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Successes and challenges of the shell model

Calvin W. Johnson

“This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award Number DE-FG02-03ER41272 ”

Celebration for Prof. James Vary, IMP-CAS Lanzhou, June 5, 2023

Congratulations James!

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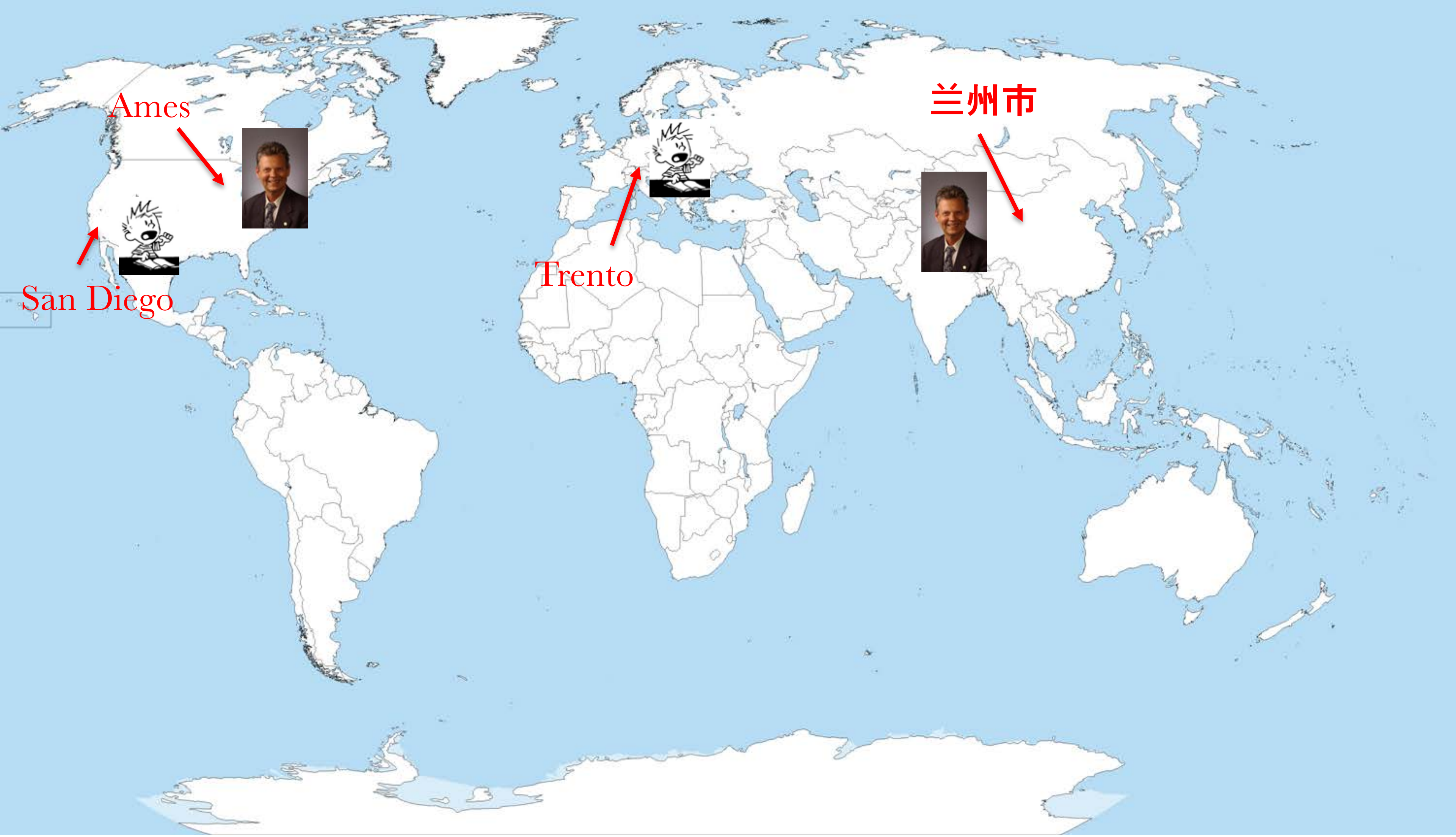
Congratulations James!

Congratulations James!



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There are many approaches to the many-body problem
(I'm going to focus on low-energy nuclear physics)

- Green's function Monte Carlo
- Coupled cluster
- Self-consistent Green's function
- Generator-coordinate/Monte Carlo shell model/ other "beyond mean-field"
- Algebraic methods
- Many-body perturbation theory
- …..
- **Configuration-interaction shell model**

To get the many-body states, we use the matrix formalism (a.k.a *configuration-interaction)*

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle \qquad H_{\alpha\beta} = \langle\alpha|\hat{\mathbf{H}}|\beta\rangle$$

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha} \quad \text{if} \quad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}$$

A brief and incomplete history

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1949: Goeppert-Mayer and Axel, Jensen & Suess show spin-orbit splitting explain magic numbers. Single-particle picture describes many measured magnetic moments. (*Non-interacting shell model*)

1956: Edith Halbert and J. B. French perform early configuration-interaction *(interacting shell model*) calculations.

1965: Cohen-Kurath empirical interaction for **valence** *p*-shell
1977: Whitehead introduces Lanczos method
1980s: **Valence** *sd*-shell calcuations
1990s: V**alence** *pf*-shell calculations

A brief and incomplete history

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c raction (interacting shell model)

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What's all this emphasis on **valence** shell calculations?

1965: Cohen-Kurath empirical interaction for **valence** *p*-shell
1977: Whitehead introduces Lanczos method
1980s: **Valence** *sd*-shell calcuations
1990s: **Valence** *pf*-shell calculations

A brief and incomplete history

What's all this emphasis on **valence** shell calculations?

Empirical valence shell calculations were *very* successful!

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But extending to multi-shell spaces proved challenging!

at's all this
is on **valence**
culations?

Empirical valence shell calculations were *very* successful!

But extending to multi-shell spaces proved challenging!

Multi-shell calculations *starting* from valence space empirical interactions tended to go awry

Empirical valence shell calculations were *very* successful!

A brief and incomplete history

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1970 Barrett and Kirson, 1972 Schucan and Weidenmuller:
intruder states can cause perturbative expansions
to ultimately diverge.

This in particular applies to particle-hole states.

This makes expanding beyond the valence space problematic,
and **almost** kills the field (except for a stubborn few) for
twenty years.

A brief and incomplete history

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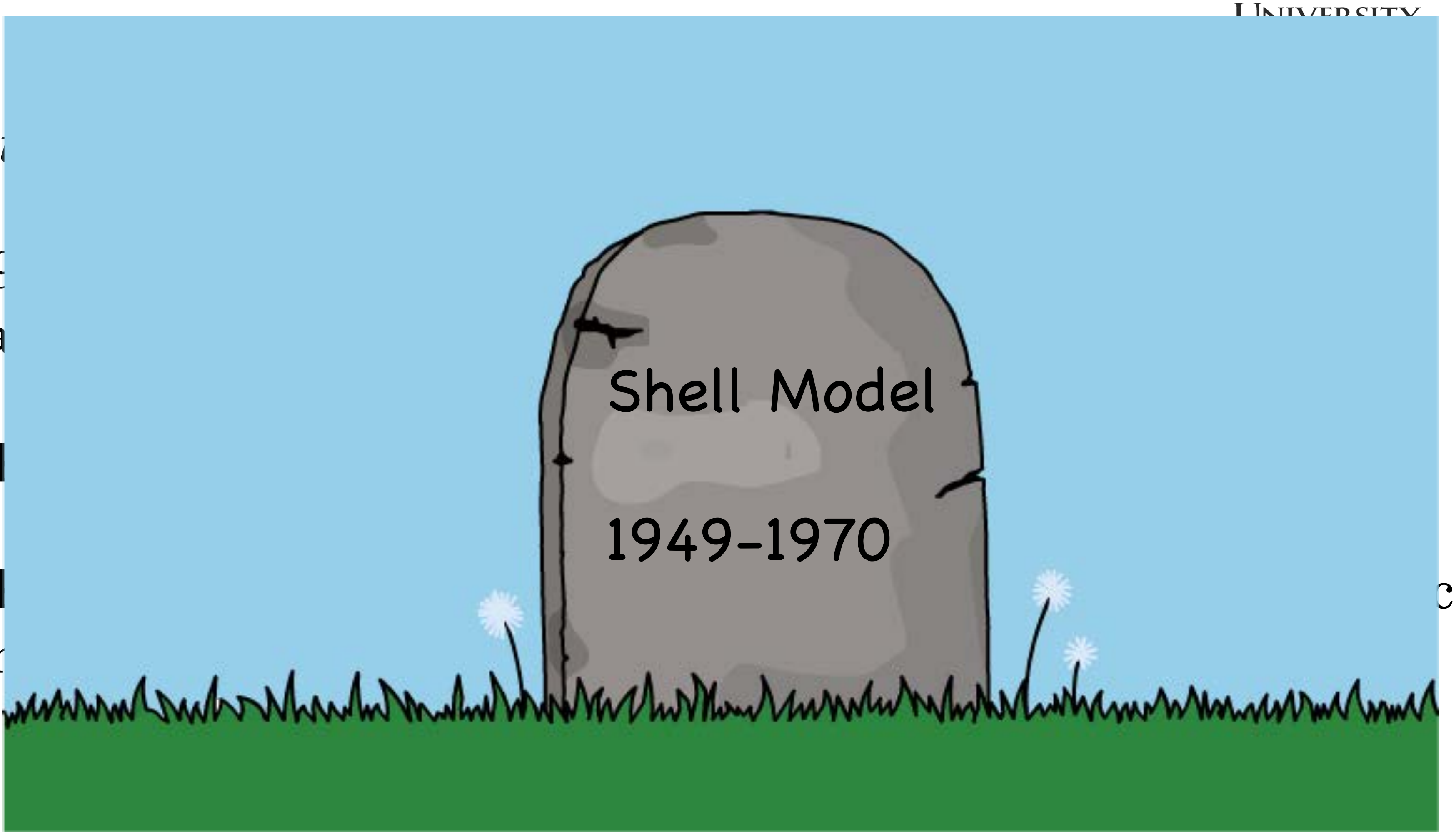

A brief and incomplete history

1991-1993: Barrett and Vary introduce the **no-core shell model** (cf. PRC **48**, 1083 (1993))
Without a core, there is no ”particle-hole” expansion.

Around this same time high-precision phase shift data from NN scattering became available.

Fitted to this data, the Argonne potential showed one could reproduce nuclear data.

Then chiral EFT gave a systematic way to characterize nuclear forces

The field lurches back to life!

A brief and incomplete history

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The field lurches back to life!


alamy stock photo

Modern many-body calculations

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No-core shell model: in harmonic oscillator basis, “all” particles active (up to N_{max} h.o. excitation quanta), with high-precision interaction (e.g. chiral EFT, Daejeon16, etc.) fit to *few-body* data

e.g. *p*-shell nuclides up to N_{max} = 10 … 22

Ab initio/ “No-core shell model”: take to infinite limit

Two parameters: h.o. basis frequency Ω
and model space cutoff N_{max}

Naïve expectation: take N_{max} -> infinity
Converged results independent of Ω

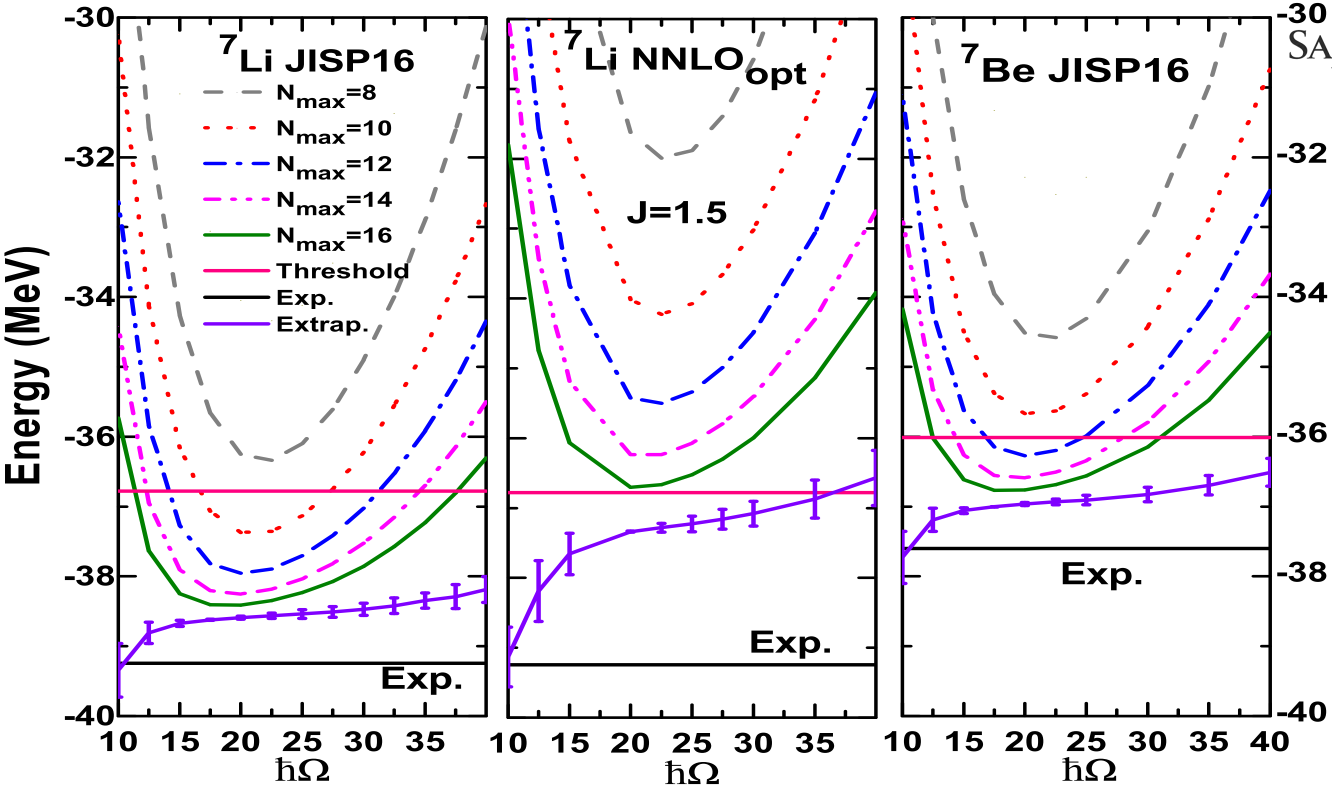


FIG. 1. (Color online) The energy of the ground state (J=$\frac{3}{2}$) for ^{7}Be and ^{7}Li with the JISP16 and NNLO$_{\text{opt}}$ interactions as a function of HO energy. In this figure and the following figures, for ^{7}Li and ^{7}Be, the $N_{\max}$ value ranges from 8 up to 16. The increment of $N_{\max}$ is 2. Extrapolated ground state energies are shown in purple with uncertainties depicted as vertical bars.

From Heng, Vary, Maris: arXiv:1602.00156

Extrapolation via assumed exponential $E(N_{\max}) = E(\infty) + a\exp(-cN_{\max})$

Natural orbitals

Natural orbitals arise from diagonalizing the (g.s.) one-body density matrix. Widely used in quantum chemistry.

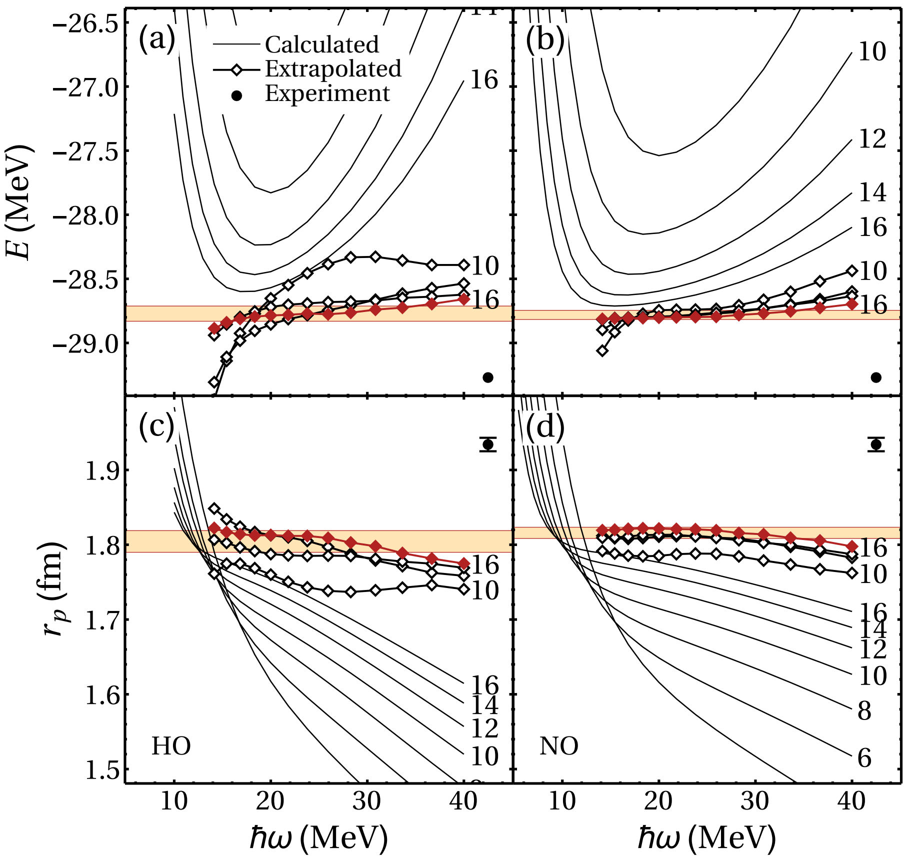
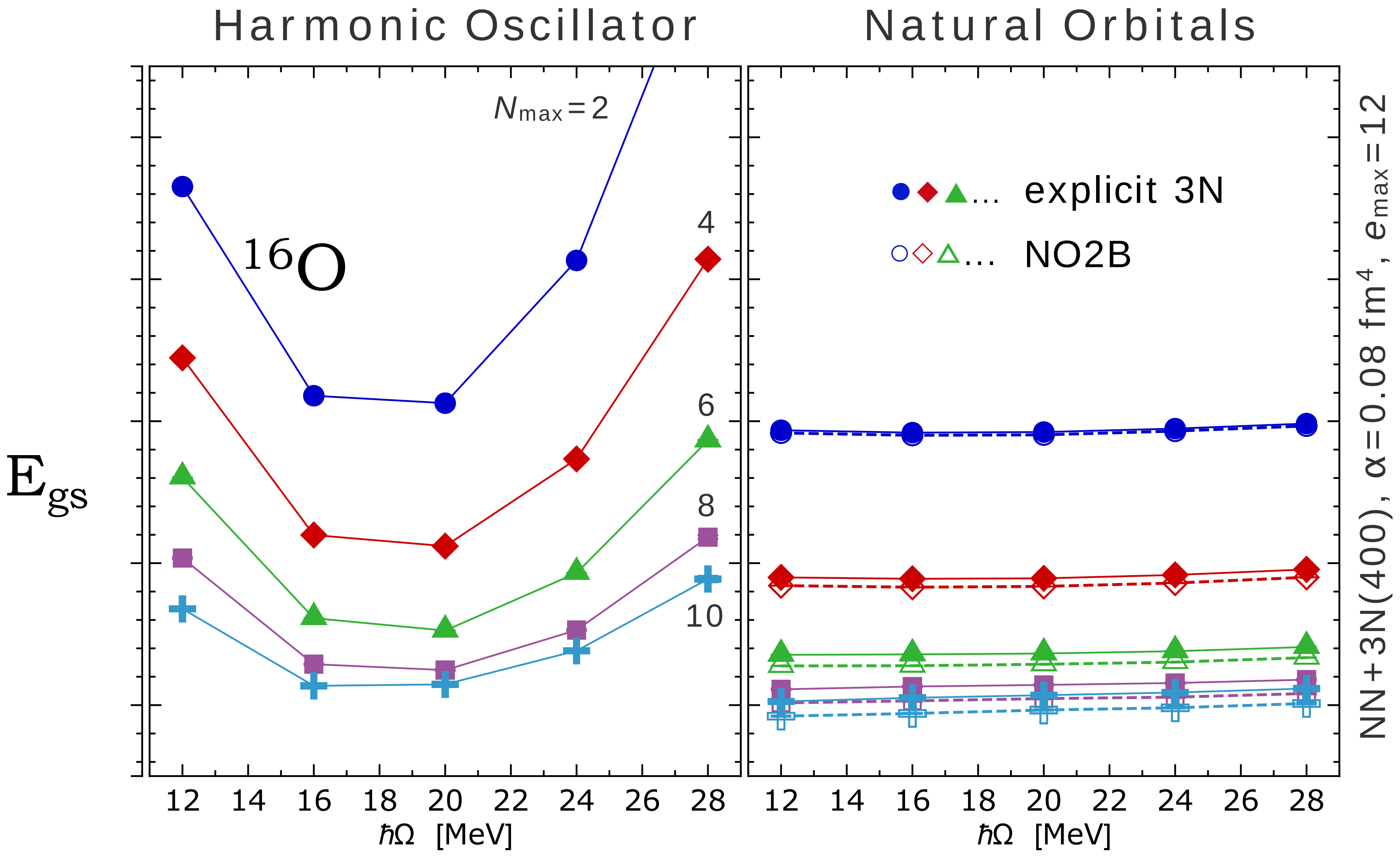


