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Challenges to the shell model

Calvin W. Johnson

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FRIB-TA Workshop, May 26 2023

Configuration-interaction shell model

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Matrix formalism:
expand in some (many-body) basis $\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$

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

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$

Disadvantage:

- not size-extensive, basis grow exponentially

Advantages:

- Excited states easy to generate
- Direct access to wave function allows for detailed analysis

Outline of talk

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- The rise and fall and rise of the shell model
- The challenge of intruders
- ^{11}Li & ^{29}F as case studies

- Possible paths forward

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
1984: Wildenthal interaction for **valence** *sd*-shell
1991: FPD6 interaction for **valence** *pf* shell

A brief and incomplete history

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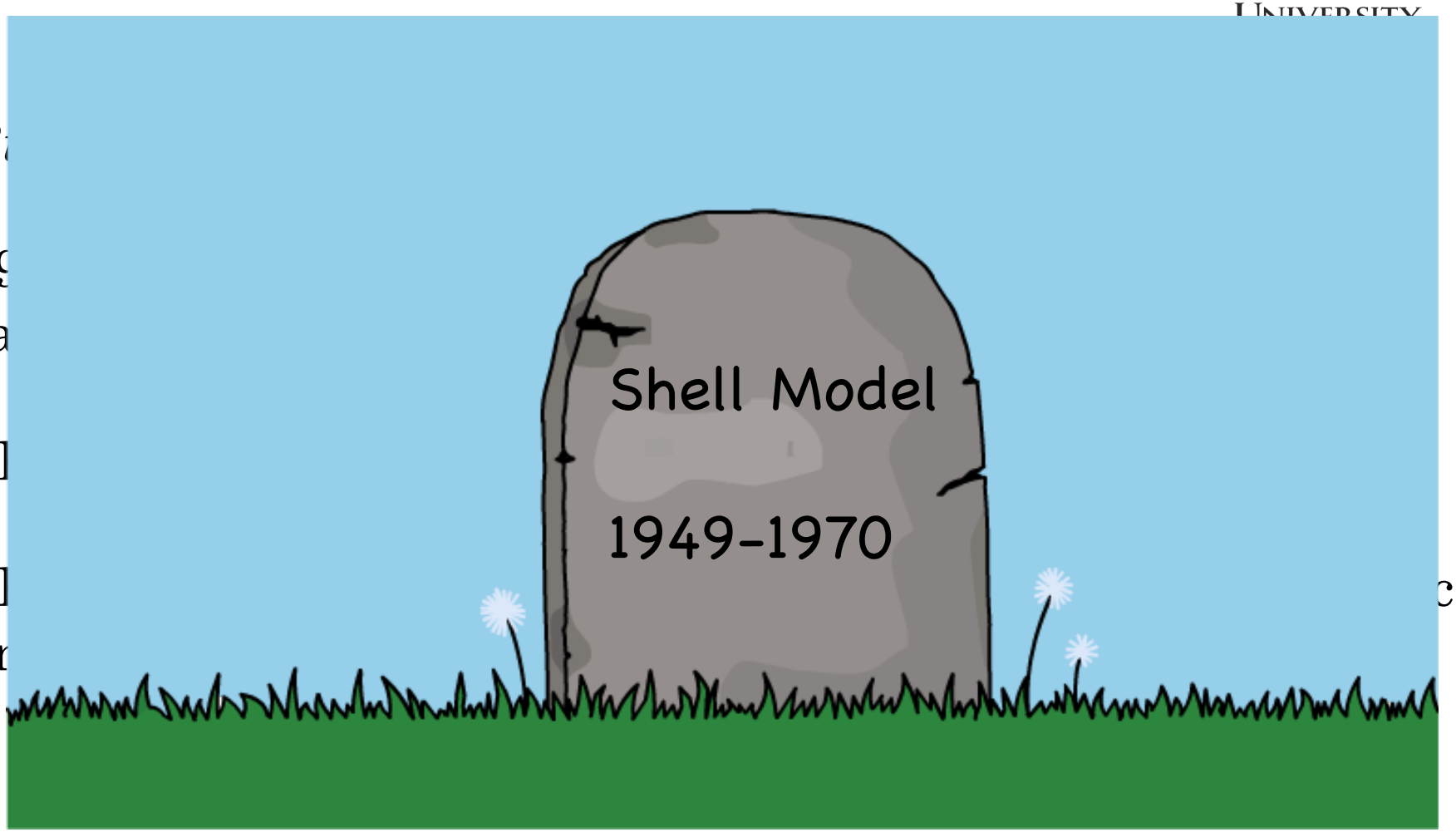
But….

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



A brief and incomplete history

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1991-1993: Barrett and Vary introduce the **no-core shell model**:
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 many-body 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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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, HOBET, etc.) fit to *few-body* data

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

(cf talks by Anna McCoy and Mark Caprio)

