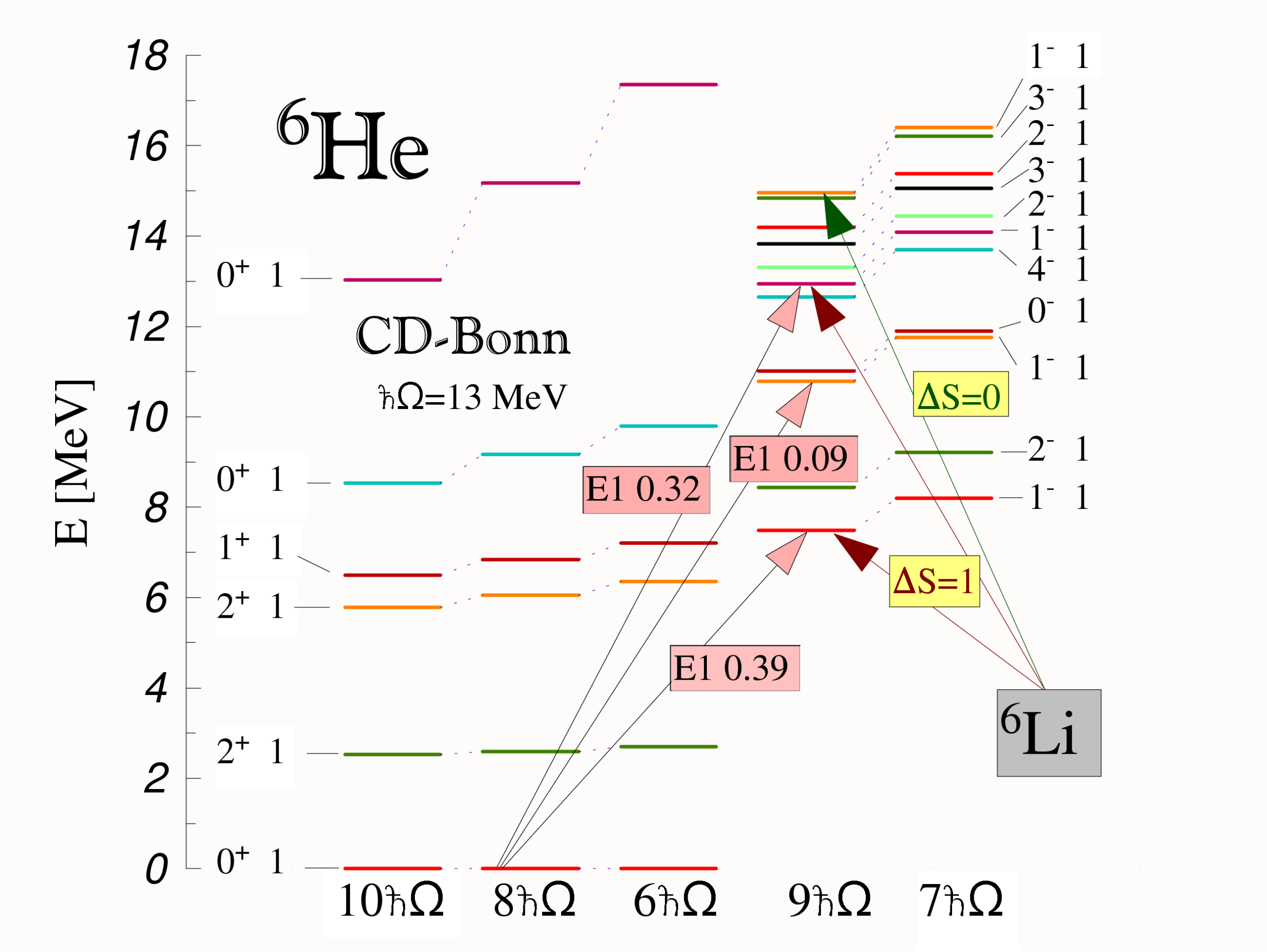
$\hbar\Omega = 28$

$\hbar\Omega = 24$

in MeV

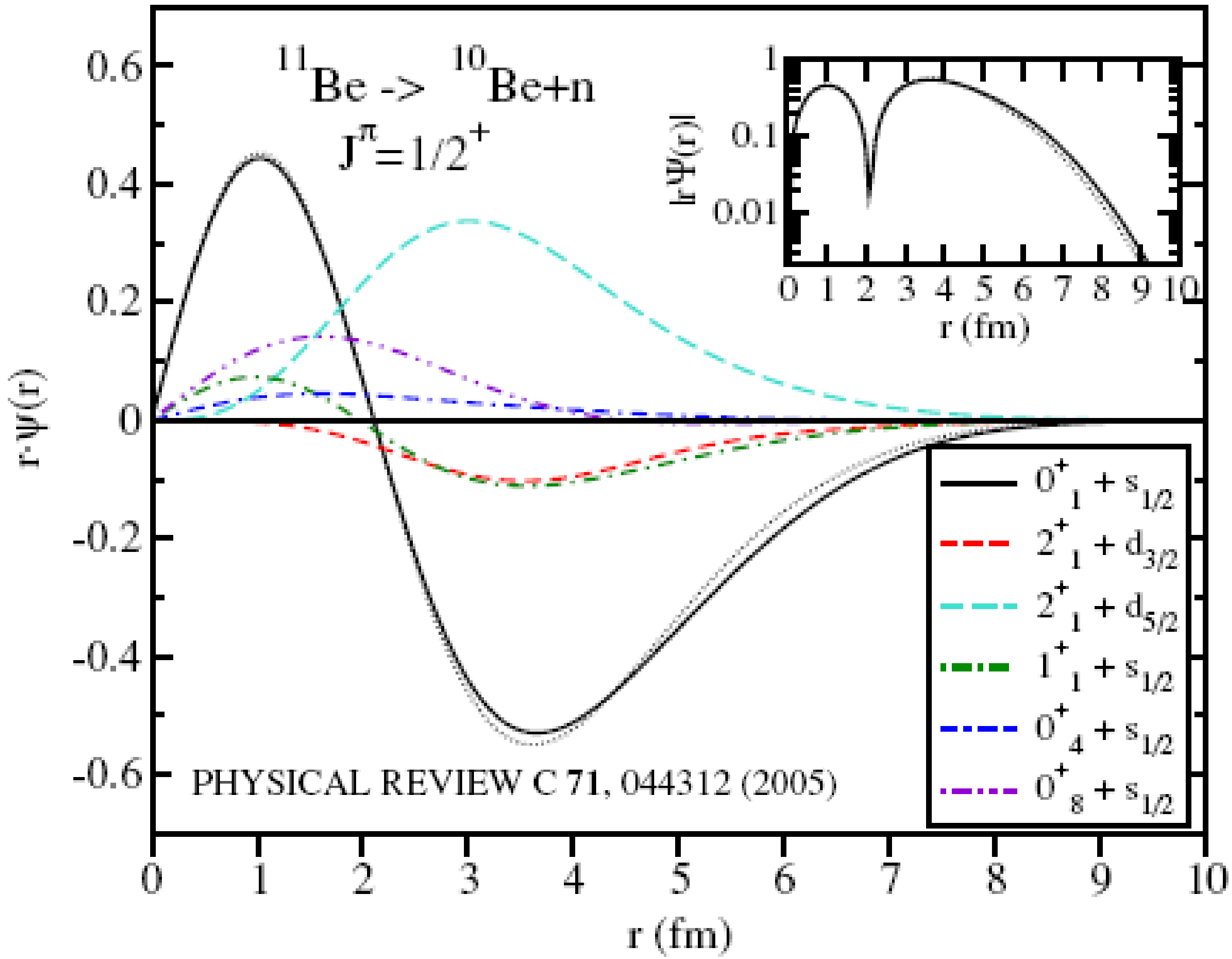


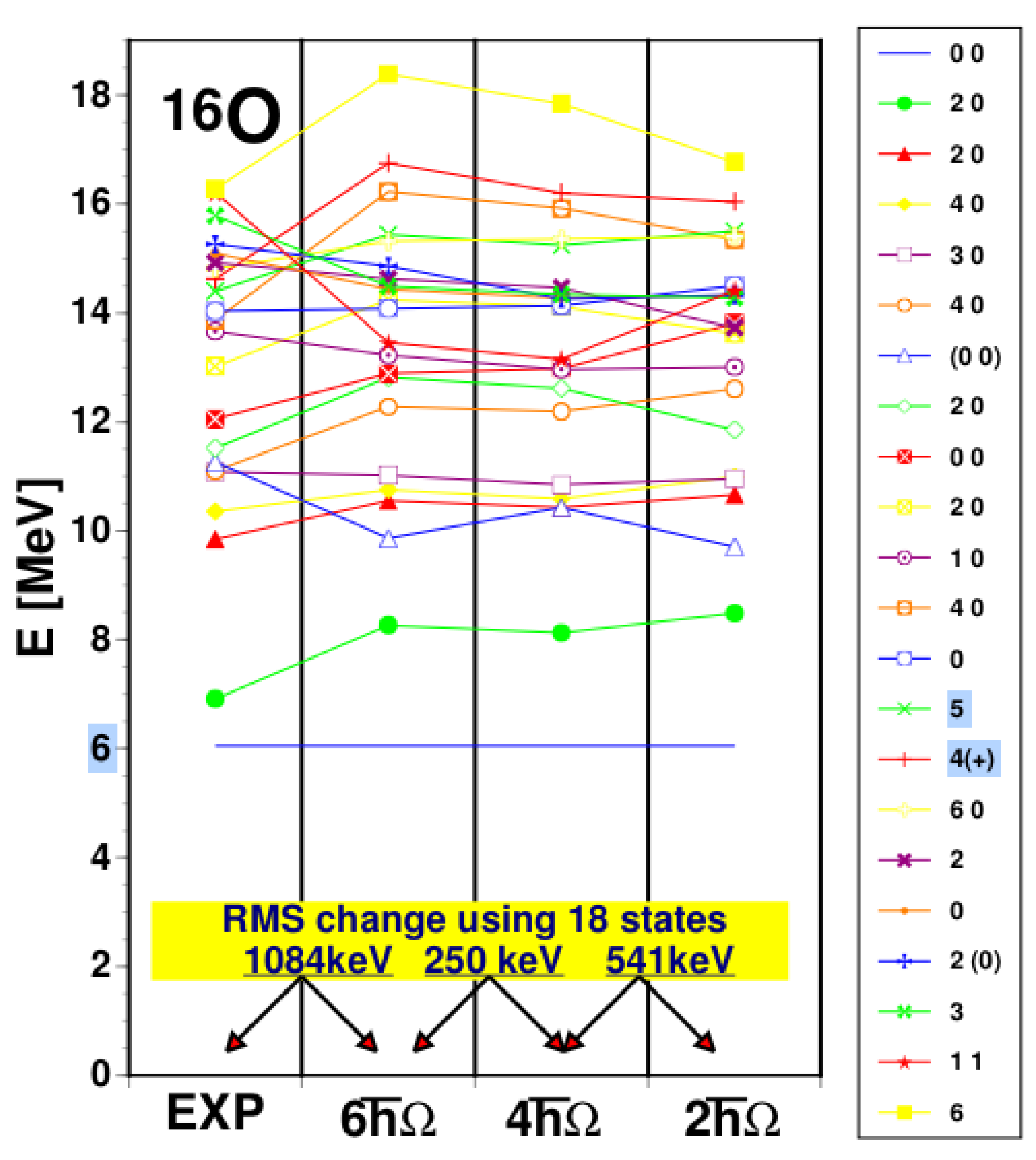
-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N max
4He
CD-Bonn
46.0
43.0
40.0
40.0
37.0
31.0
31.0
22.0
22.0
19.0



P. Navrátil, *et al.*, Phys.Rev. Lett. **87**, 172502 (2001)

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





The spectra are aligned with the experimental first excited 0+ state

J. P. Vary et al., Eur. Phys. J A25, s01, 475 (2005).