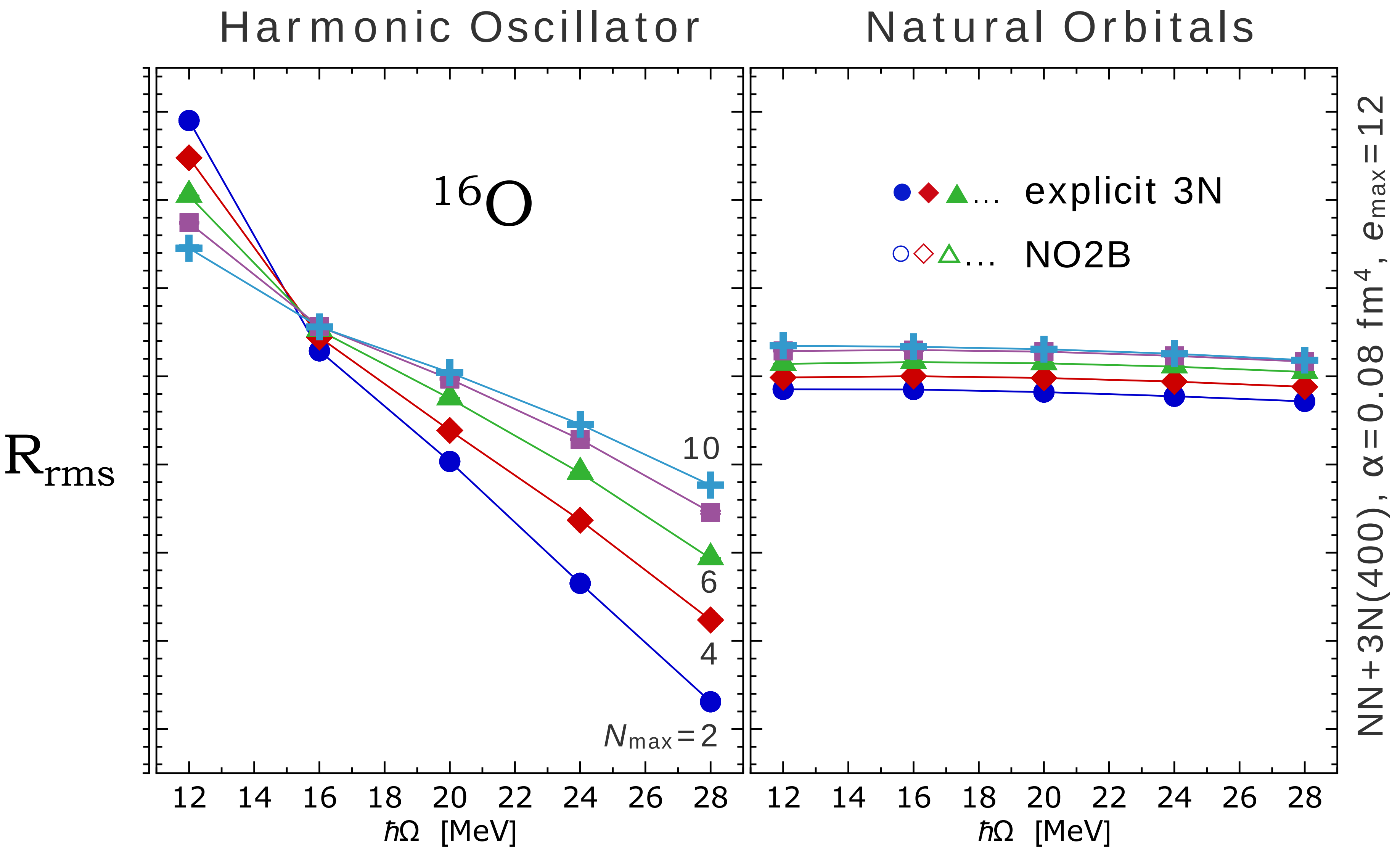
FIG. 4: Infrared basis extrapolations for the ^{6}He ground state energy (top) and point proton radius (bottom), based on calculations in the harmonic oscillator basis (left) and natural orbital basis (right). The extrapolations (diamonds) are shown along with the underlying calculated results (plain lines) as functions of $\hbar\omega$ at fixed $N_{\max}$ (as indicated). Experimental values (circles) are shown with uncertainties. The shaded bands reflect the mean values and standard deviations of the extrapolated results, at the highest $N_{\max}$, over the $\hbar\omega$ range considered.

From Constantinou *et al*,

arXiv:1605.04976



From R. Roth, talk at TRIUMF, Feb 2018



From R. Roth, talk at TRIUMF, Feb 2018

Some highlight achievements:

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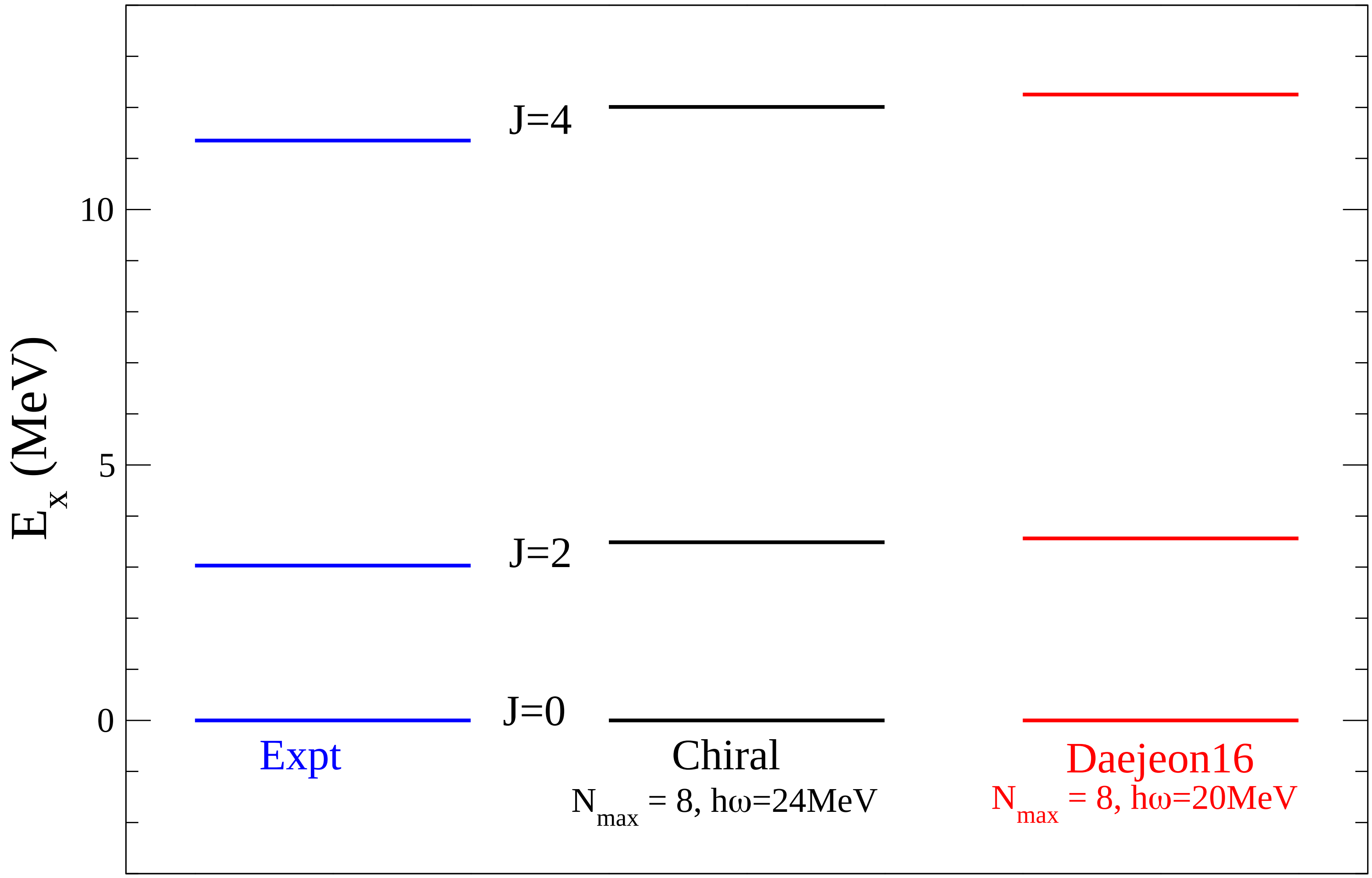
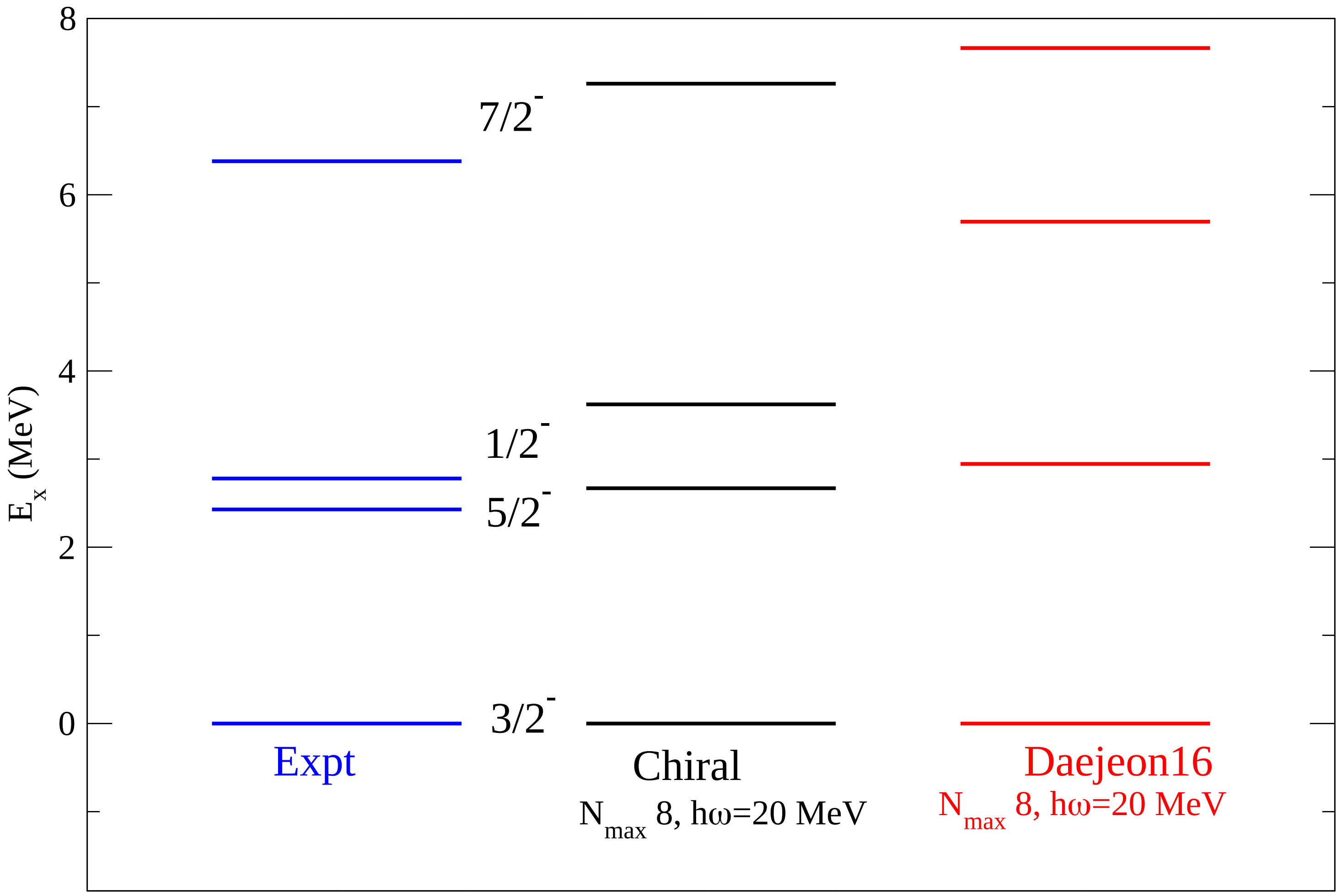
Some highlight achievements:

- Can get spectra of light nuclei ”from first principles”

^{8}Be


E$_x$ (MeV)
10
5
0
J=4
J=2
J=0
Expt
Chiral
N$_{max}$ = 8, hω=24MeV
Daejeon16
N$_{max}$ = 8, hω=20MeV

^{9}Be


8
6
4
2
0
E_x (MeV)
7/2$^-$
1/2$^-$
5/2$^-$
3/2$^-$
Expt
Chiral
N_{max} 8, hω=20 MeV
Daejeon16
N_{max} 8, hω=20 MeV

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Some highlight achievements:

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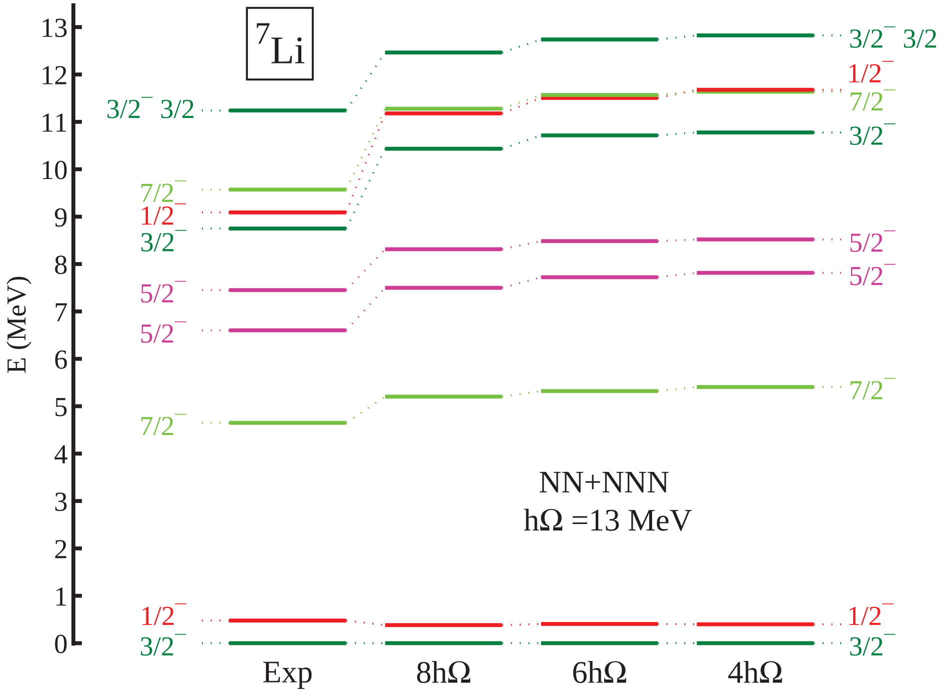
PHYSICAL REVIEW C **87**, 014327 (2013)

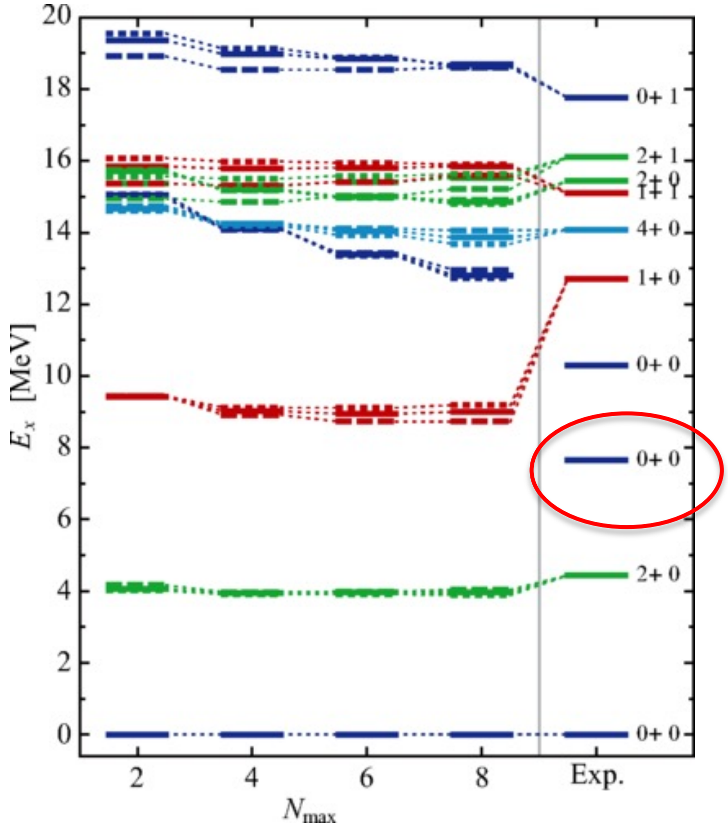


Maris , Vary, Navratil
PRC **87**, 014327 (2013)

chiral 2+3 body forces

Some highlight achievements:

- Can get spectra of light nuclei ”from first principles”



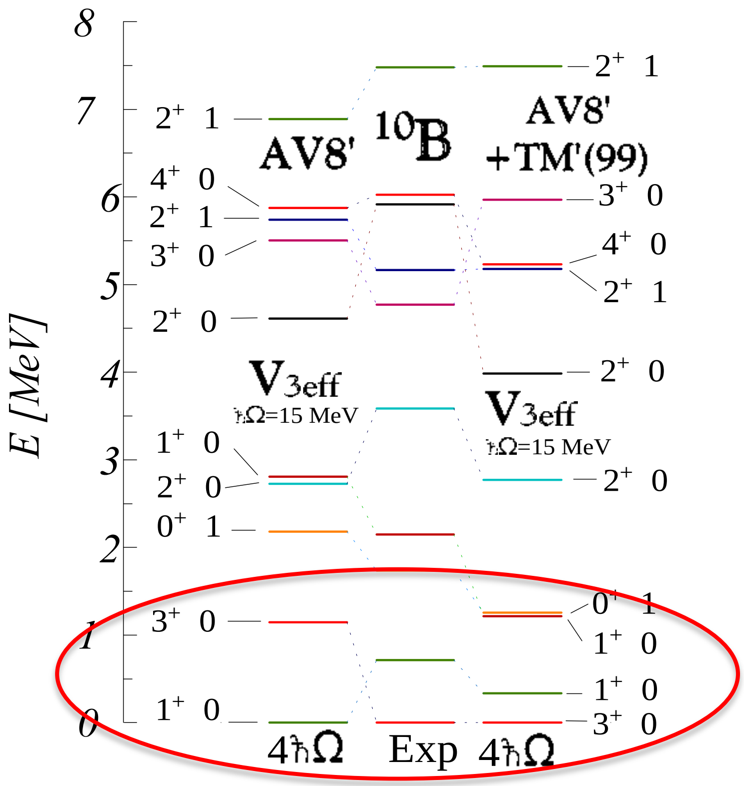
Hoyle state

Maris *et al* PRC **90**, 014314 (2014)

^{12}C with chiral 2+3 body forces

Some highlight achievements:

- Can get spectra of light nuclei ”from first principles”



Navratil and Ormand, PRC **68**, 034305 (2003)

^{10}B. with 2+3 body forces

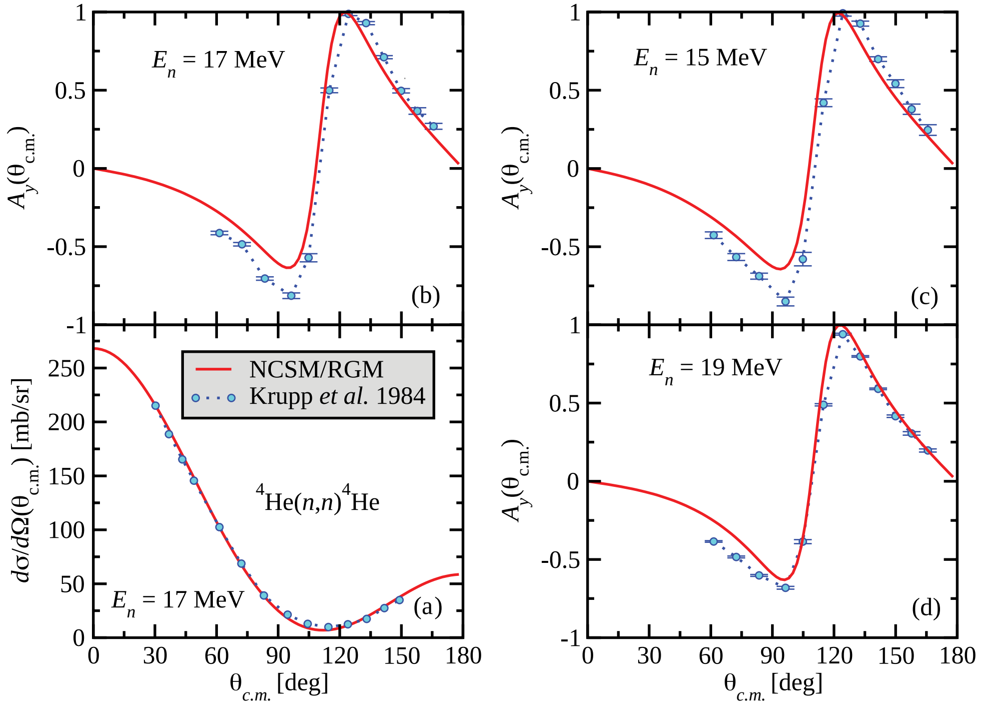
Here 3-body needed to get correct ordering of spectra

Some highlight achievements:

- Can compute anomalously long lifetime of ^{14}C from first principles: Maris *et al*, PRL **106** 202502 (2011) (requires 3-body forces)

Some highlight achievements:

- Can compute scattering/reactions from first principles



Navratil, Roth, Quaglioni
PRC **82**, 034609 (2010)

FIG. 5. (Color online) Calculated n-^{4}He differential cross section for neutron laboratory energy of (a) $E_n = 17$ MeV, and analyzing power for (b) $E_n = 17$, (c) 15, and (d) 19 MeV compared to experimental data from Ref. [36]. The NCSM/RGM results include the ^{4}He ground state and the first 0^+0 excited state and were obtained by using the SRG-N^{3}LO NN potential with $\Lambda = 2.02$ fm^{-1} for an HO frequency $\hbar\Omega = 20$ MeV and basis space size $N_{\max} = 17$.