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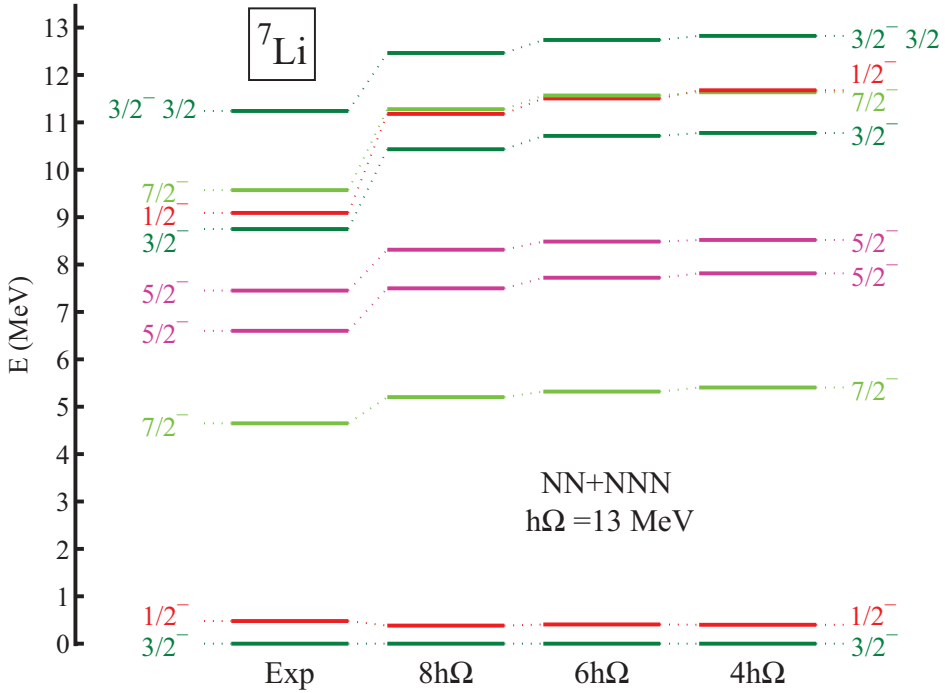
Some highlight achievements:

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

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



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

chiral 2+3 body forces

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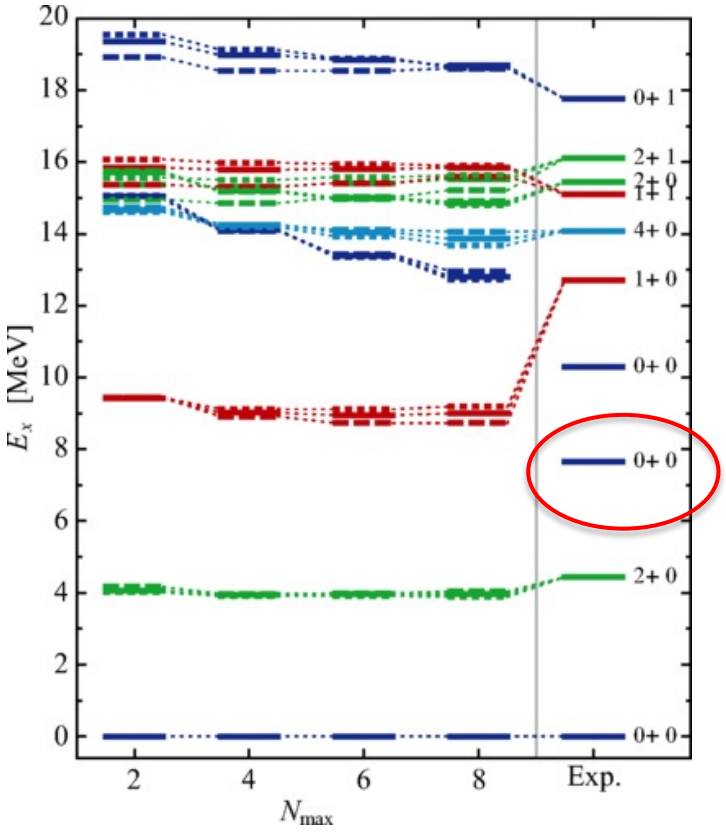
Some highlight achievements:

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

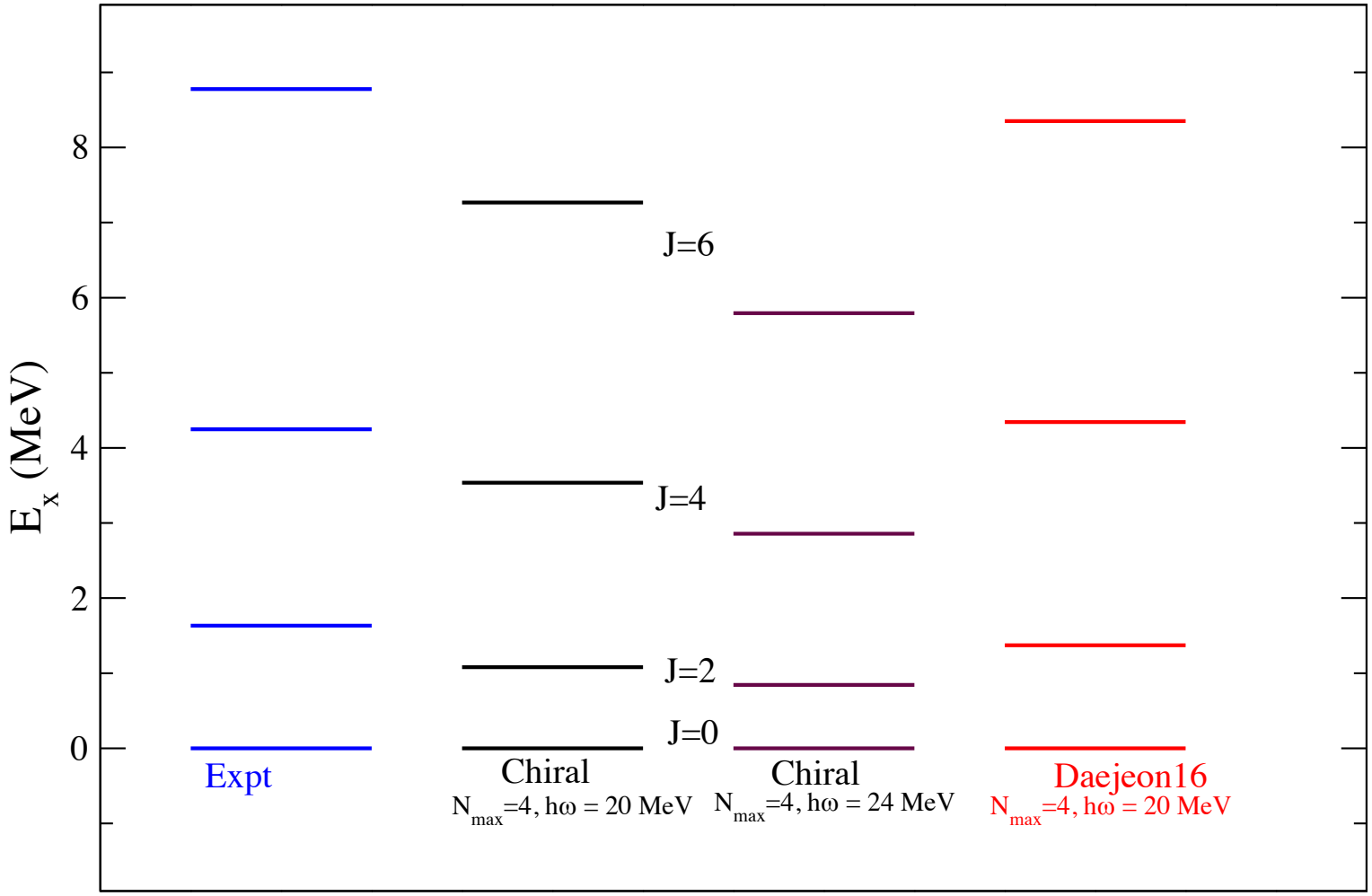


Hoyle state

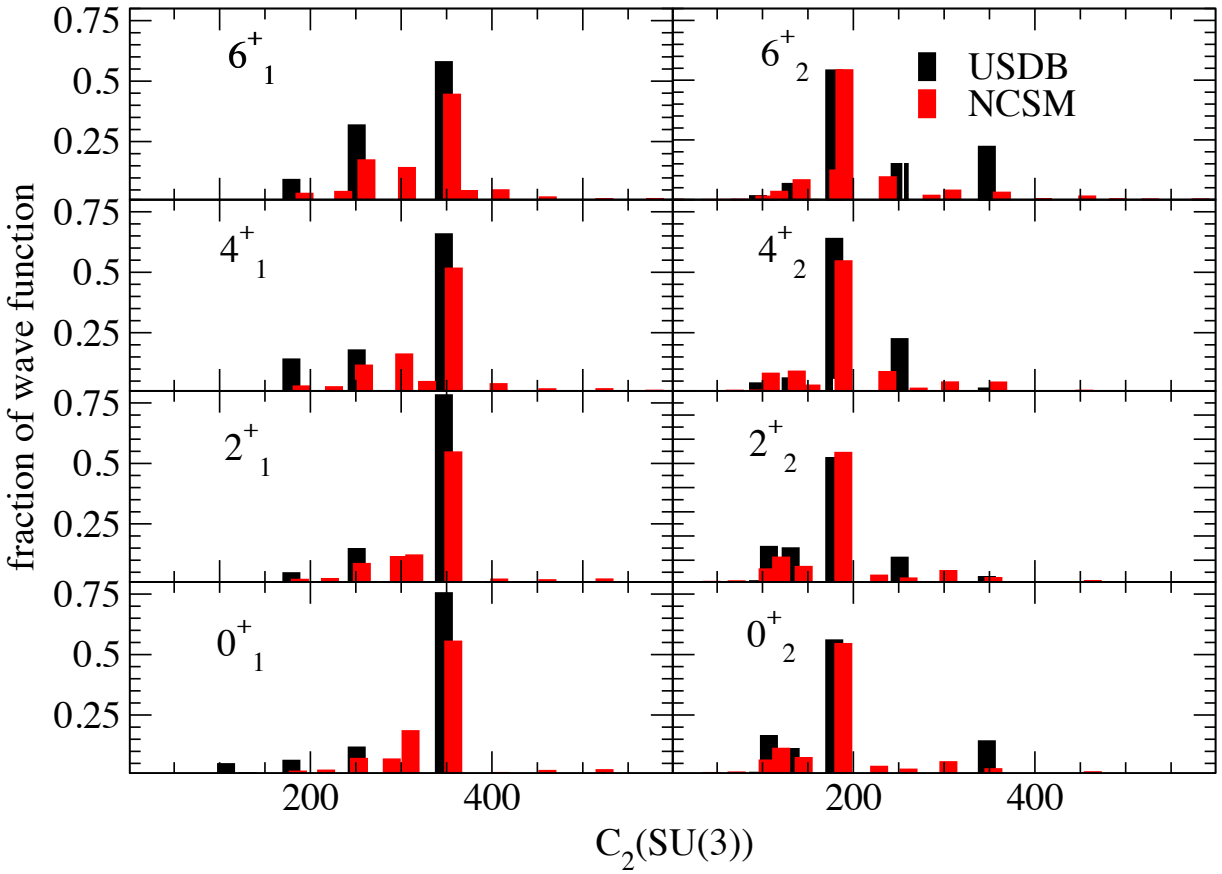
Maris *et al* PRC **90**, 014314 (2014)