Some highlight achievements:

- Can compute scattering/reactions from first principles

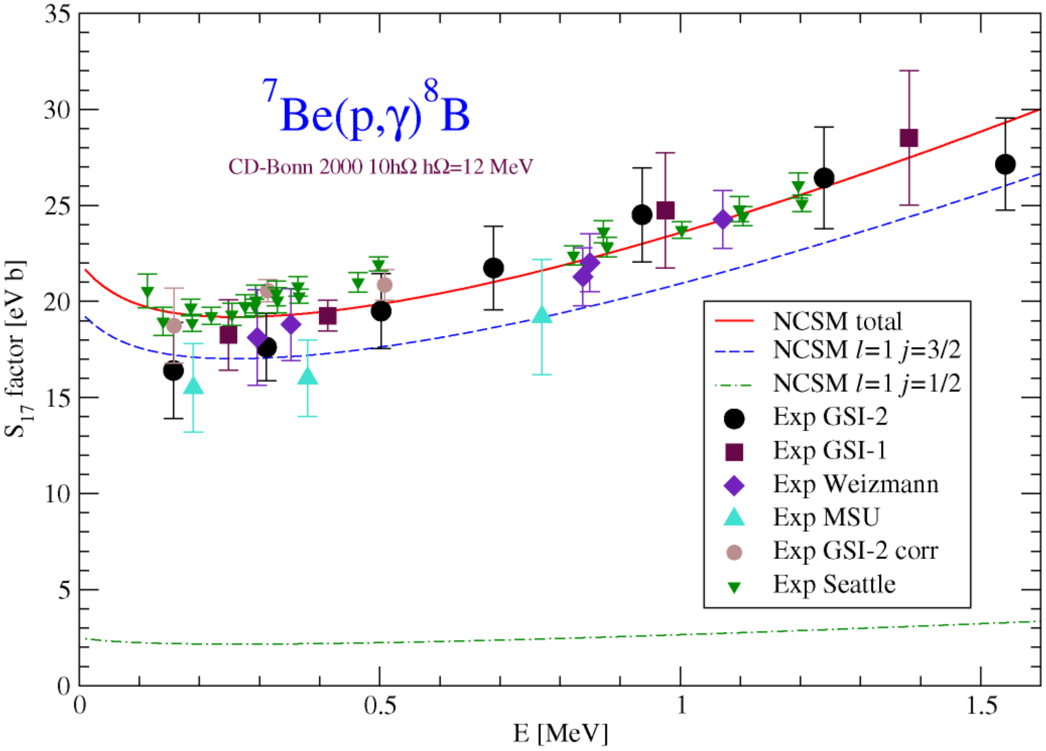
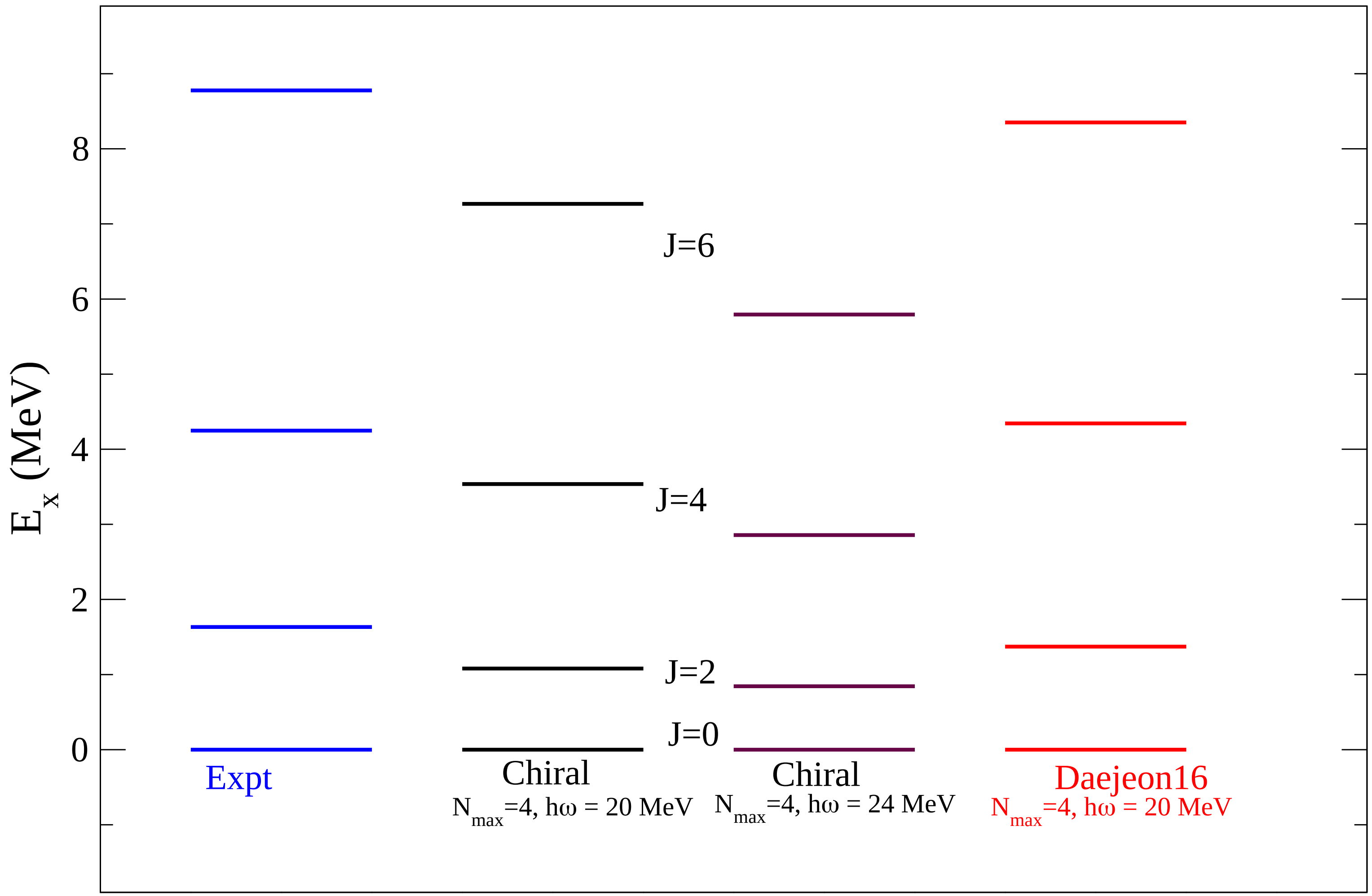


Fig. 3. The ^{7}Be(p, γ)^{8}B S-factor obtained using the NCSM cluster form factors with corrected asymptotics by the WS solution fit. Experimental values are from Refs. [6,7,9].

Navratil, Bertulani, Caurier
Phys Lett B **634**, 191 (2006)

^{20}Ne


E$_x$ (MeV)
0
2
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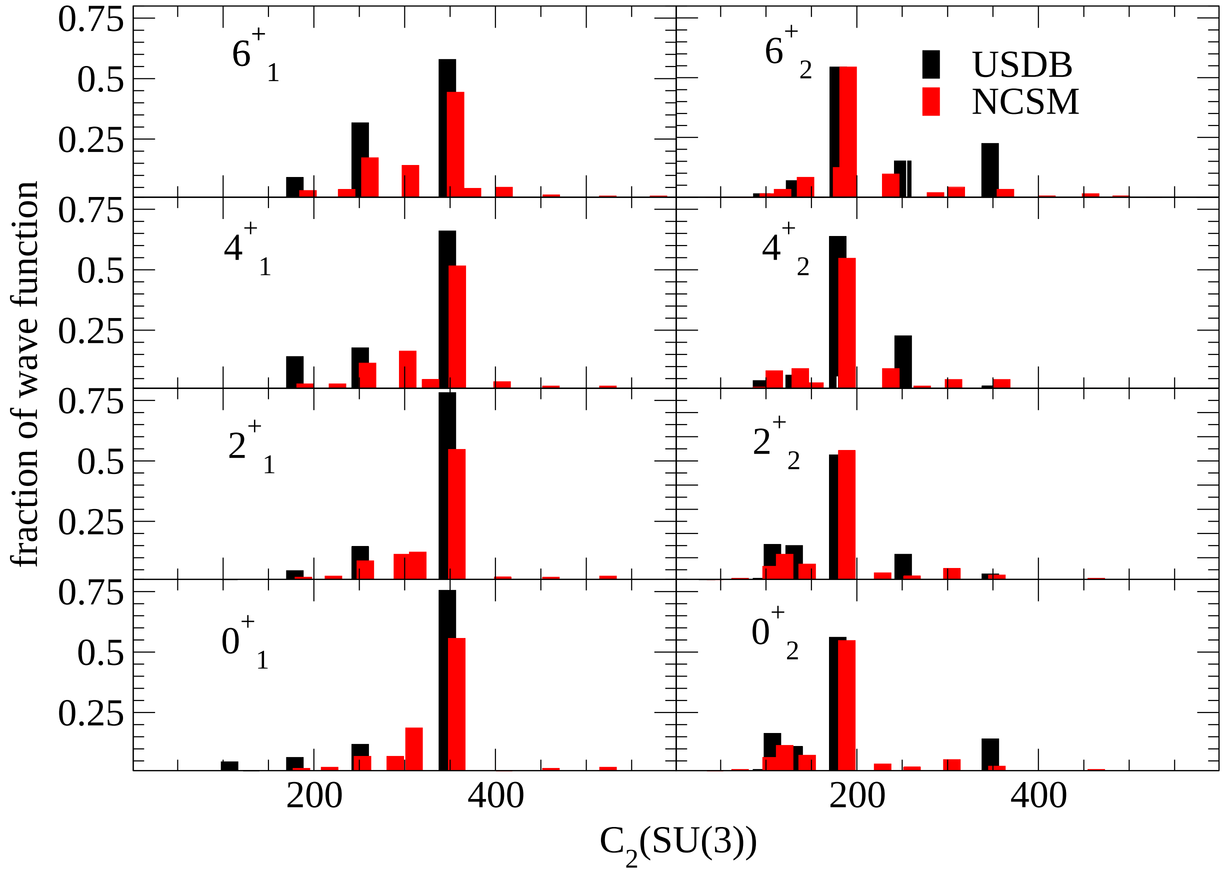
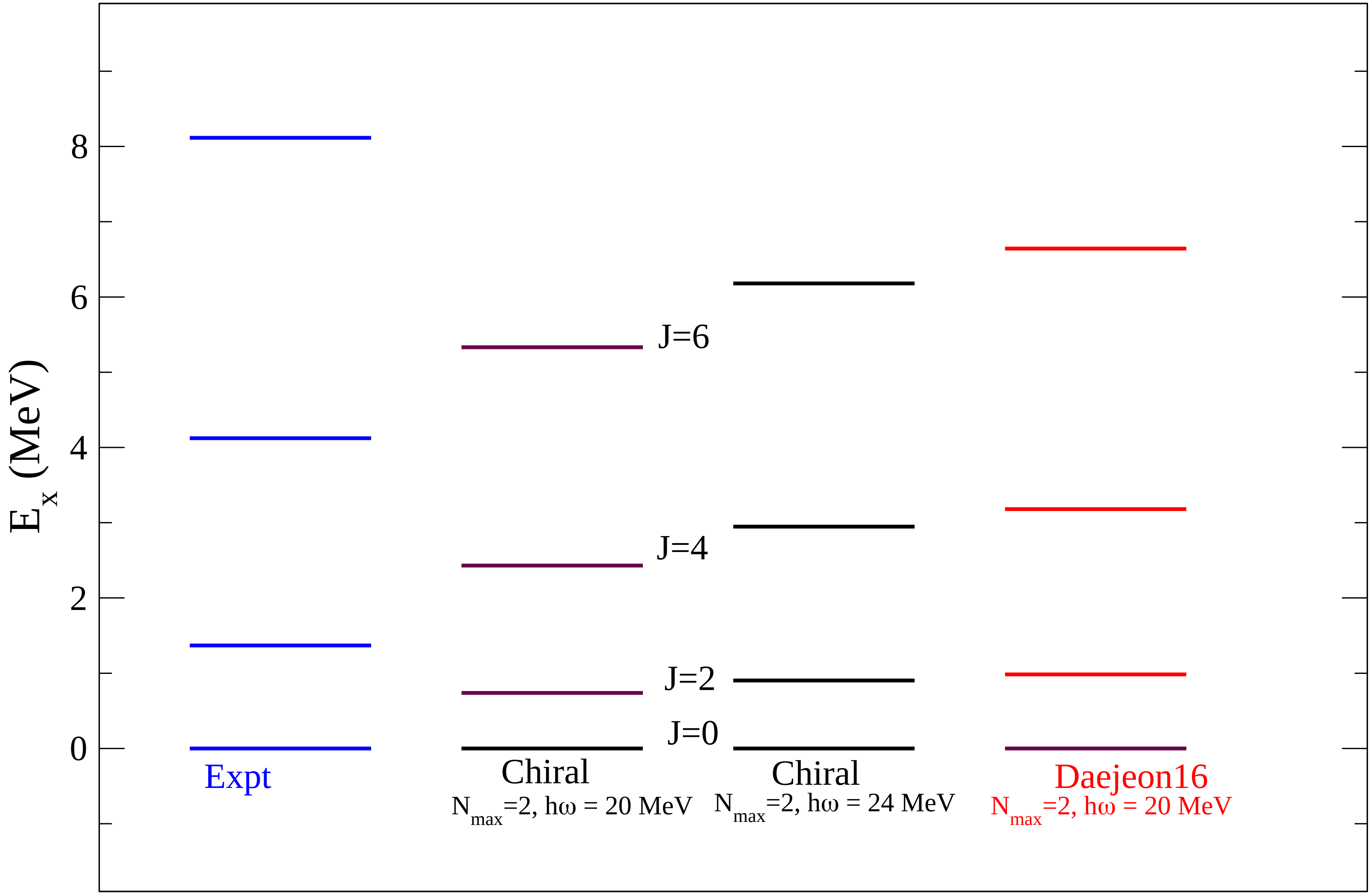
Chiral
N$_{max}$=4, hω = 20 MeV
Chiral
N$_{max}$=4, hω = 24 MeV
Daejeon16
N$_{max}$=4, hω = 20 MeV

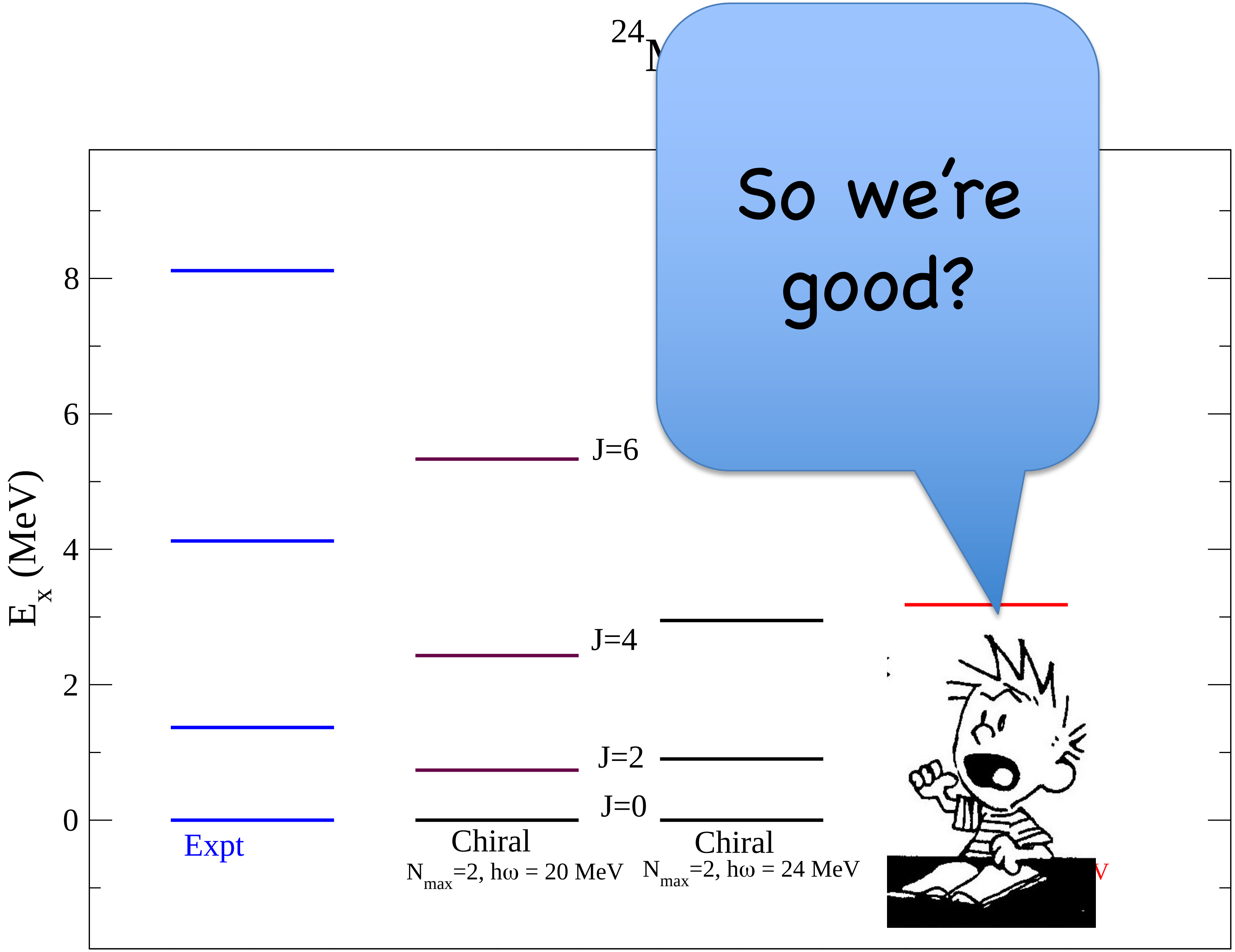
^{20}Ne

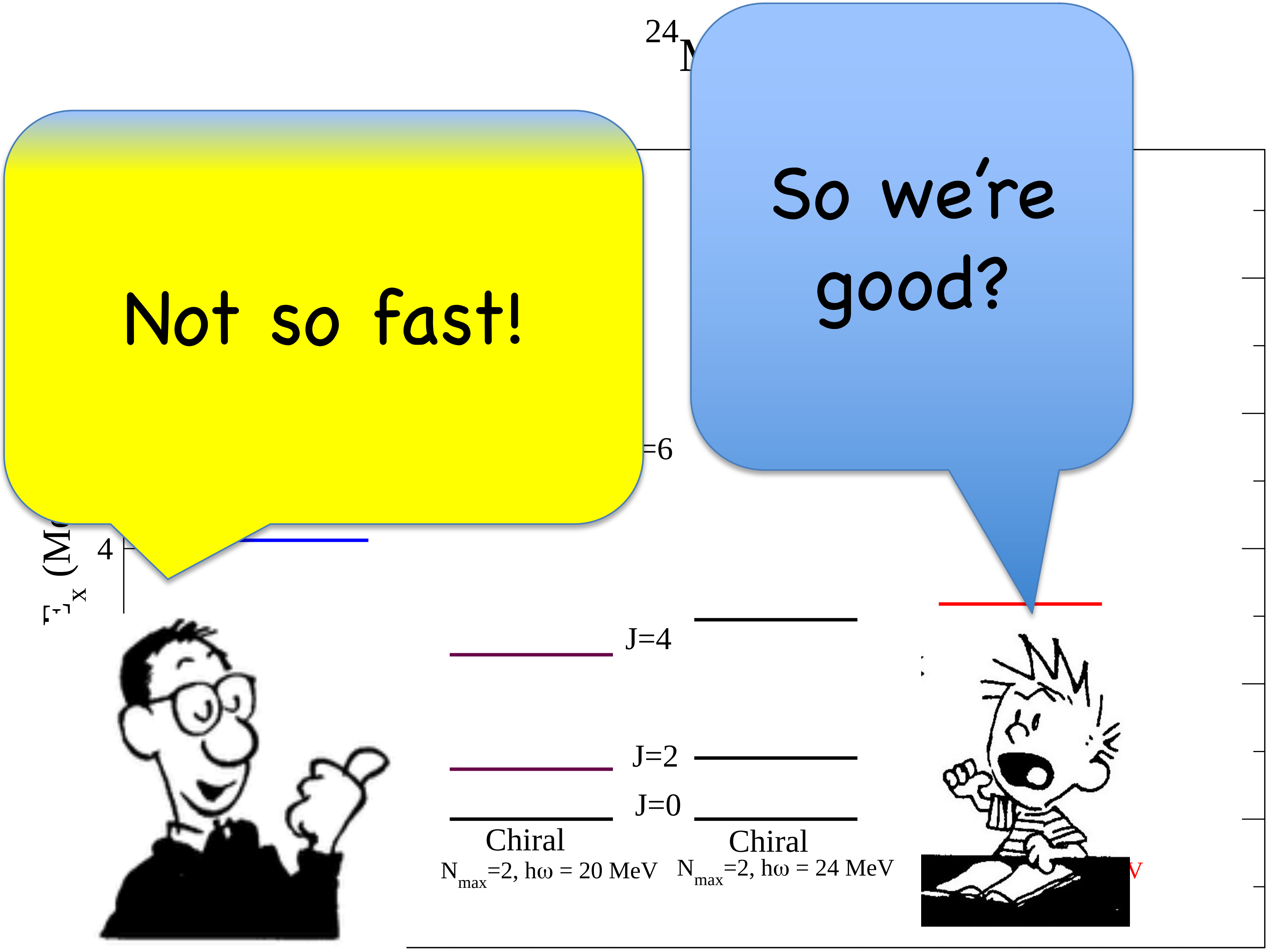


By looking at the group-theoretical decomposition, we can even show that the valence-space empirical and *ab initio* multi-shell wave functions have similar structure!

^{24}Mg

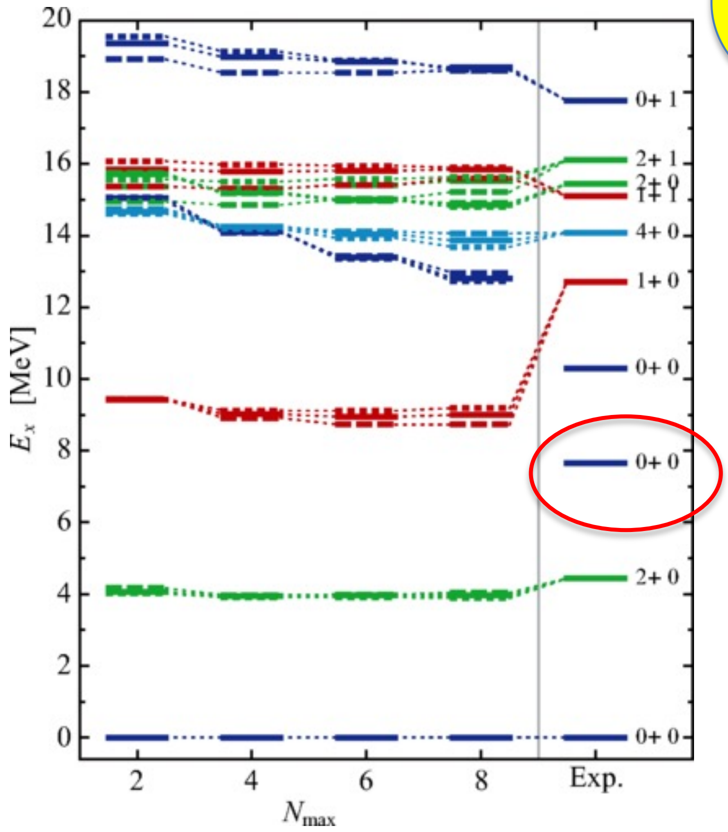

E_x (MeV)
8
6
4
2
0
J=6
J=4
J=2
J=0
Expt
Chiral
N_{max}=2, hω = 20 MeV
Chiral
N_{max}=2, hω = 24 MeV
Daejeon16
N_{max}=2, hω = 20 MeV


^{24}M
So we're good?
E_x (MeV)
0
2
4
6
8
J=0
J=2
J=4
J=6
Expt
Chiral
N_{max}=2, hω = 20 MeV
Chiral
N_{max}=2, hω = 24 MeV
V


Not so fast!
So we're good?
24
M
=6
4
(Me
E_x
J=4
J=2
J=0
Chiral
N_max=2, hω = 20 MeV
Chiral
N_max=2, hω = 24 MeV
V

Maris *et al* PRC **90**, 014314 (2014)

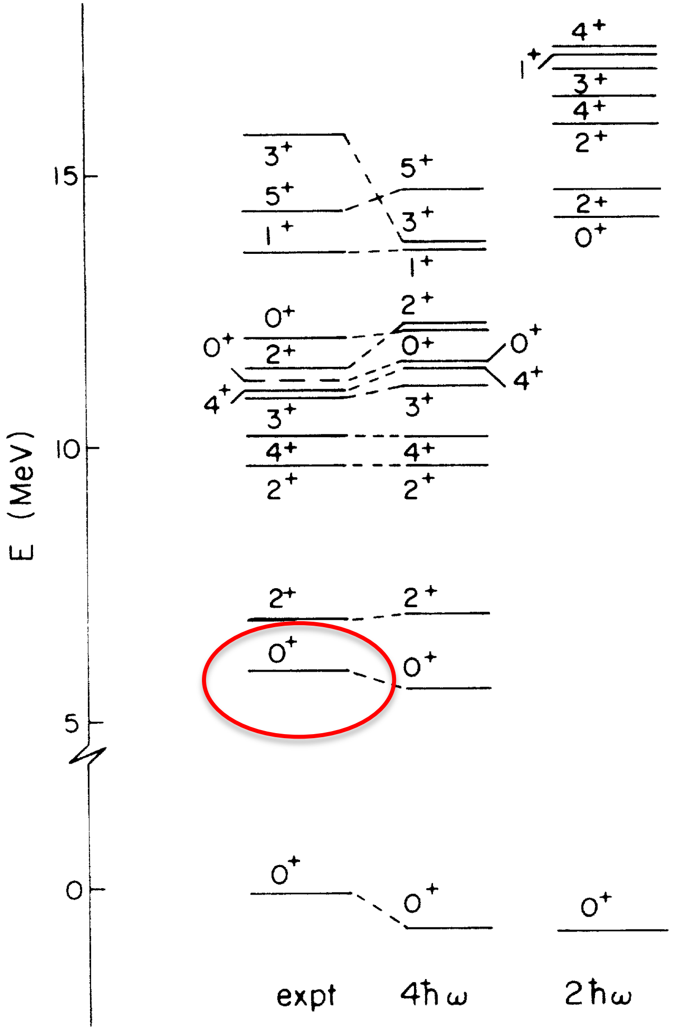
^{12}C with chiral 2+3 body forces



Hoyle state

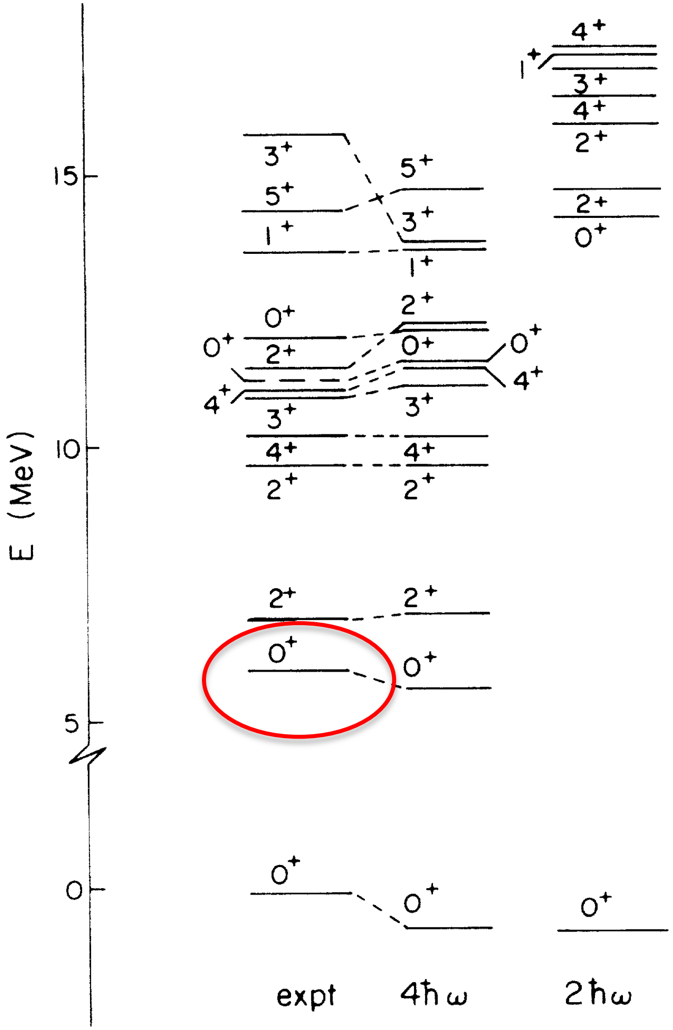
The Hoyle state in ^{12}C is a problem!

Haxton and Johnson, PRL **65**, 1325 (1990)



There's a similar state in ^{16}O

Haxton and Johnson, PRL **65**, 1325 (1990)

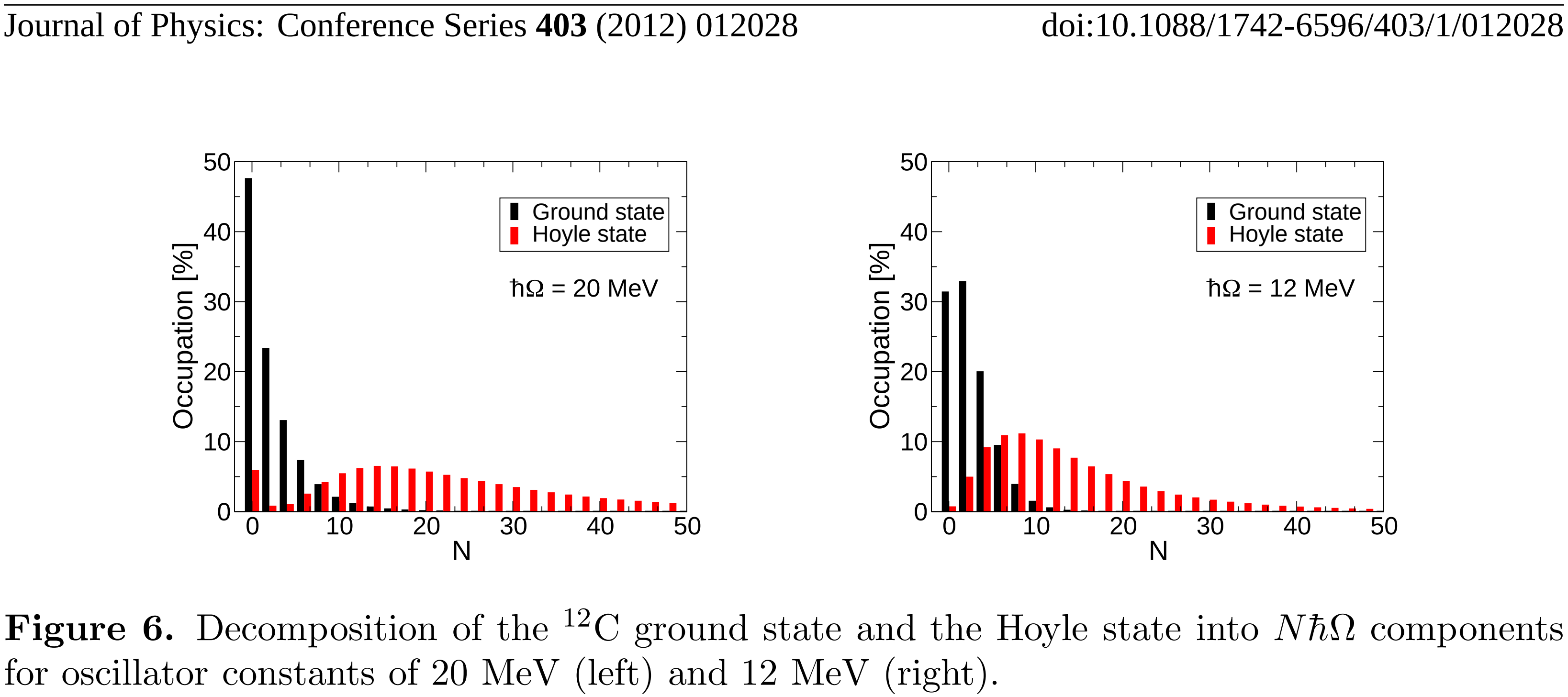


There's a similar state in ^{16}O

One can think of these as alpha-cluster states

These cluster states are not easy to reproduce in the NCSM.
They may require as much as $30h\omega$ excitations in a h.o. basis (T. Neff), yet they appear low in the spectrum

T. Neff, J. Phys. Conf. Ser. **403** 012028 (2012)

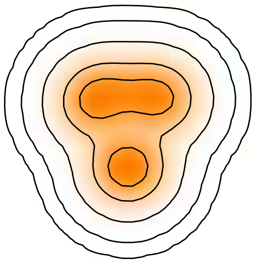


Journal of Physics: Conference Series **403** (2012) 012028 doi:10.1088/1742-6596/403/1/012028

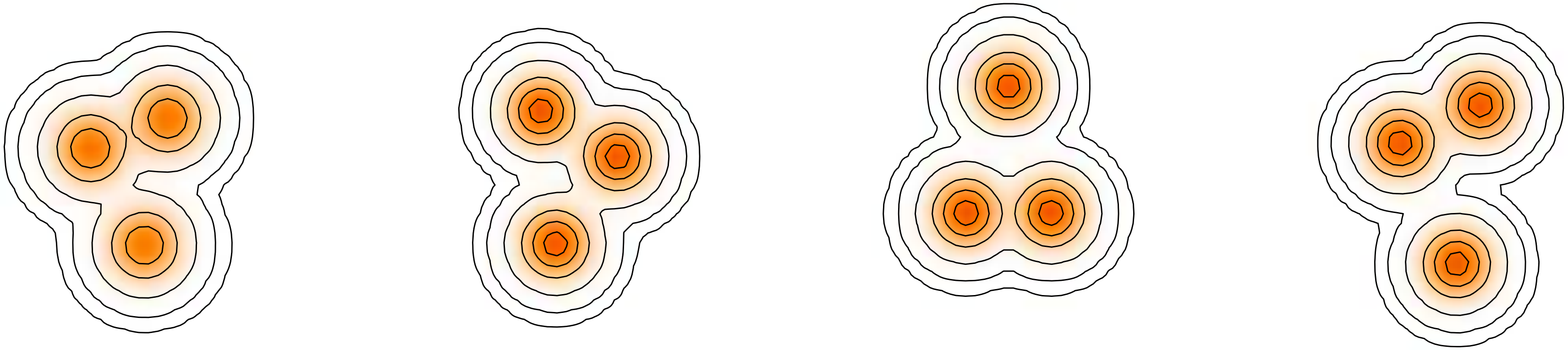
Figure 6. Decomposition of the ^{12}C ground state and the Hoyle state into $N\hbar\Omega$ components for oscillator constants of 20 MeV (left) and 12 MeV (right).

Fermionic molecular dynamics calculation with Argonne V18 potential

T. Neff, J. Phys. Conf. Ser. **403** 012028 (2012)



See also: S. Shen, D. Lee, et al, Nat. Commun. 14 (2023) 2777 (arXiv:2202.13596) for similar results on the lattice

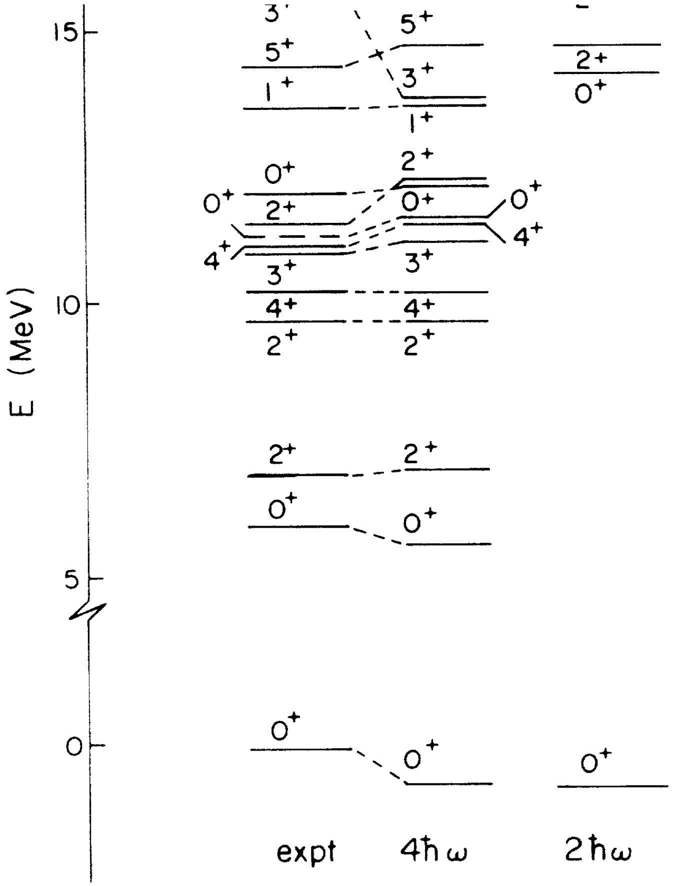


^{12}C Hoyle state main FMD configurations.

These cluster states are not easy to reproduce in the NCSM.
They may require as much as 30hω excitations in a h.o. basis (T. Neff), yet they appear low in the spectrum

So basically we have the intruder state problem all over again!

One can phenomenologically reproduce spectra for example, by adjusting single particle energies



^{16}O Haxton & CWJ, PRL **65** (1990) 1325

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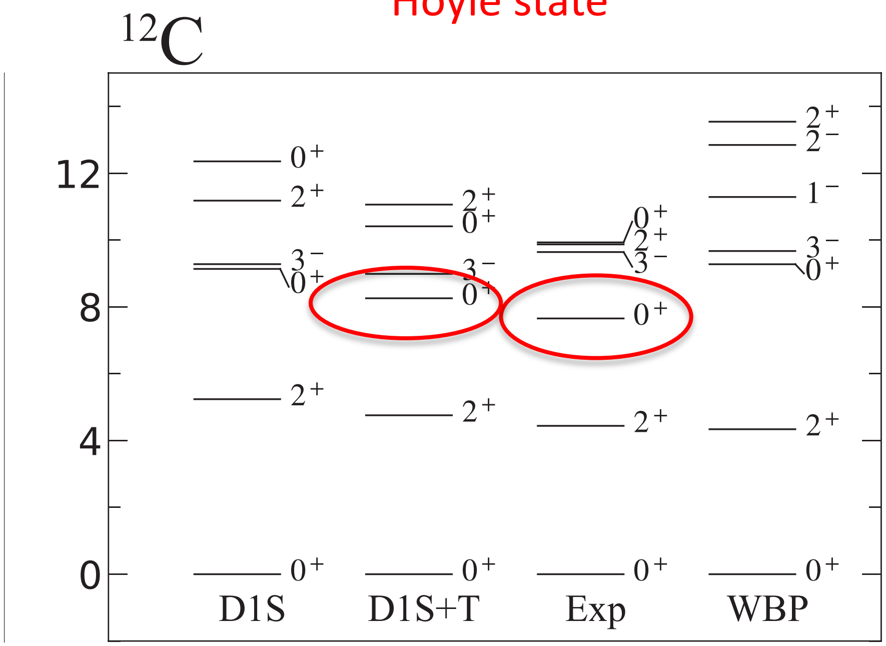
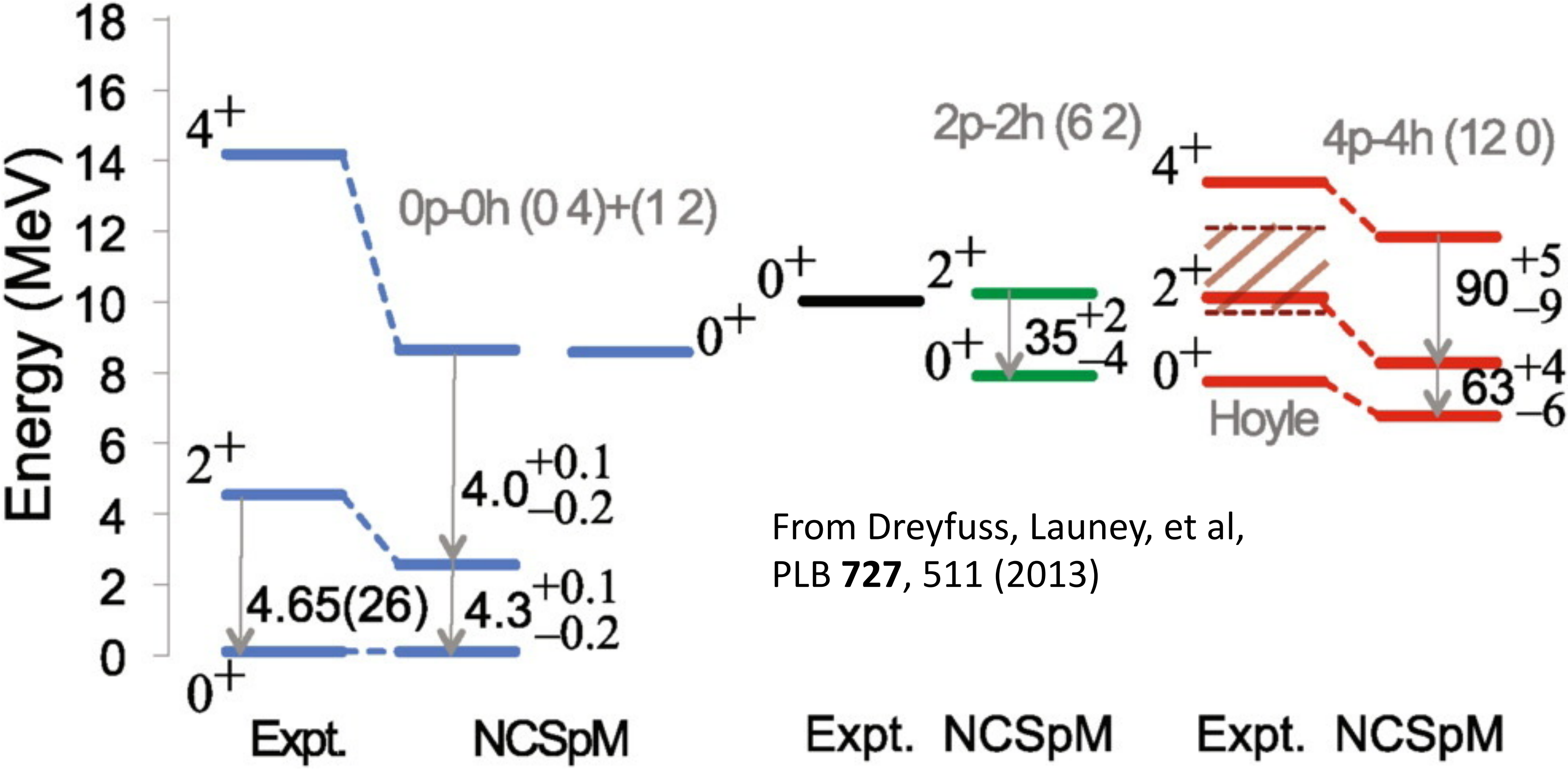


Hoyle state

B. Dai, CWJ, et al, PRC 103, 064327 (2021)

(adjust s.pe.s to fit levels in ^{15,17}O relative to ^{16}O)

One can phenomenologically reproduce spectra or by adjusting the strength of an SU(3) Casimir