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

^{20}Ne

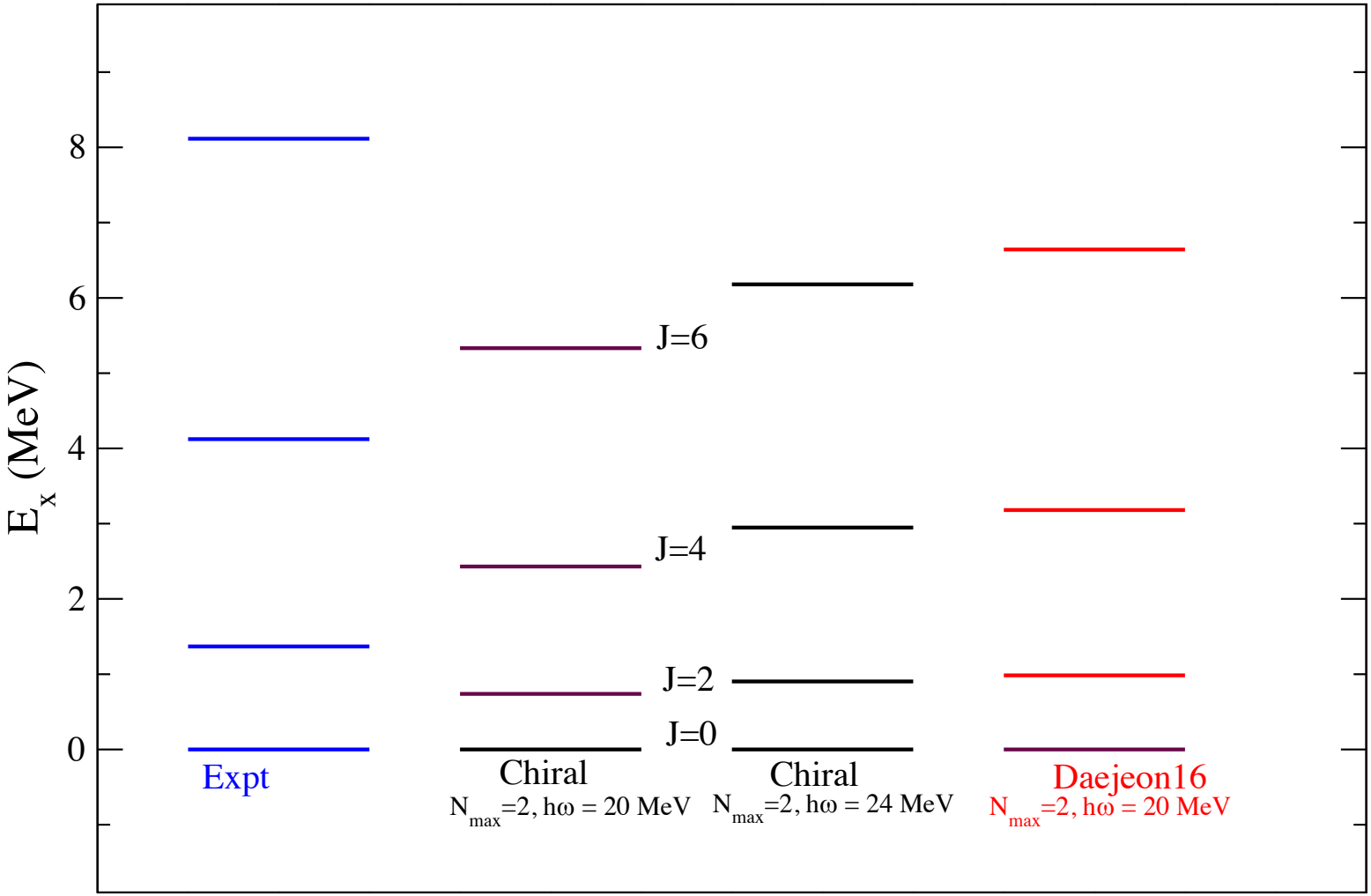

E_x (MeV)
0
2
4
6
8
J=6
J=4
J=2
J=0
Expt
Chiral
N_max=4, hω = 20 MeV
Chiral
N_max=4, hω = 24 MeV
Daejeon16
N_max=4, hω = 20 MeV