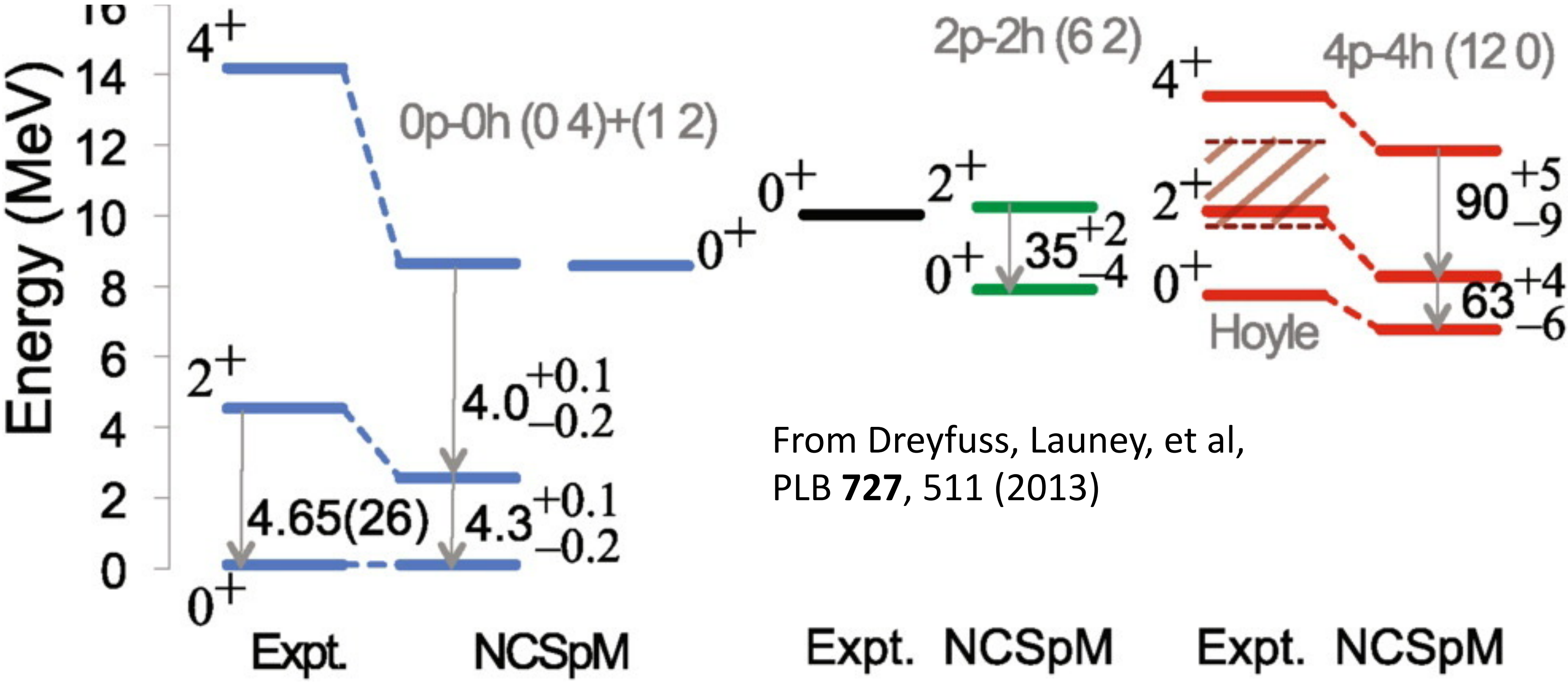
From Dreyfuss, Launey, et al, PLB **727**, 511 (2013)

$$H_\gamma = \sum_{i=1}^{A}\left(\frac{\mathbf{p}_i^2}{2m} + \frac{m\Omega^2\mathbf{r}_i^2}{2}\right) + \frac{\chi}{2}\frac{(e^{-\gamma Q\cdot Q} - 1)}{\gamma}$$

$$-\kappa\sum_{i=1}^{A} l_i \cdot s_i .$$

a

r



From Dreyfuss, Launey, et al,
PLB **727**, 511 (2013)

Furthermore,
the islands of inversions
and halo nuclei
form a similar **challenge** to
standard shell-model pictures

CASE STUDY: ^{11}LI

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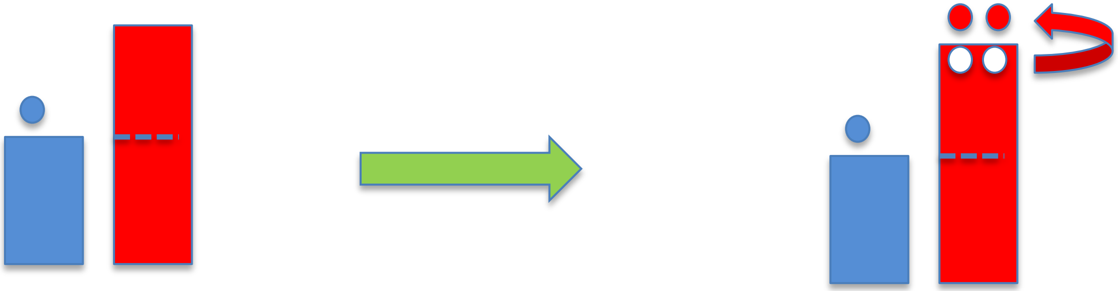
^{11}Li makes for an excellent case study:

- Example of “island of inversion”
- Halo or extended state
- Small enough to be tackled numerically
- Testbed for techniques

CASE STUDY: ^{11}LI



One proton outside a filled shell
+ filled neutron shell

One proton outside a filled shell
+ neutron 2p-2h

"island of inversion"

CASE STUDY: ^{11}LI

^{11}Li makes for an excellent case study

(The following results are **preliminary**)

3/2- g.s. is a halo state and on an island of inversion

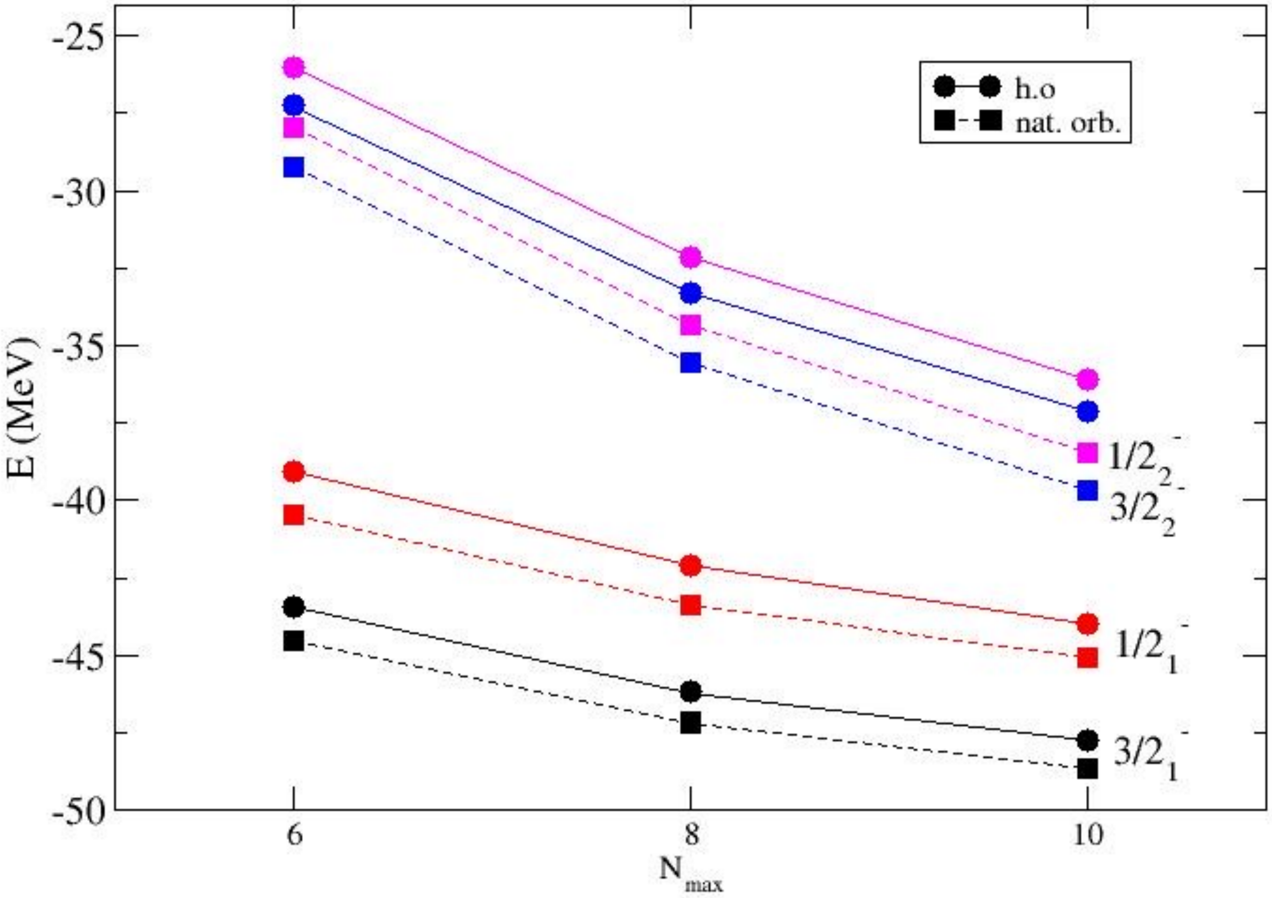
CASE STUDY: ^{11}LI

^{11}Li makes for an excellent case study

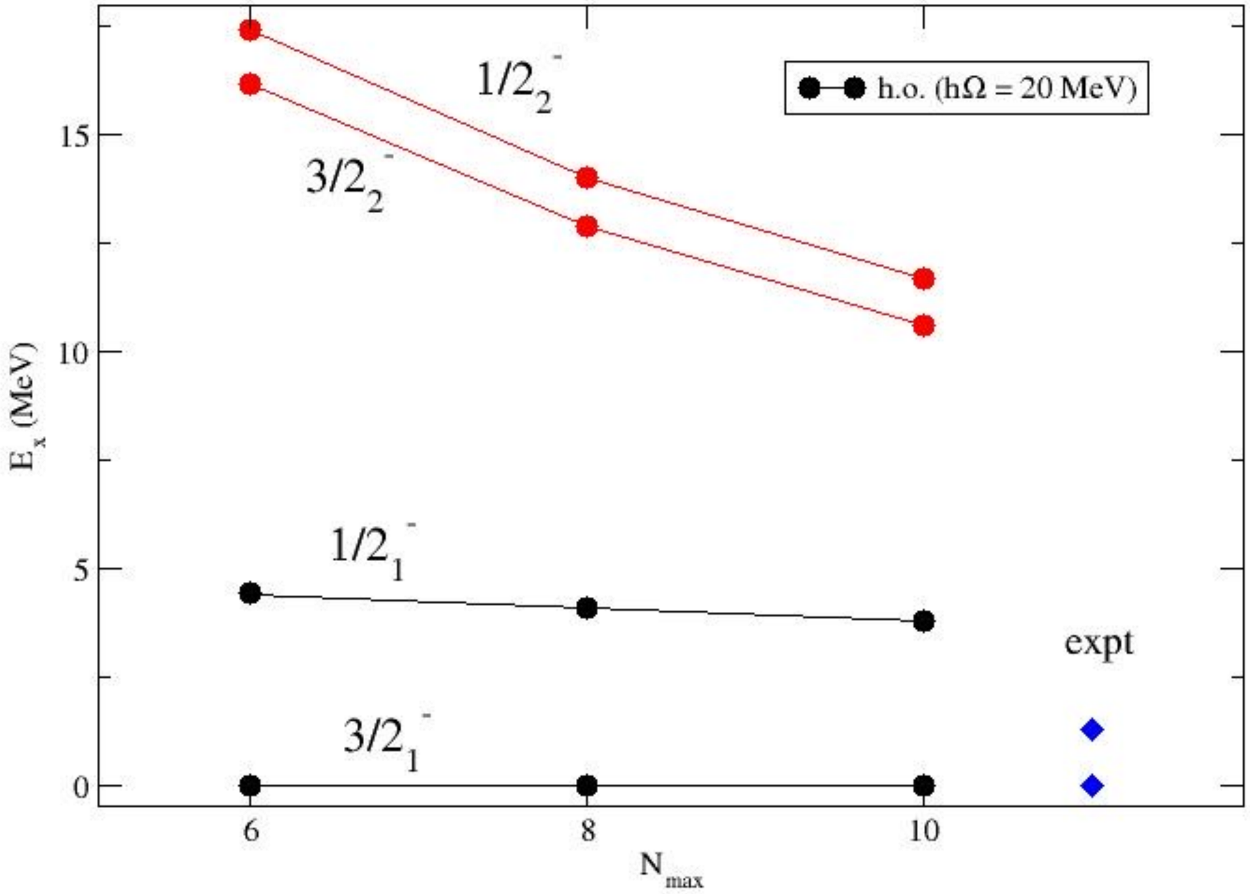
Calculations with Entem-Machleidt N3LO chiral (no 3-body) at hΩ = 20 MeV.

Also computed with natural orbitals

CASE STUDY: ^{11}LI



CASE STUDY: ^{11}LI



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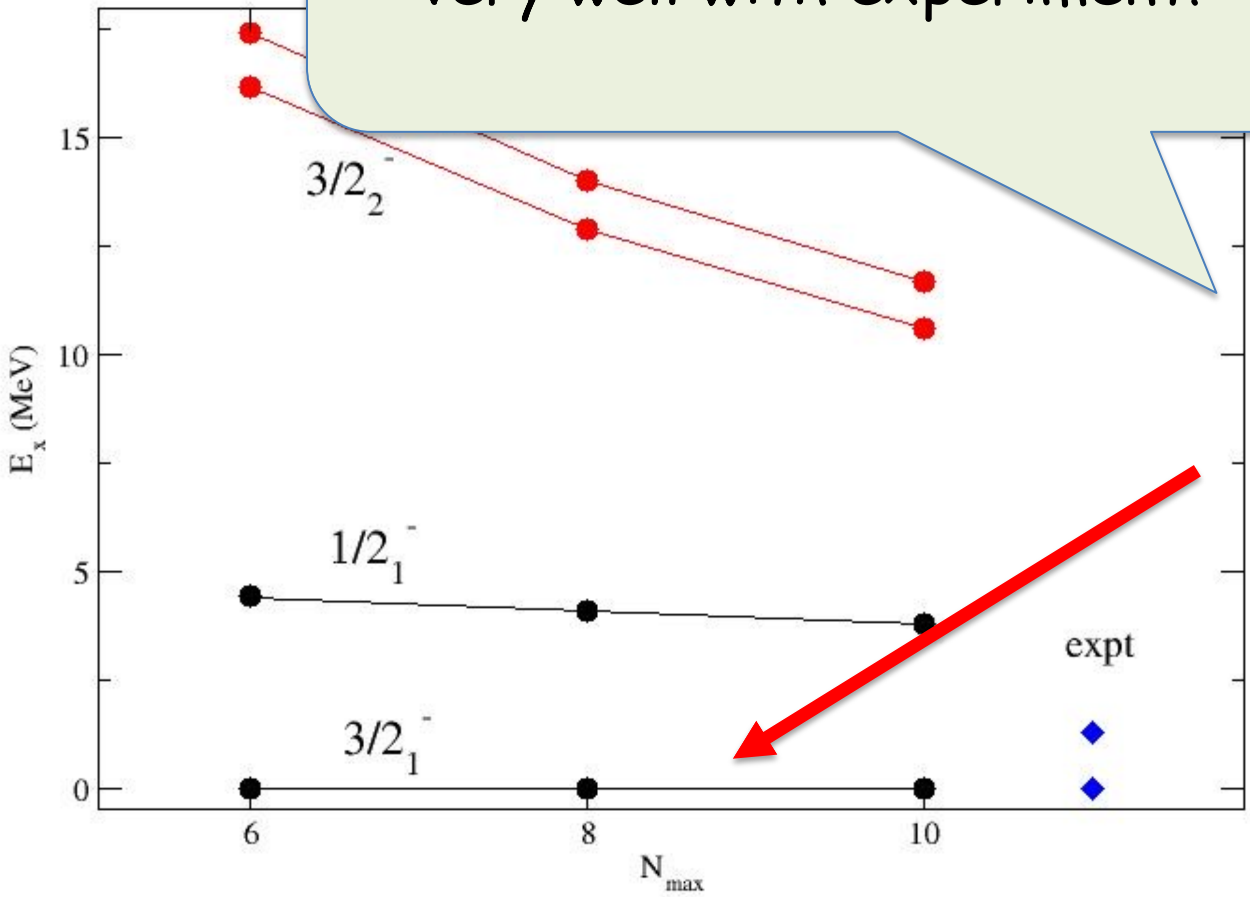
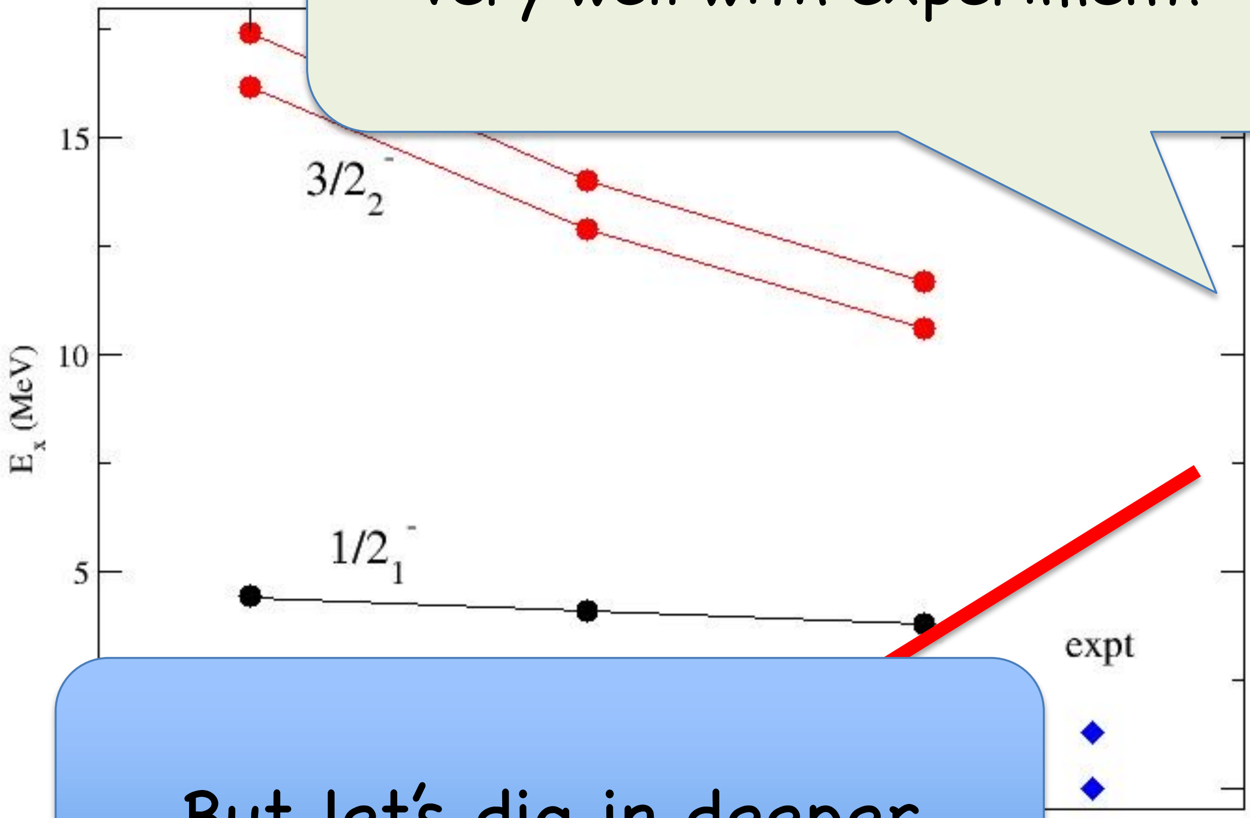
“The ratio Q_p/r^2_p agrees very well with experiment!”



Mark Caprio

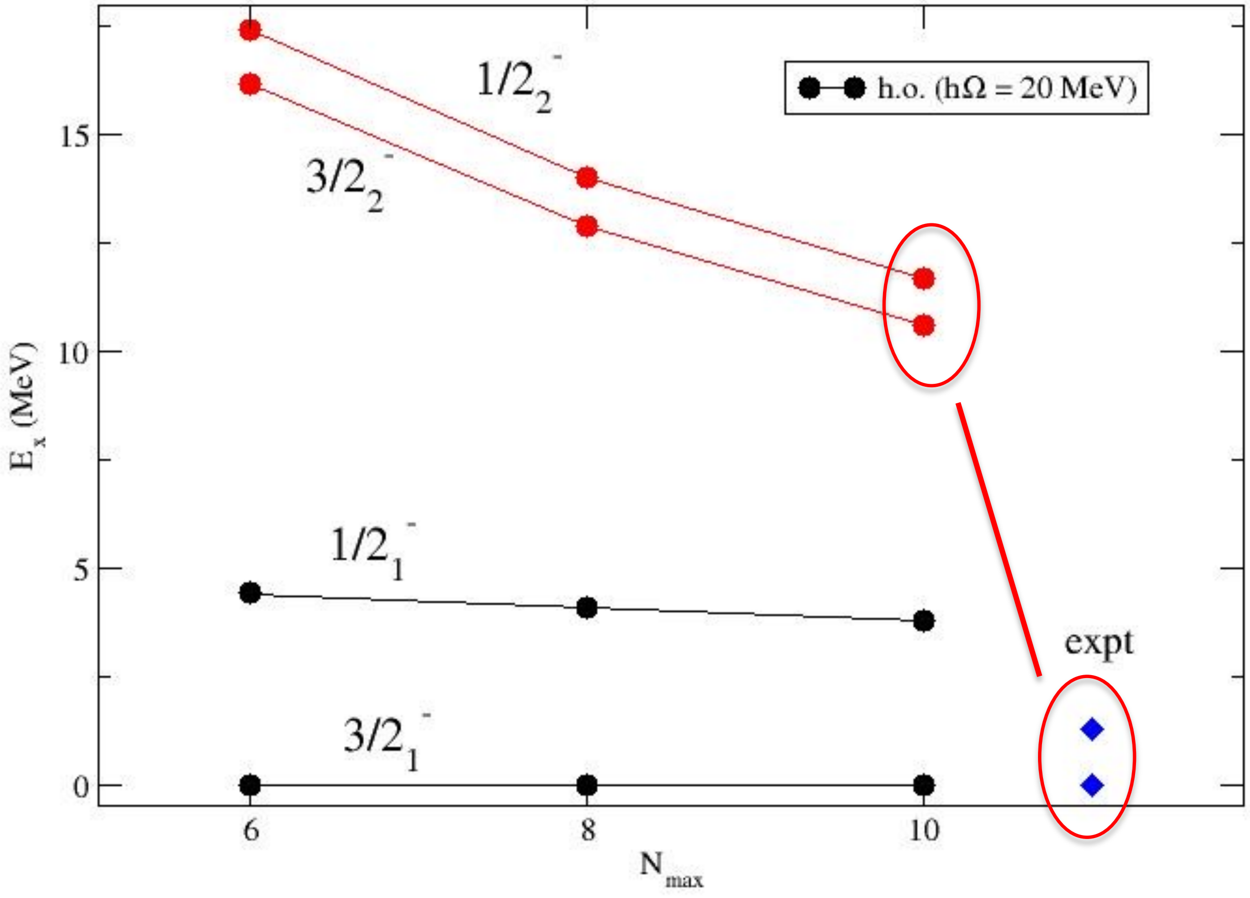
“The ratio Q_p/r^2_p agrees very well with experiment!”