^{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)
0
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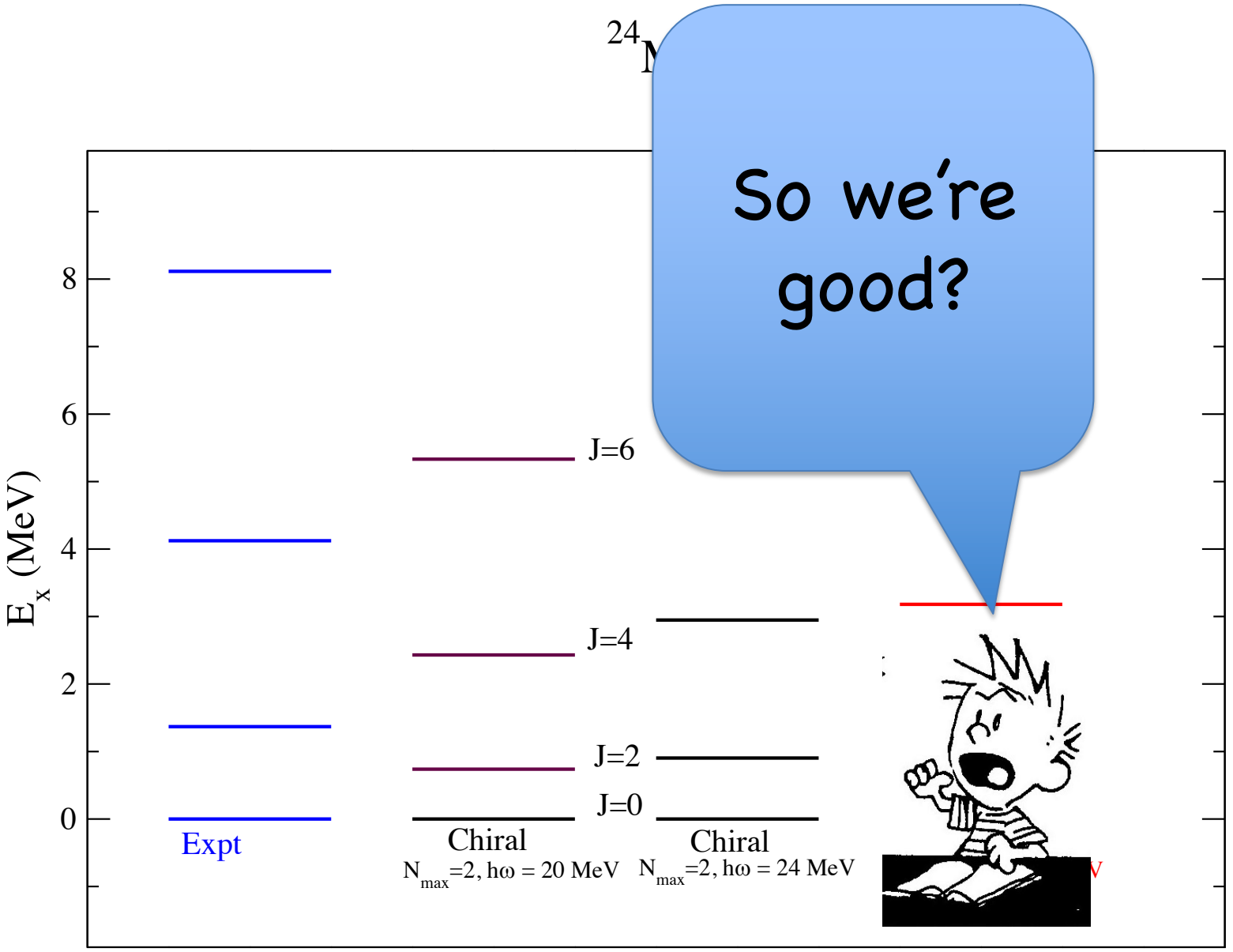
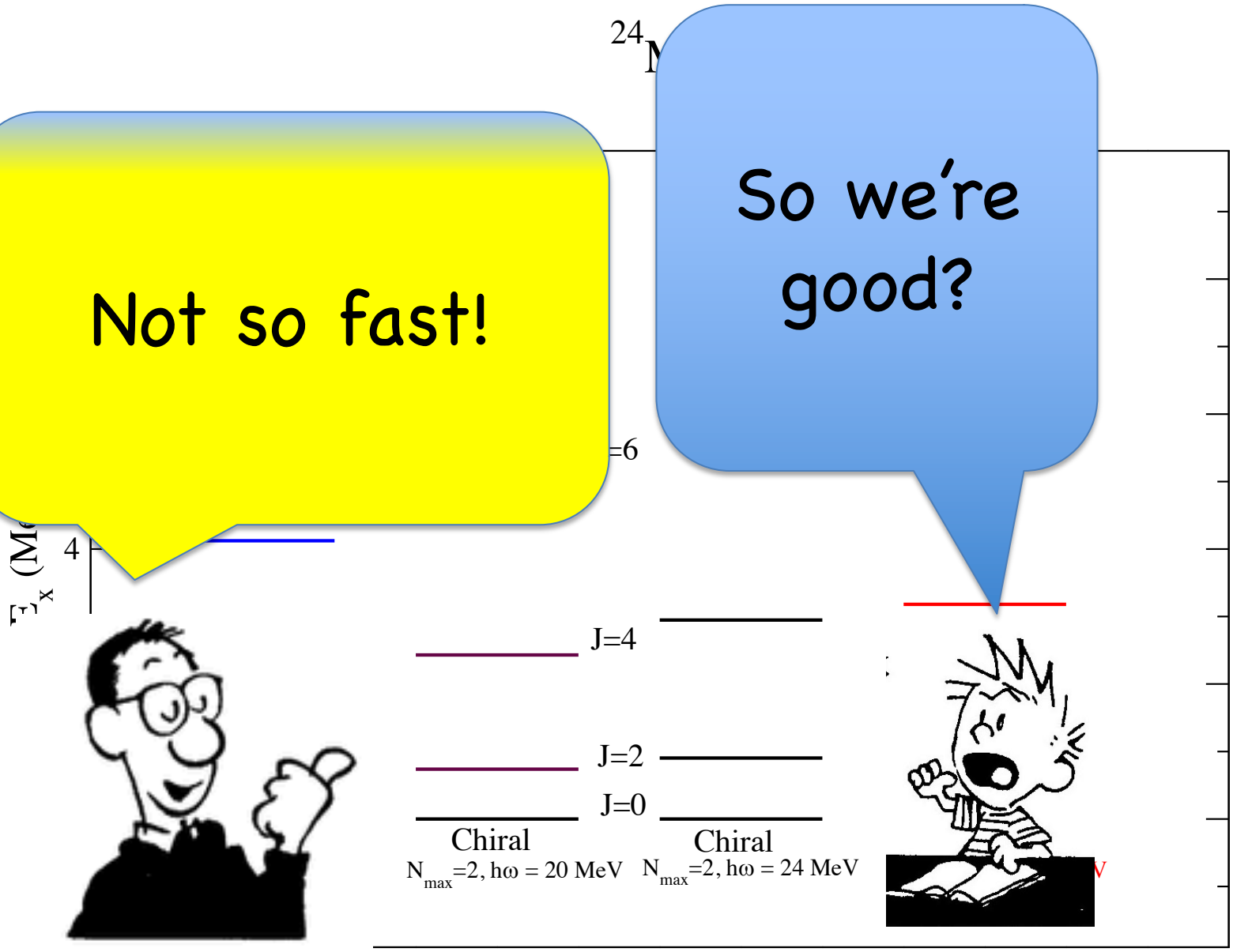
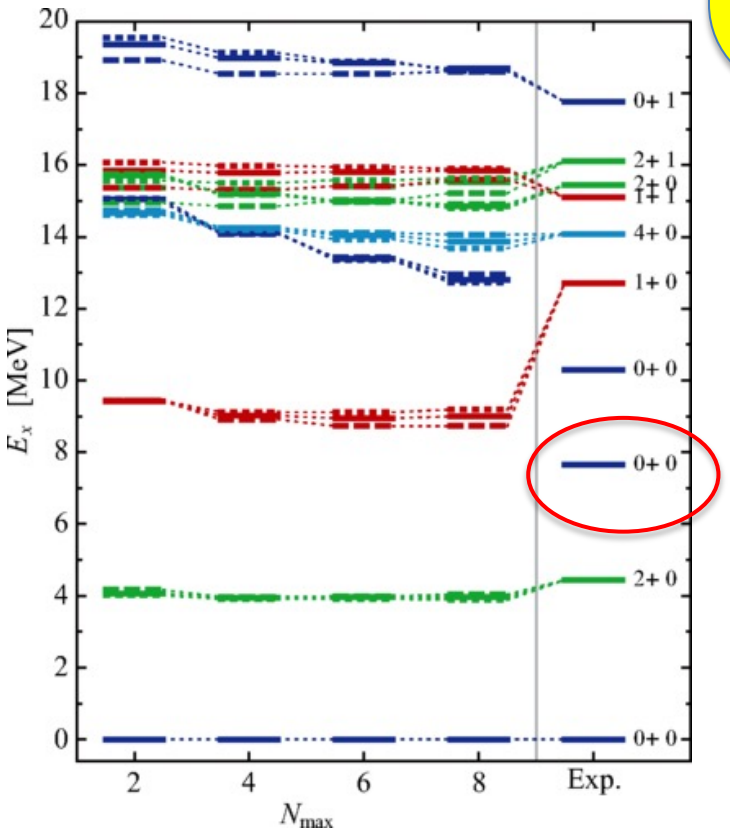

24
So we're good?
8
6
4
2
0
E_x (MeV)
J=6
J=4
J=2
J=0
Expt
Chiral
N_max=2, hω = 20 MeV
Chiral
N_max=2, hω = 24 MeV


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

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

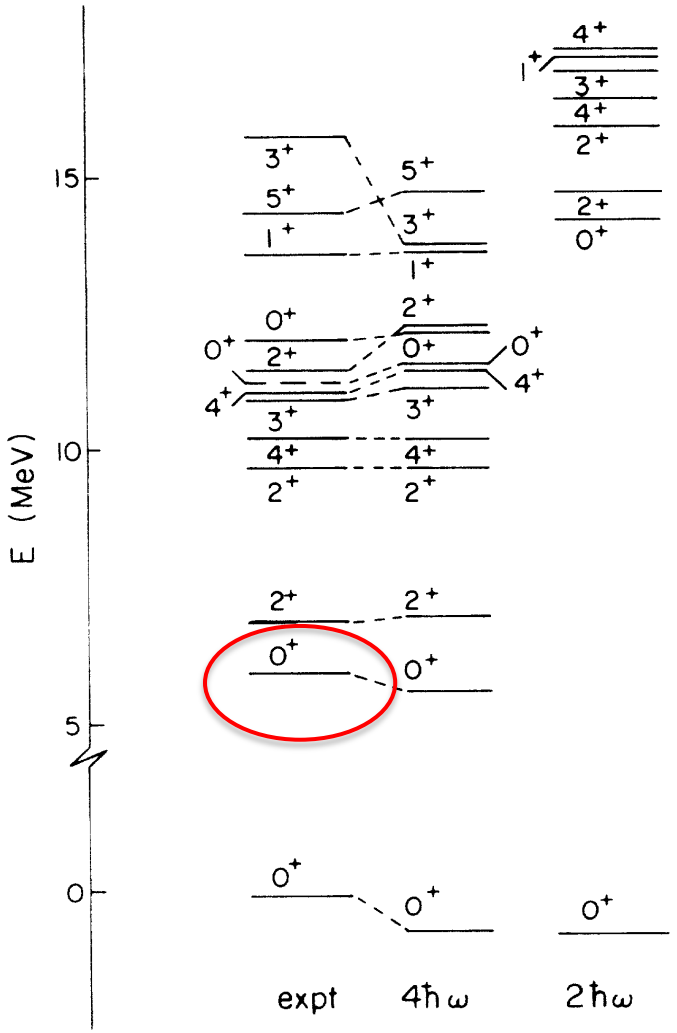
^{12}C with chiral 2+3 body forces



Hoyle state

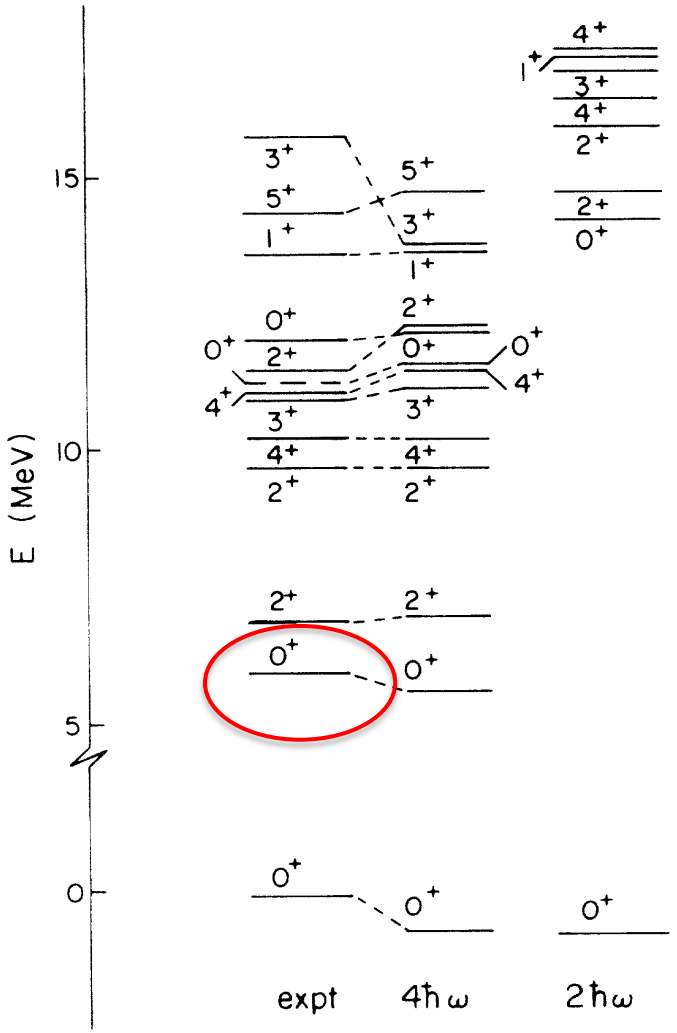
The Hoyle state in ^{12}C is a problem!