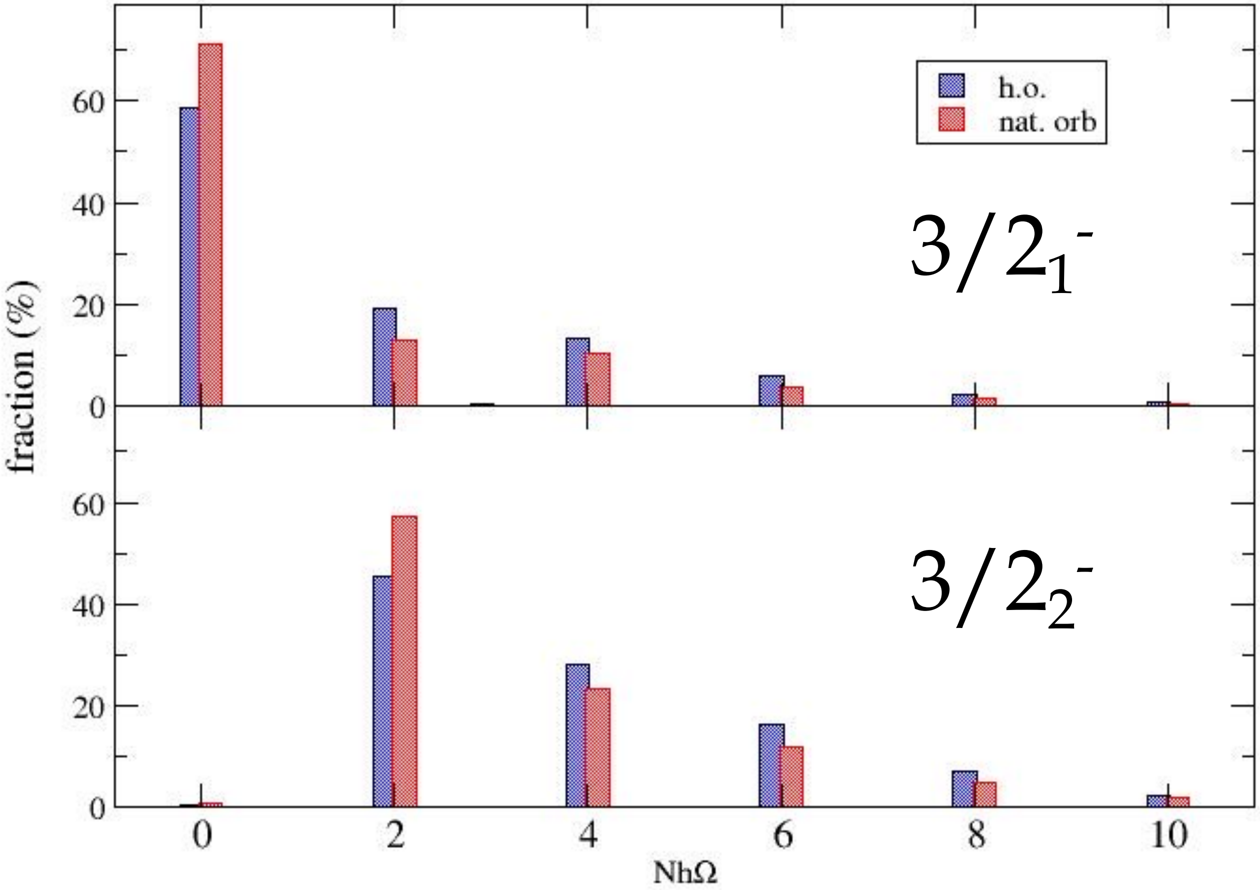
Mark Caprio

But let’s dig in deeper

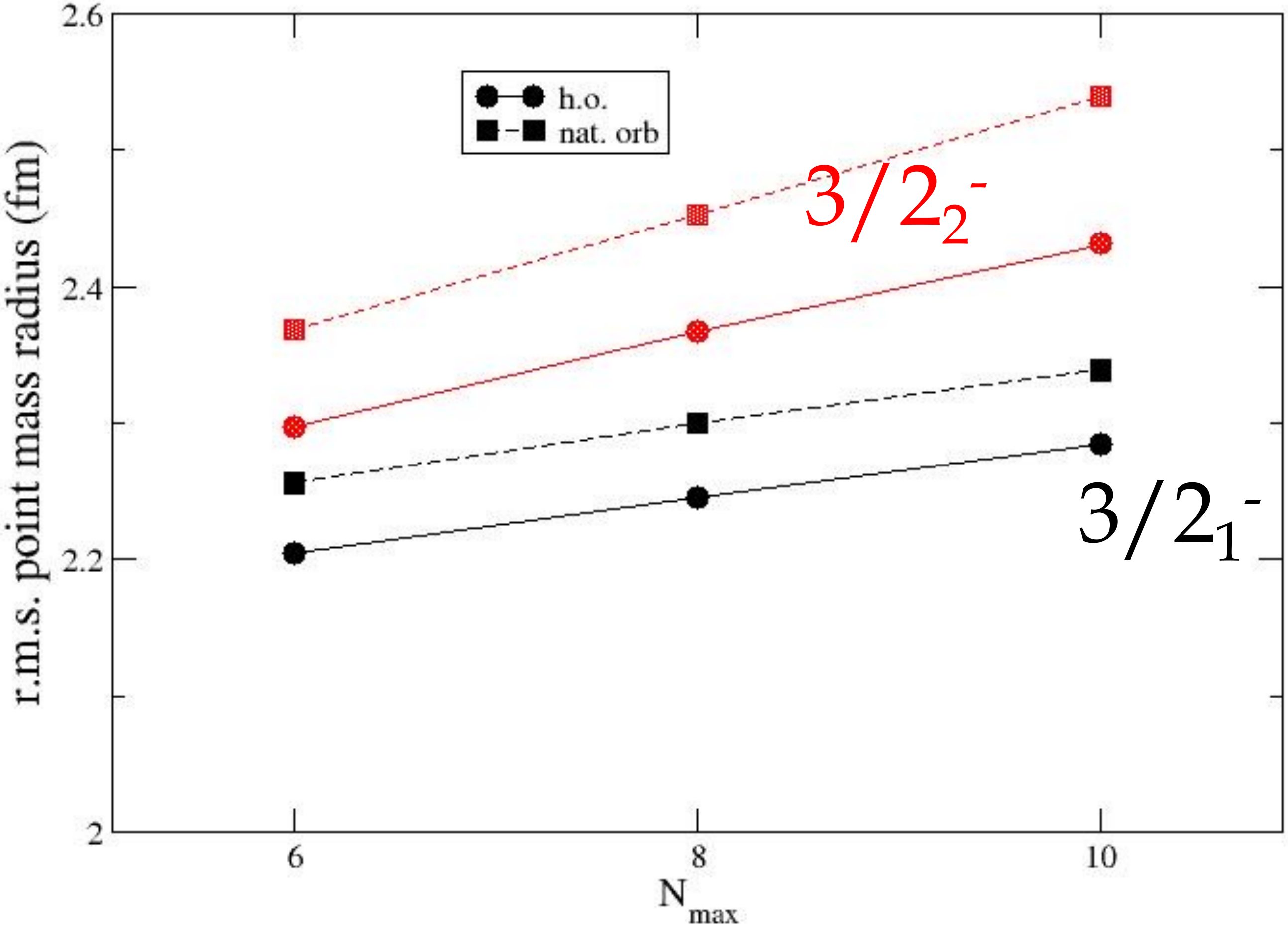
CASE STUDY: ^{11}LI



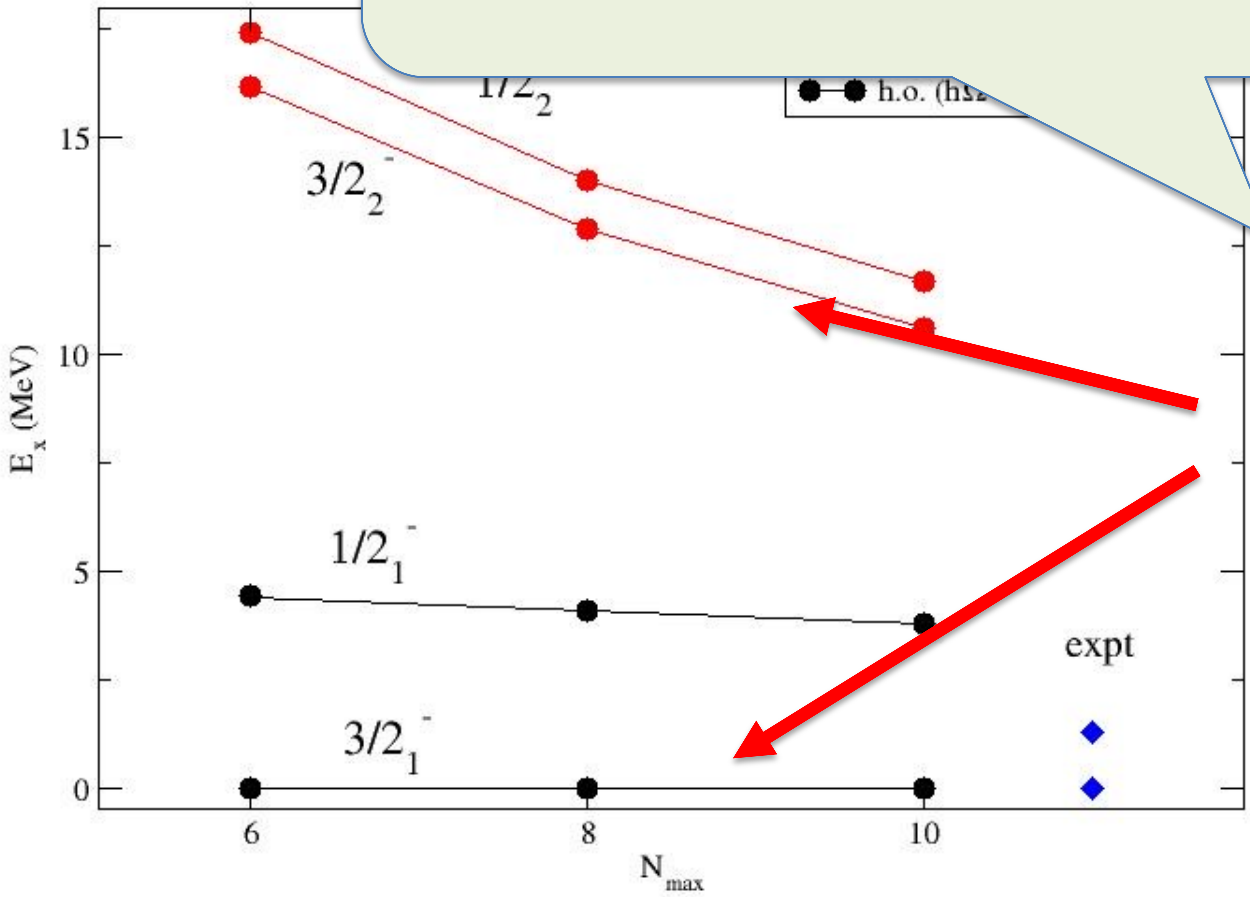
CASE STUDY: ^{11}LI



CASE STUDY: ^{11}LI

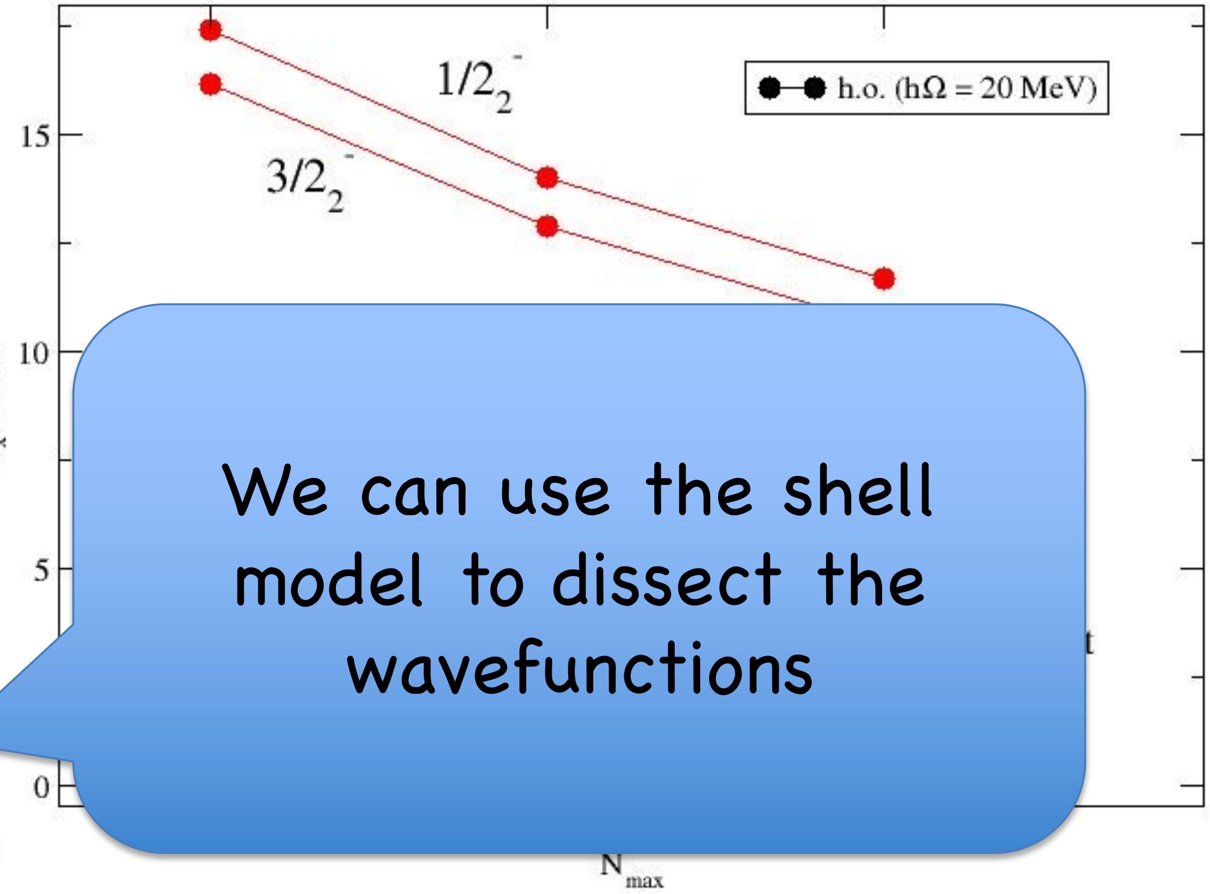


“The ratio Q_p/r^2_p agrees very well with experiment… for both 3/2- states!”



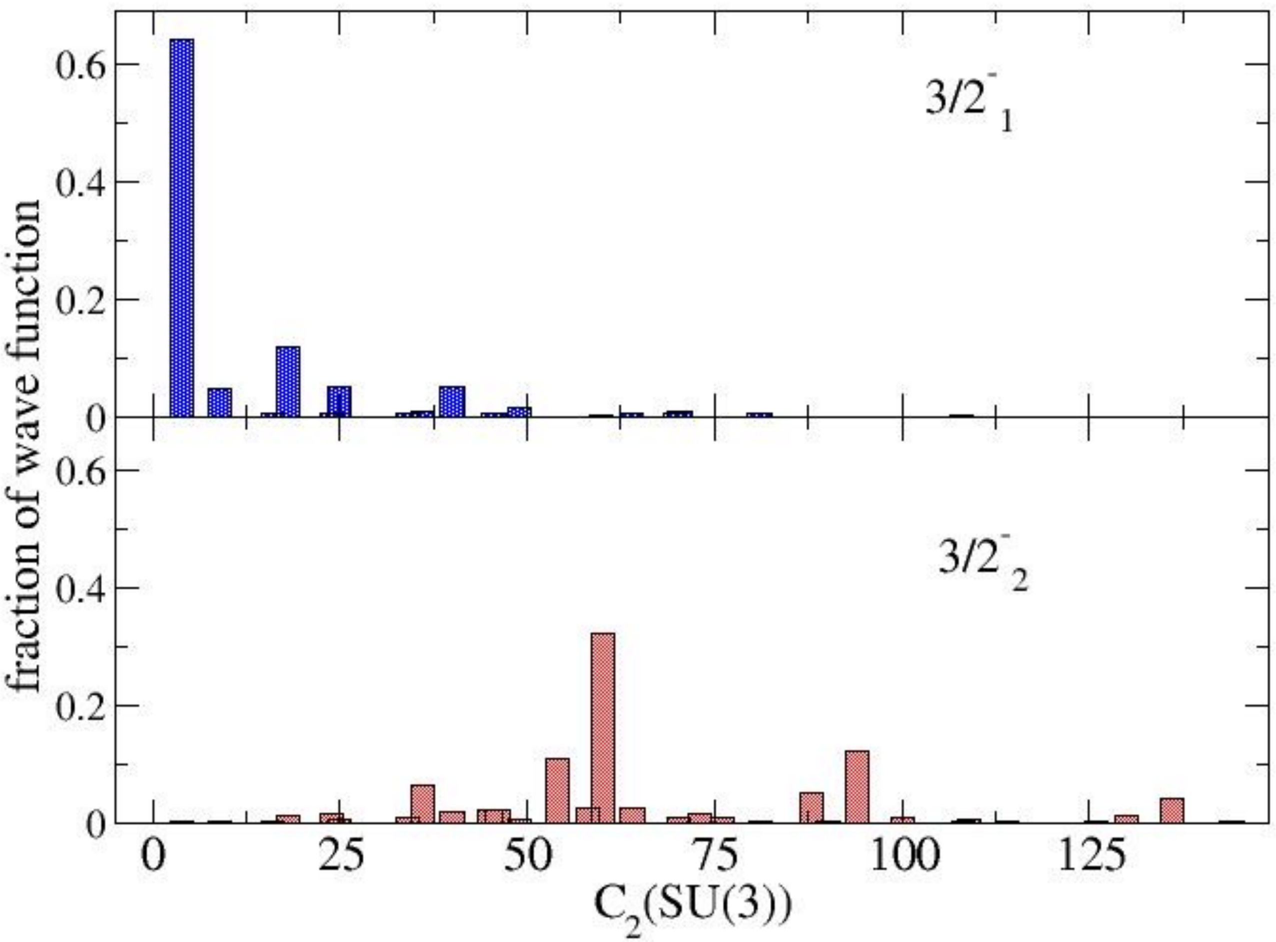
Mark Caprio

CASE STUDY: ^{11}LI



We can use the shell model to dissect the wavefunctions

CASE STUDY: ^{11}LI



Group-theoretical Decomposition

Elliot SU(3)

CASE STUDY: ^{11}LI

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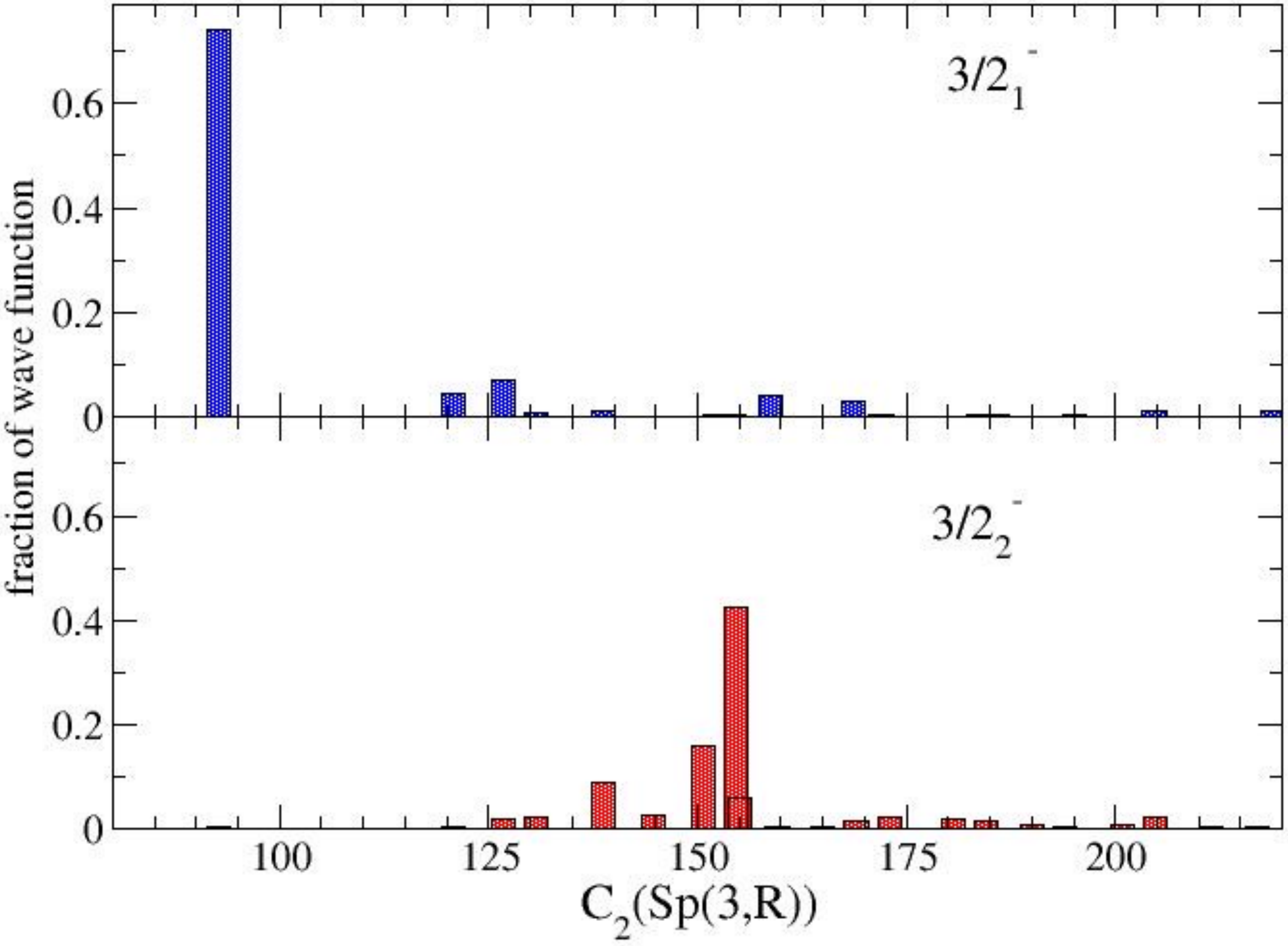