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

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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

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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

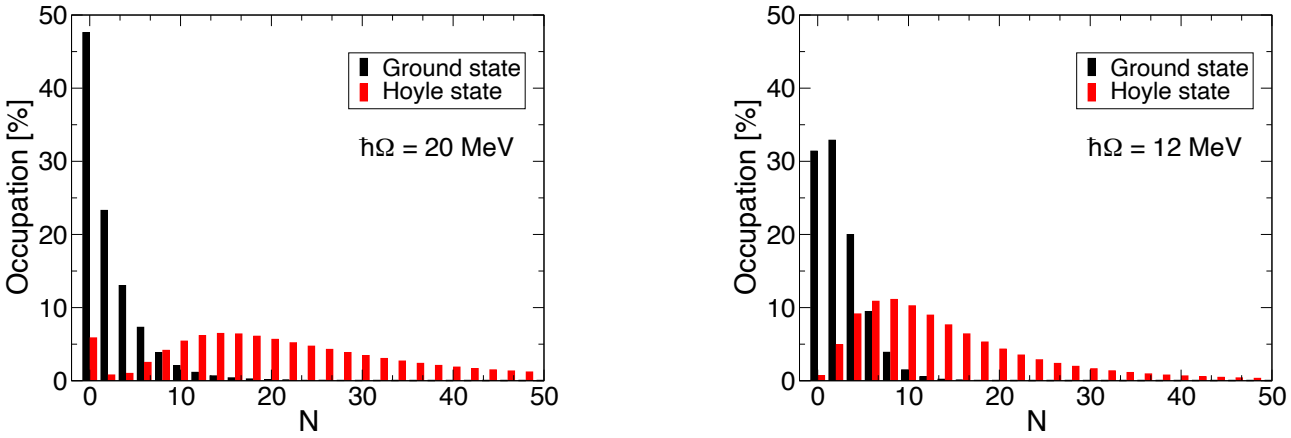

Figure 6. Decomposition of the ^{12}C ground state and the Hoyle state into $N\hbar\Omega$ components for oscillator constants of 20 MeV (left) and 12 MeV (right).

Fermionic molecular dynamics calculation with Argonne V18 potential

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

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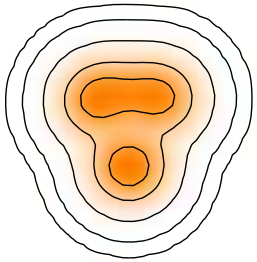
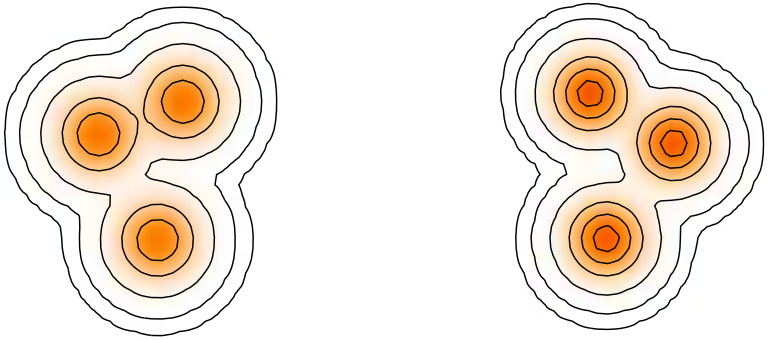
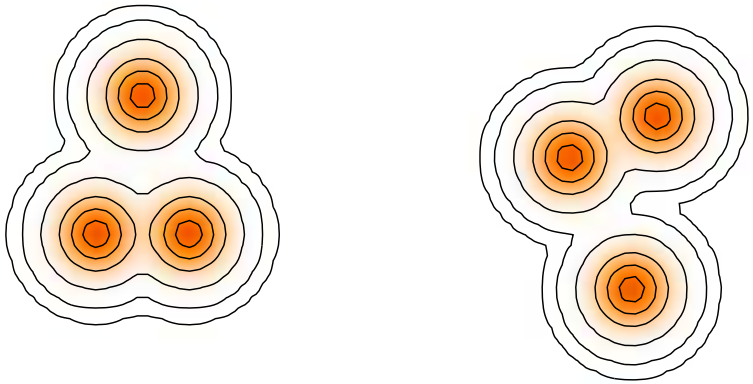


^{12}C g.s. (fermionic molecular dynamics FMD calculation)





^{12}C Hoyle state main FMD configurations.