Group-theoretical Decomposition

Symplectic Sp(3,R)

CASE STUDY: ^{29}F

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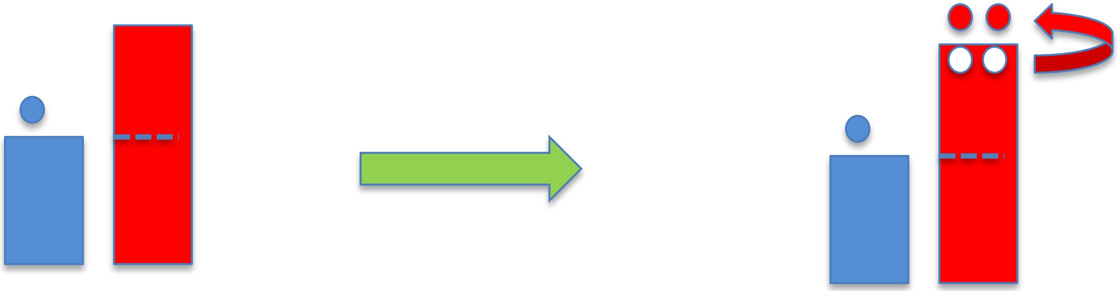
^{29}F is an analog of ^{11}Li



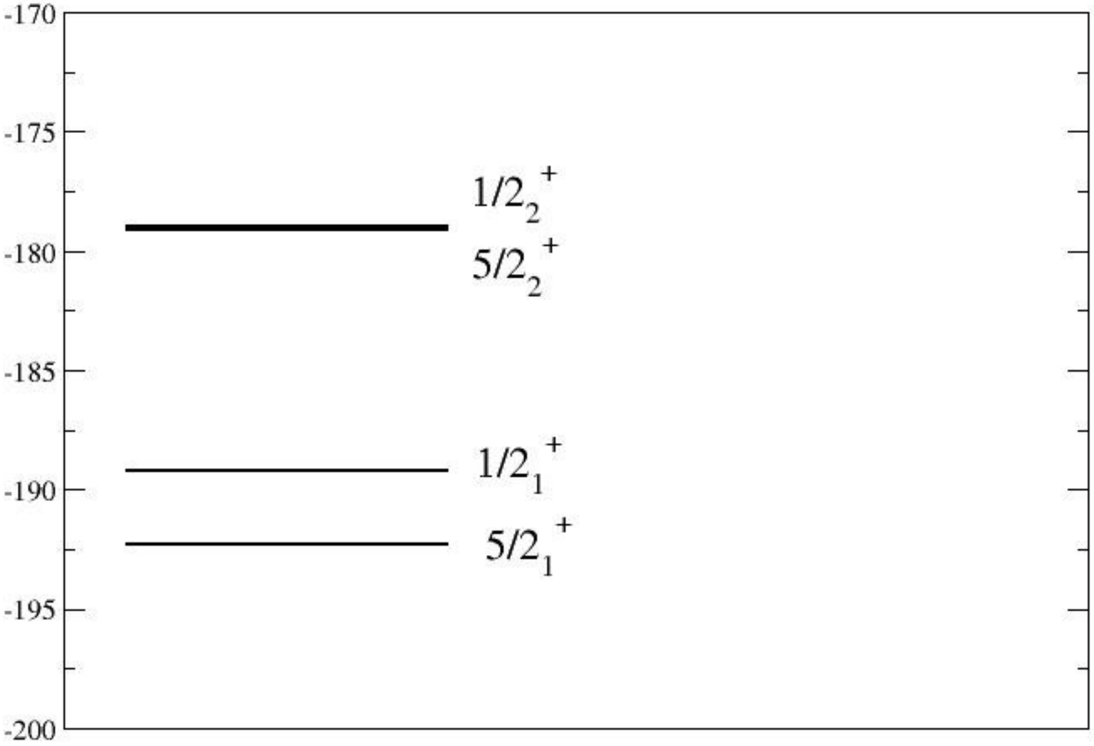
One proton outside a filled shell
+ filled neutron shell

One proton outside a filled shell
+ neutron 2p-2h

"island of inversion"

CASE STUDY: ^{29}F

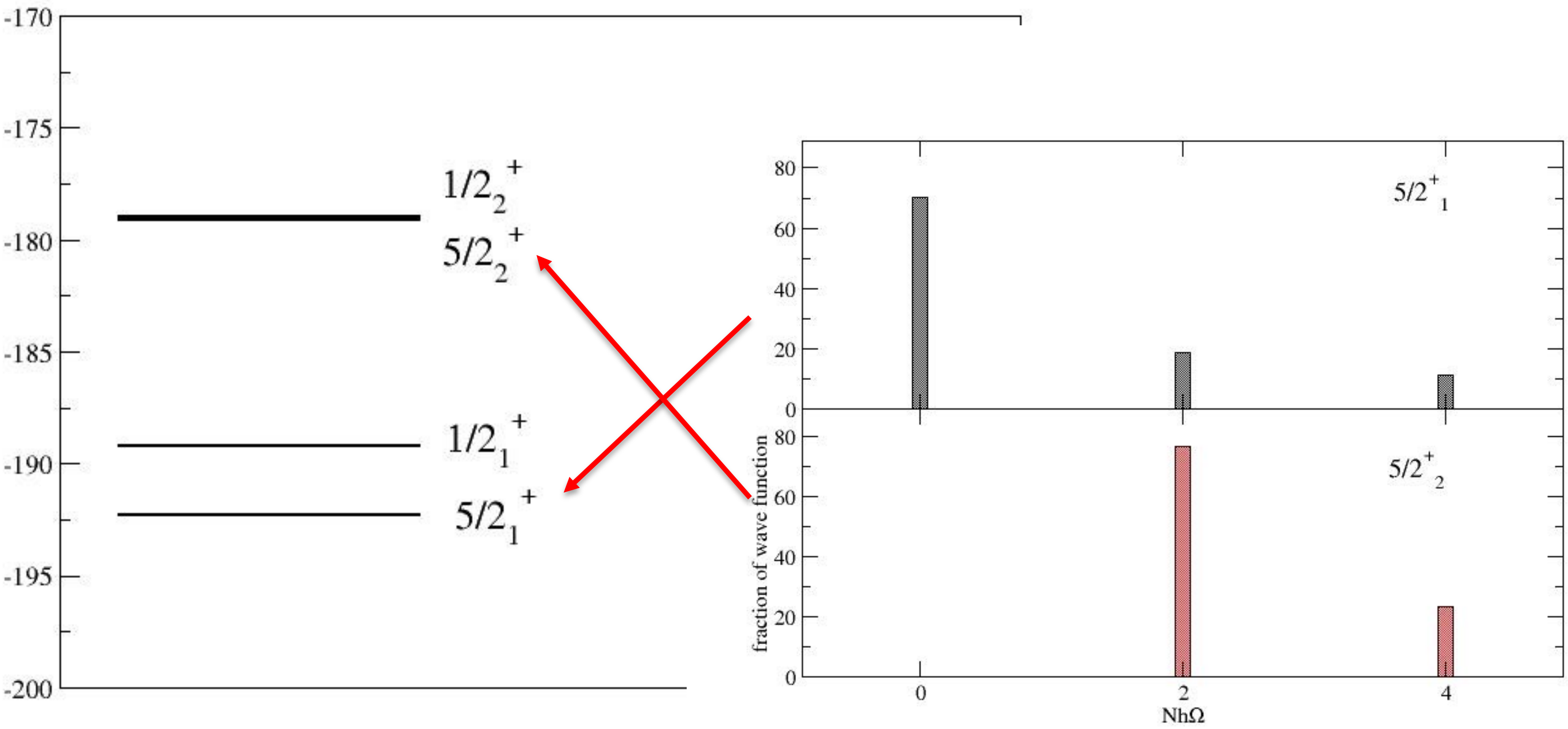
^{29}F is an analog of ^{11}Li



N_{max} = 4, natural orbitals

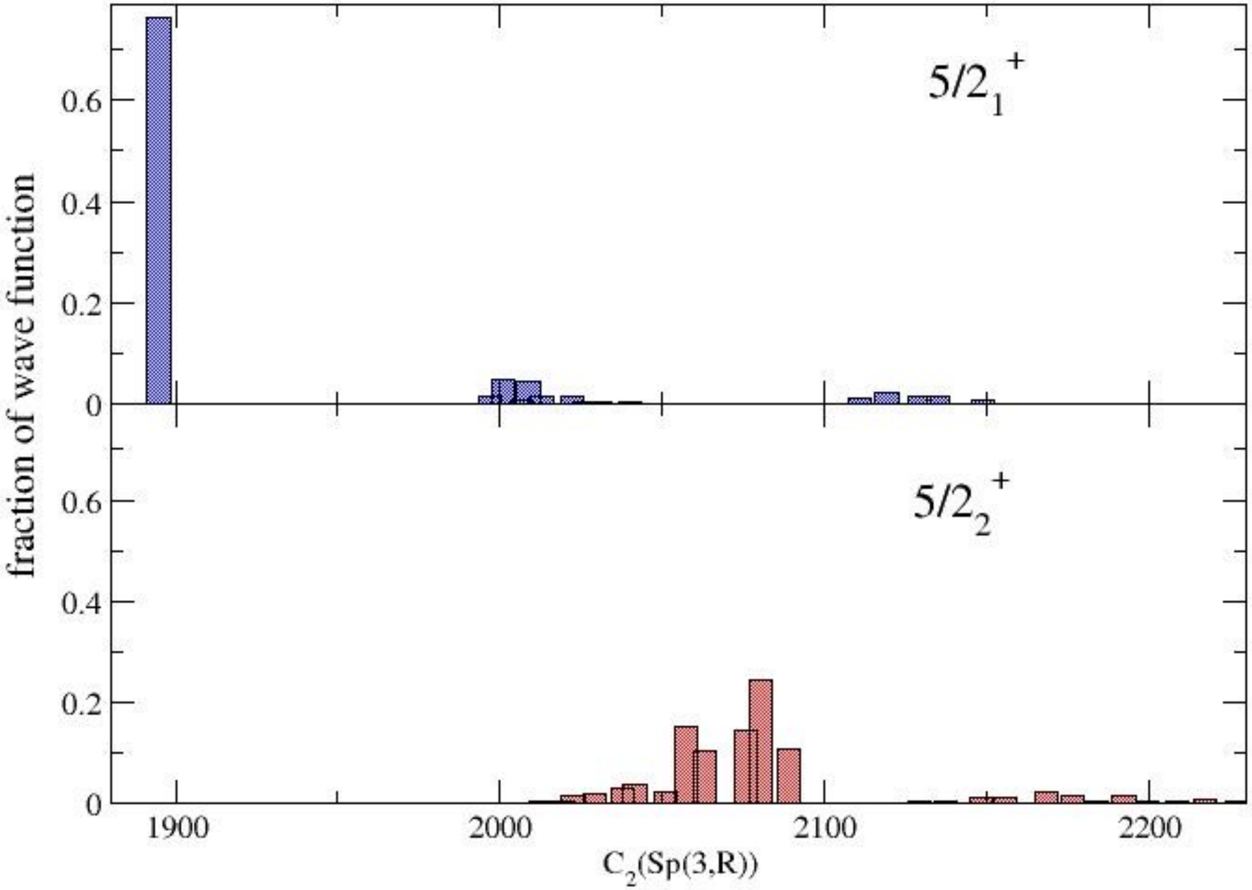
CASE STUDY: ^{29}F

^{29}F is an analog of ^{11}Li



N_{max} = 4, natural orbitals

CASE STUDY: ^{29}F



$N_{max} = 4$

Group-theoretical Decomposition

Symplectic Sp(3,R)

CASE STUDY: ^{29}F

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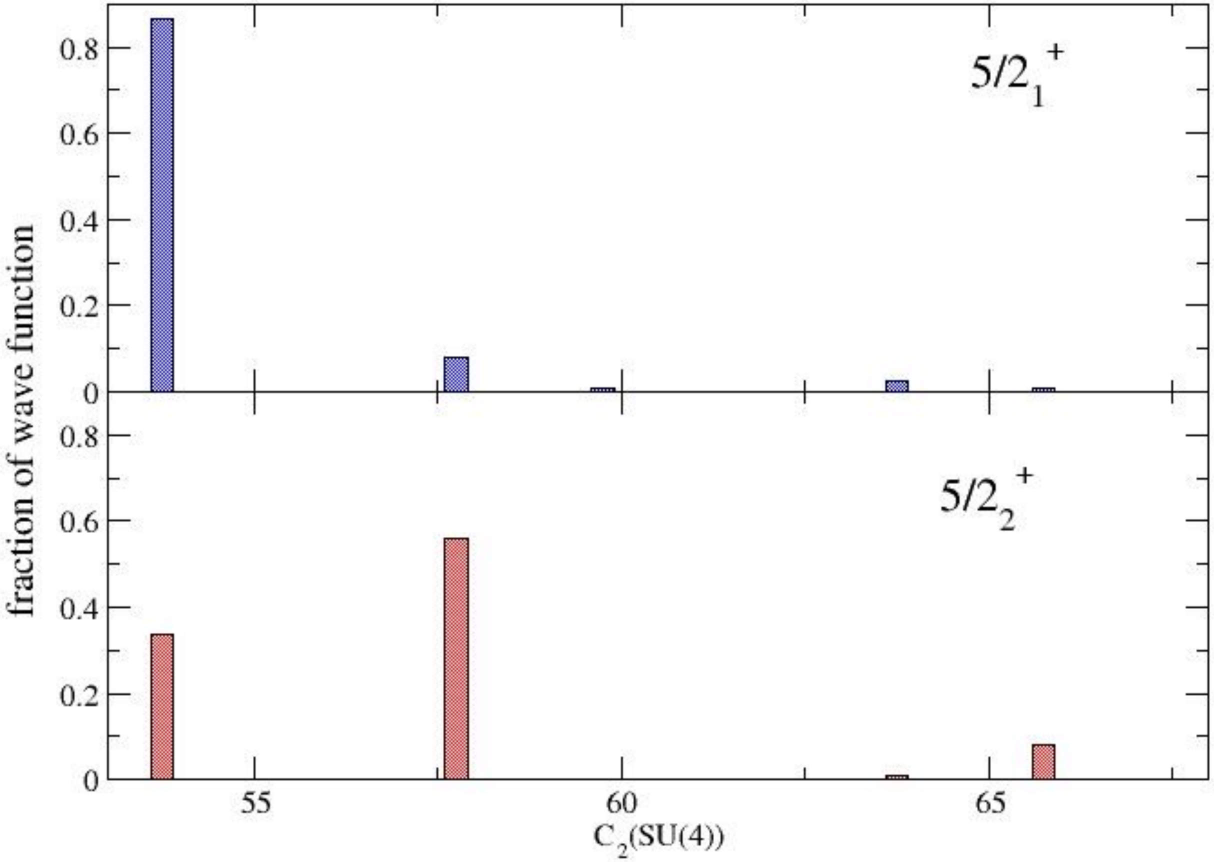

$N_{max} = 4$

Group-theoretical decomposition

SU(4)

CASE STUDIES: ^{11}LI, ^{29}F

I suggest ^{11}Li, ^{29}F as case studies for other methods (coupled cluster, IM-SRG, symmetry adapted, lattice, etc.).

CASE STUDIES: ^{11}LI, ^{29}F

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I suggest ^{11}Li, ^{29}F as case studies for other methods (coupled cluster, IM-SRG, symmetry adapted, lattice, etc.).

We should also look for experimental observables to test our calculations (since the quadrupole moment, in ^{11}Li at least, does not differentiate between states).

So what have we learned?

The no-core shell model reproduces some features **easily** but others are **very challenging!**

What are possible strategies for extending the reach of the shell model?

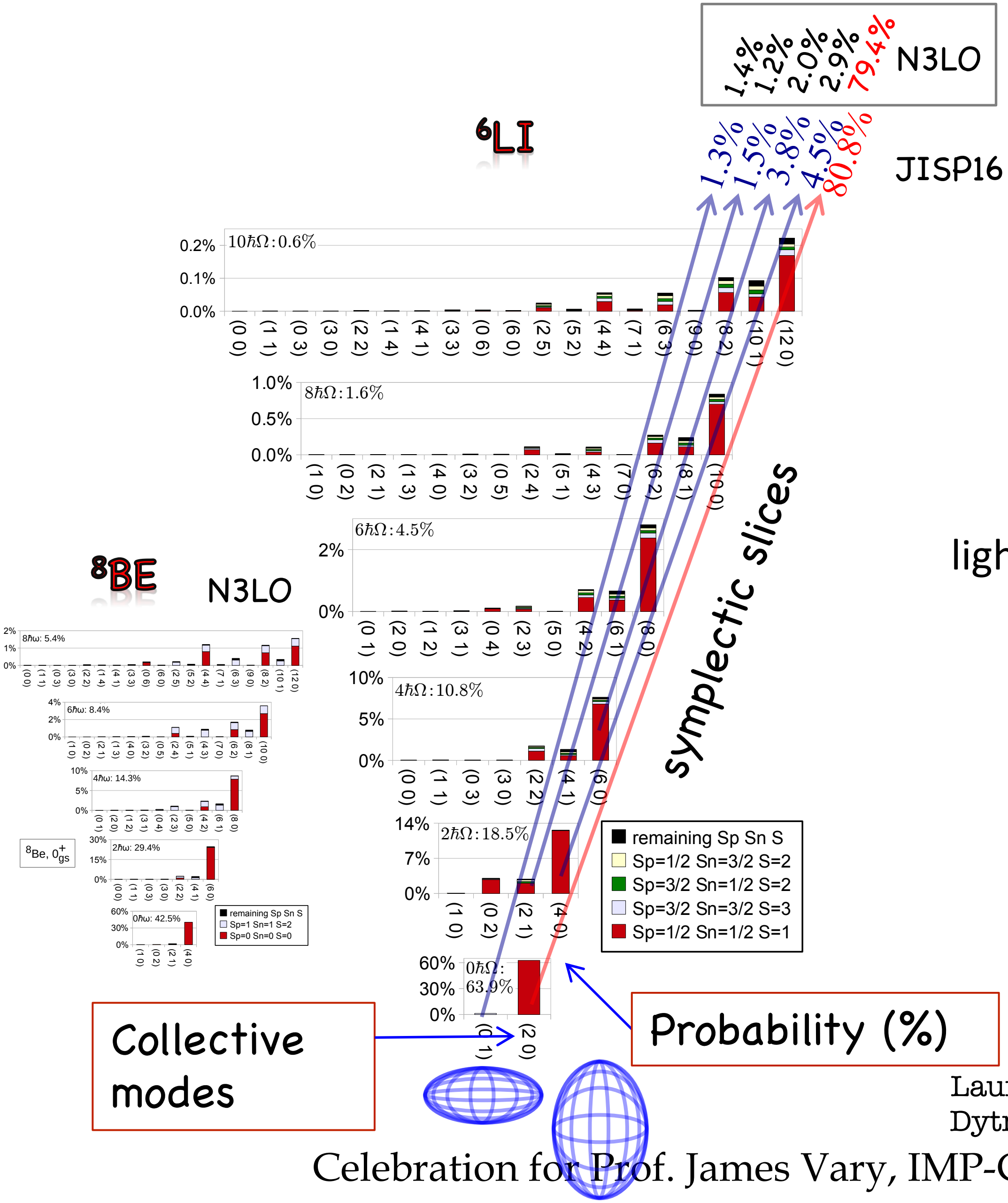
- "Beyond mean-field"/Generator-coordinate-like methods

cf. Dao & Nowacki, PRC **105**, 054314 (2023)

* Proton-neutron factorization:
cf. Papenbrock & Dean, PRC **67**, 051303(R) (2003) +
CWJ, Gorton, J. Phys. G. **50**, 045110 (2023).

* "Symmetry-adapted" approaches

Symplectic Sp(3,R) Symmetry



Collective modes

Probability (%)

(From K. Launey, LSU)

From first principles: light/intermediate-mass nuclei, low-lying states

Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

Collectivity features

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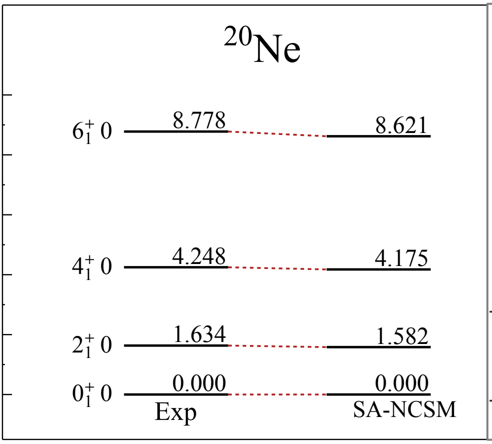
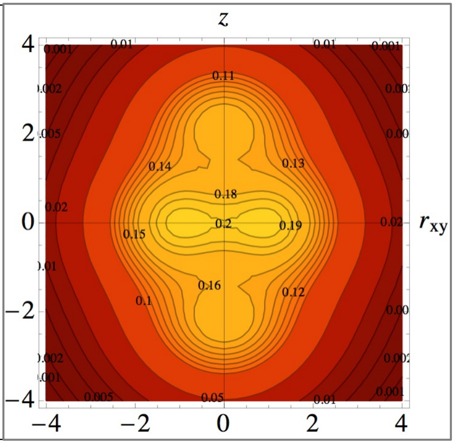
20NE





13 shells

SA-NCSM (selected model space): 50 million SU(3) states

Complete model space: 1000 billion states

Ne & Mg isotopes

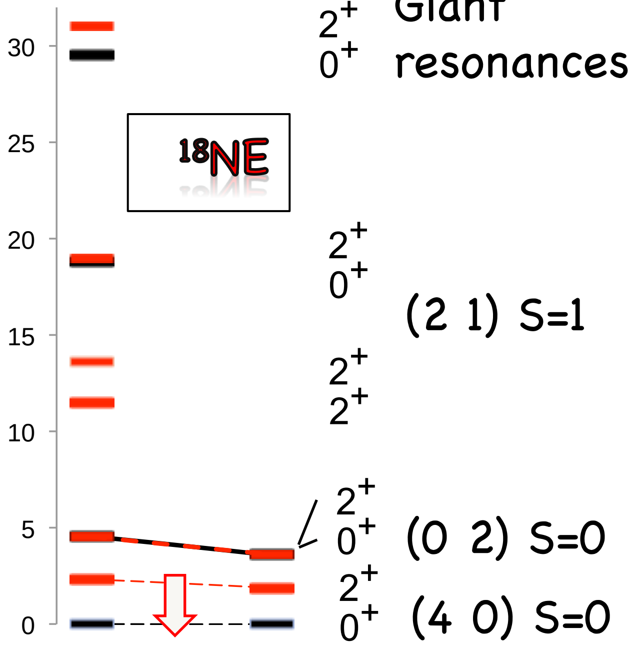
^{18}Ne, B(E2: 2^+->0^+)

Experiment……… 17.7(18) W.u.

9 shells …………… 1.13 W.u.

33 shells ………….. 13.0(7) W.u.

(no effective charges)



N2LOopt; 9 shells, ħω = 15 MeV

Grigor Sargsyan, PhD student, LSU

Group theory may be a natural framework for cluster physics

Kravvaris & Volya, PRL **119**, 062501 (2017)

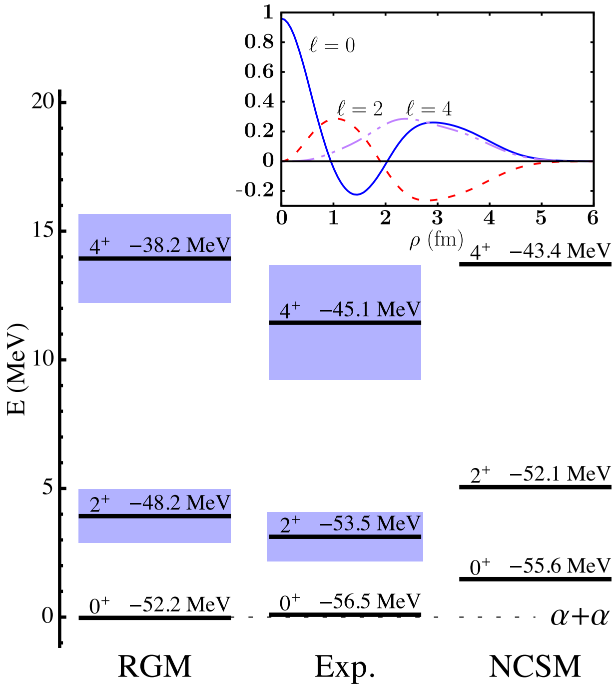


FIG. 1. Spectrum of RGM Hamiltonian with the SRG softened N3LO interaction ($\lambda = 1.5\ \mathrm{fm}^{-1}$) and $\hbar\Omega = 25$ MeV for a 2α system. Zero on the energy scale is set by the $\alpha + \alpha$ breakup threshold of the corresponding model. Levels are marked by spin and parity and by an absolute binding energy in units of MeV. The α binding energies for the $\alpha[0]$ and NCSM ($\alpha[4]$) calculations are −26.08 and −28.56 MeV, respectively. The inset shows the relative wave function of the two α clusters.

J-scheme matrices are smaller but much denser than M-scheme, and “symmetry-adapted” (i.e. SU(3)) matrices are smaller (and denser) still.

example: $^{12}C\ N_{max} = 8$

scheme	basis dim
M	6×10^{8}
J (J=4)	9×10^{7}
SU(3)	9×10^{6}

(truncated)

From Dytrych, et al, arXiv:1602.02965

J-scheme matrices are smaller but much denser than M-scheme, and “symmetry-adapted” (i.e. SU(3)) matrices are smaller (and denser) still.

example: ^{12}C $N_{max} = 8$

scheme	basis dim	# of nonzero matrix elements
M	6×10^8	5×10^{11}
J (J=4)	9×10^7	3×10^{13}
SU(3) (truncated)	9×10^6	2×10^{12}

From Dytrych, et al, arXiv:1602.02965

J-scheme matrices are smaller but much denser than M-scheme, and “symmetry-adapted” (i.e. SU(3)) matrices are smaller (and denser) still.

example: ^{12}C $N_{max} = 8$

but least amount of work!

scheme	basis dim	# of nonzero matrix elements	
M	6×10^8	5×10^{11}	4 Tb of memory!
J (J=4)	9×10^7	3×10^{13}	240 Tb of memory!
SU(3)	9×10^6	2×10^{12}	16 Tb of memory!

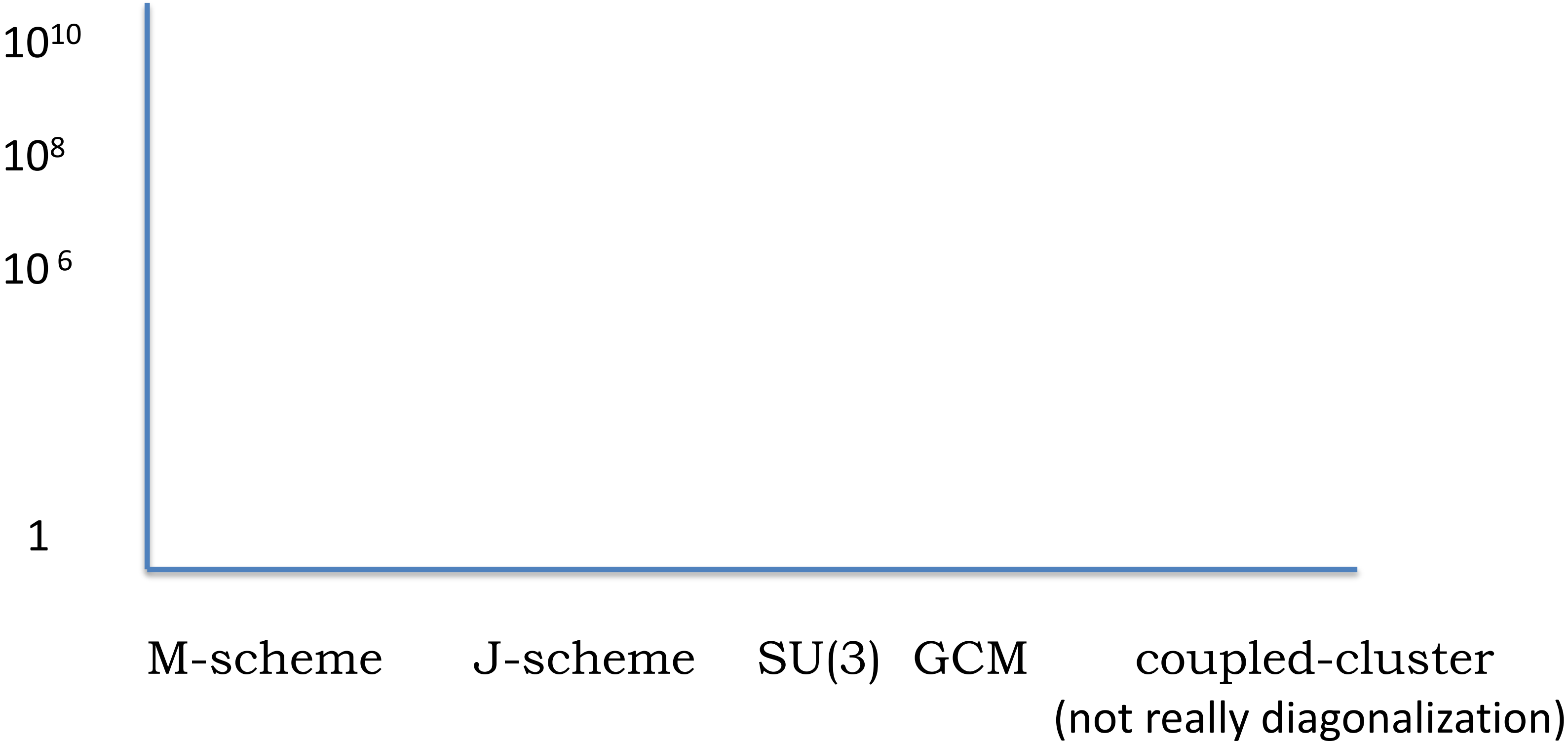
large dimension

(truncated)

From Dytrych, et al, arXiv:1602.02965

Choice of wave function basis

One chooses between *a few, complicated states* or *many simple states*



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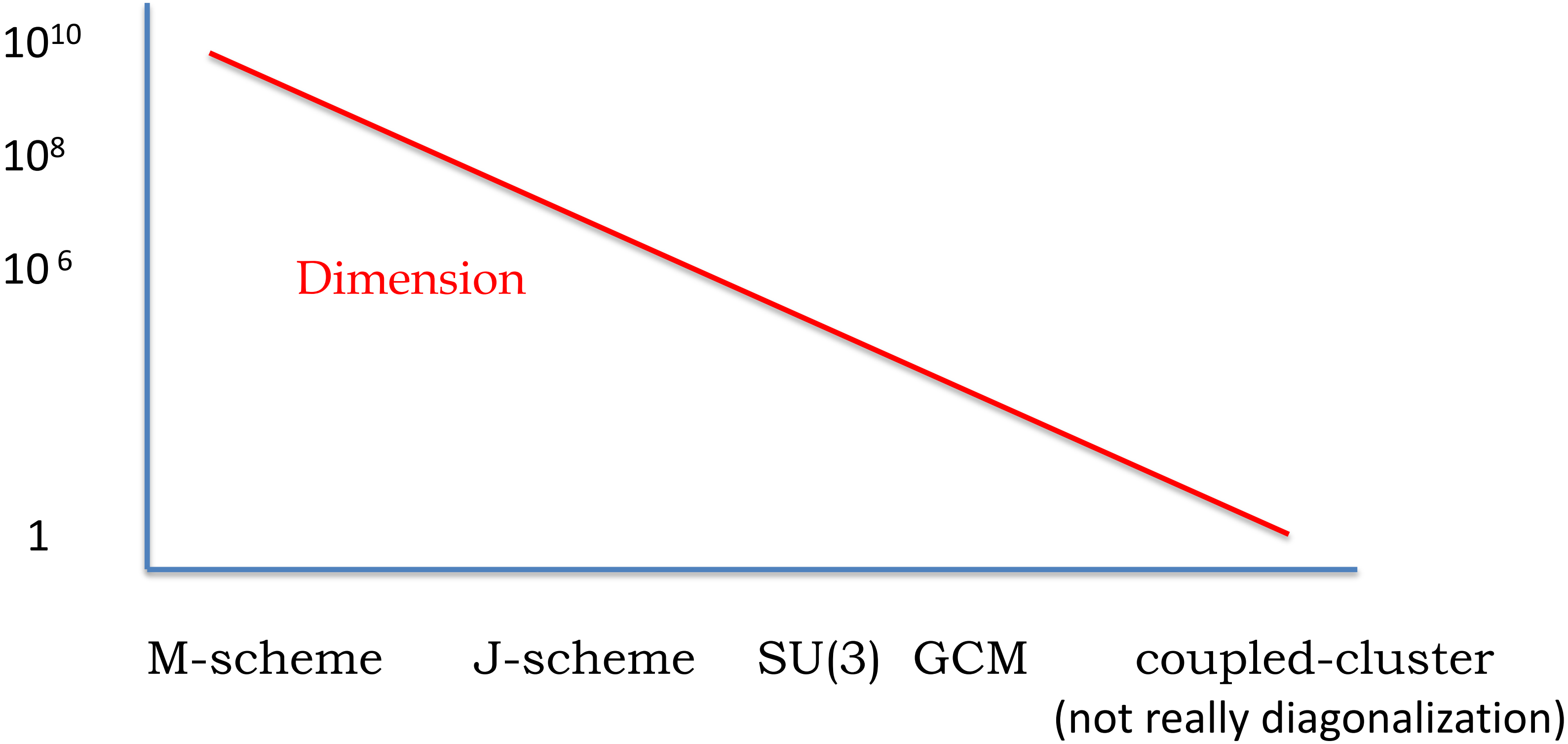

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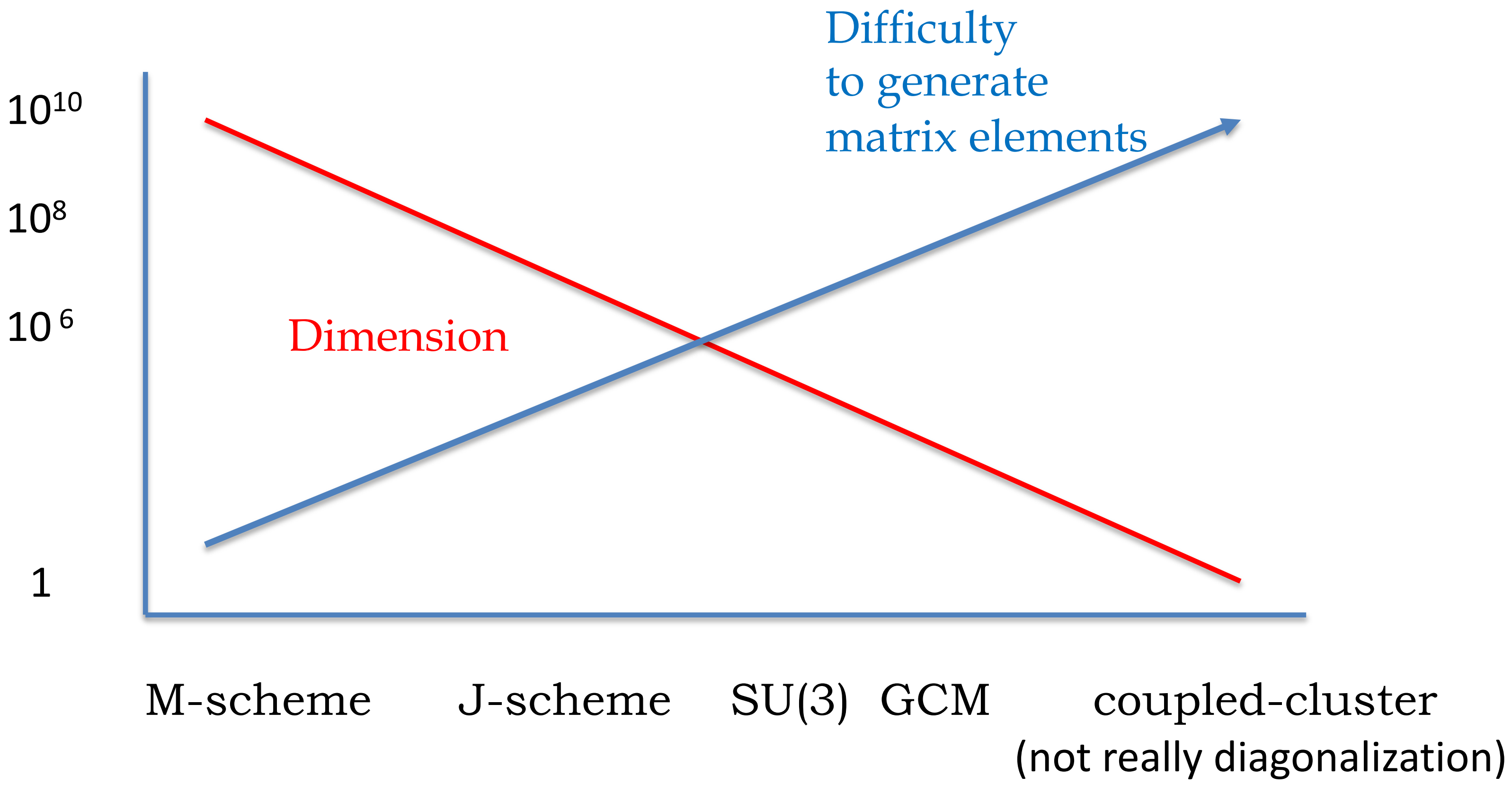
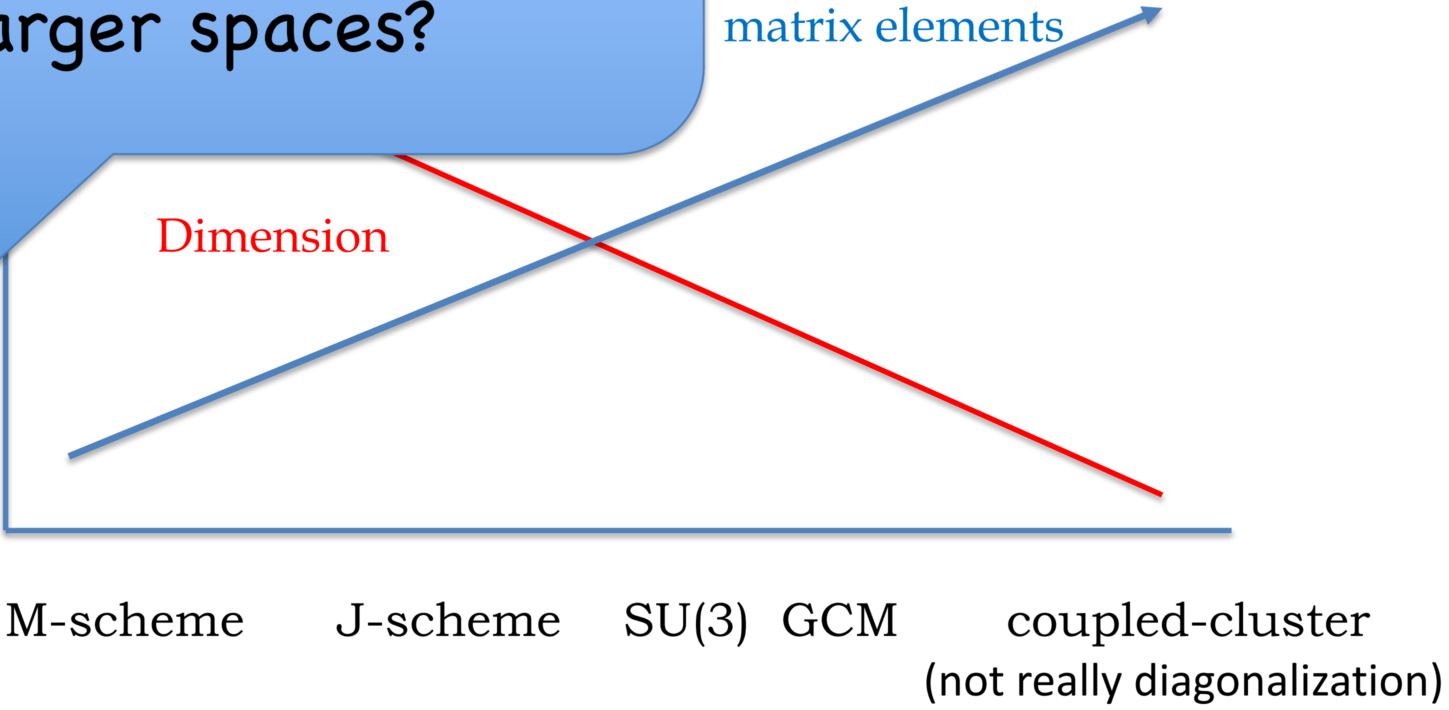


Choice of wave function basis

mplicated states

Are there ways we can harness the efficiency of M-scheme but still get to larger spaces?



Difficulty to generate matrix elements

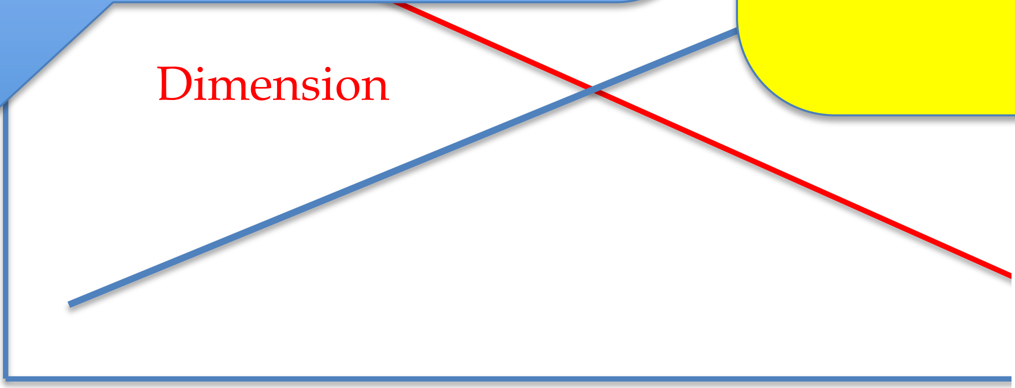
Dimension

M-scheme J-scheme SU(3) GCM coupled-cluster (not really diagonalization)

Choice of wave function basis

Are there ways we can harness the efficiency of M-scheme but still get to larger spaces?

That's the question for future research!



Summary:

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First principles calculations of nuclear structure have had many successes.

An eternal barrier are intruders—
the alpha cluster states such as the Hoyle state in ^{12}C and the 0^+_2 analog in ^{16}O, as well as halo and IoI states

A rich variety of approaches are being pursued.

I propose ^{11}Li and ^{29}F as important test cases