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

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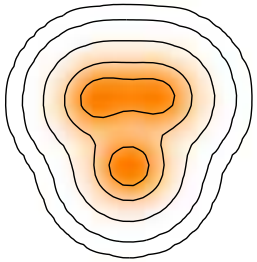
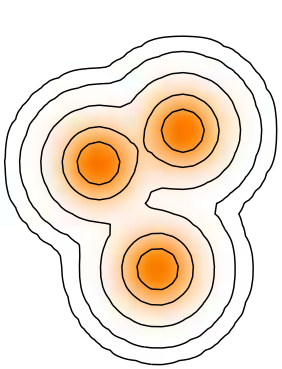
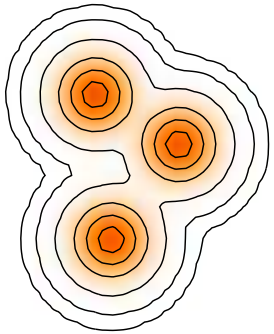
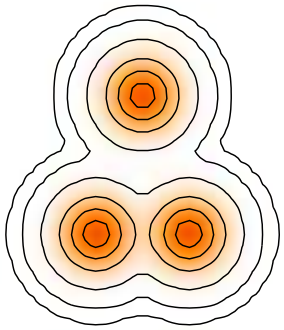
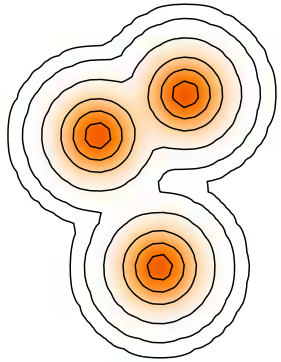


See also: S. Shen, D. Lee, et al, Nat. Commun. 14 (2023) 2777 (arXiv:2202.13596) for similar results on the lattice









^{12}C Hoyle state main FMD configurations.

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

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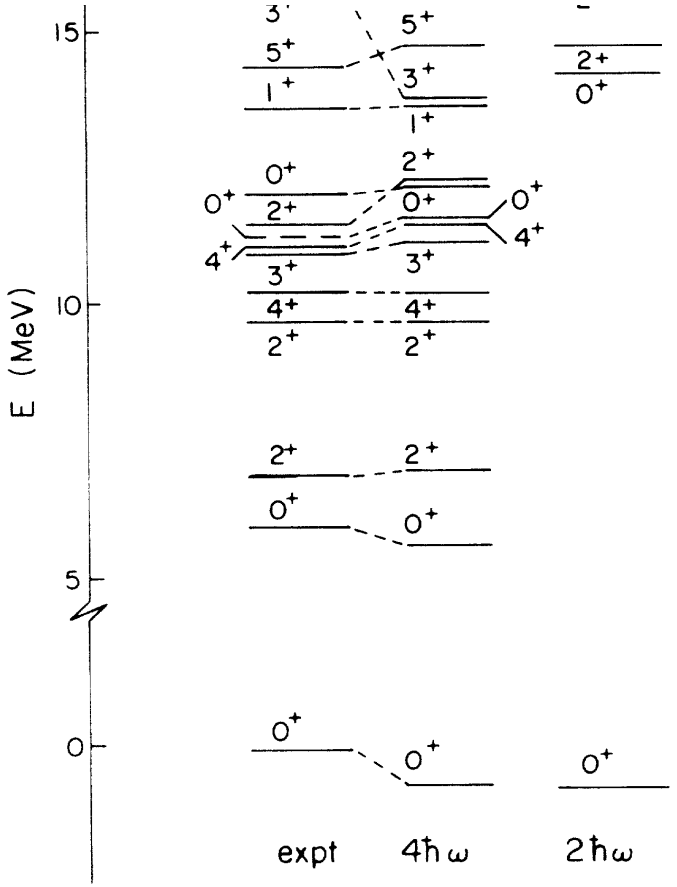
One can phenomenologically reproduce spectra for example, by adjusting single particle energies



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

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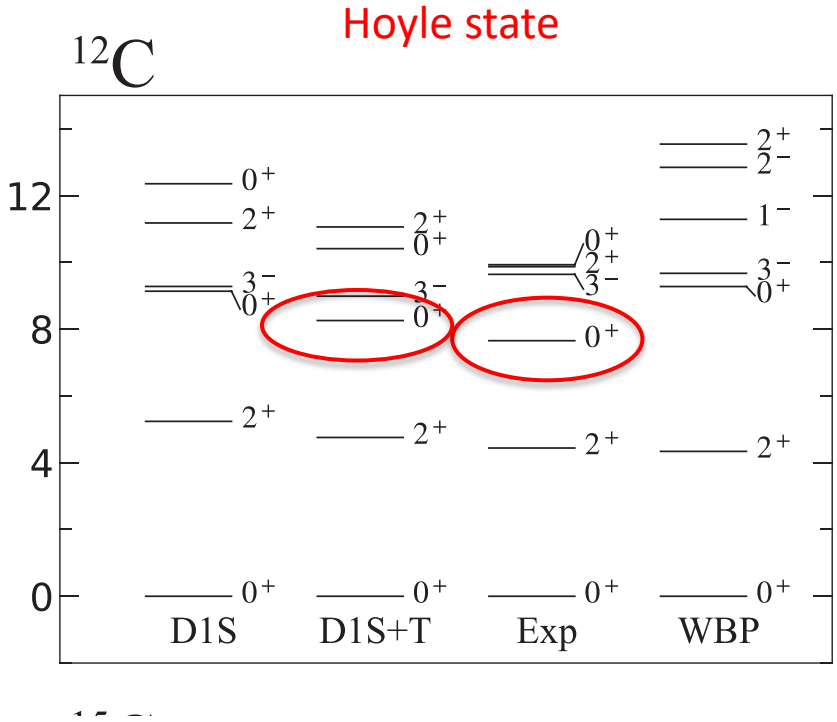

B. Dai, CWJ, et al, PRC 103, 064327 (2021)

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

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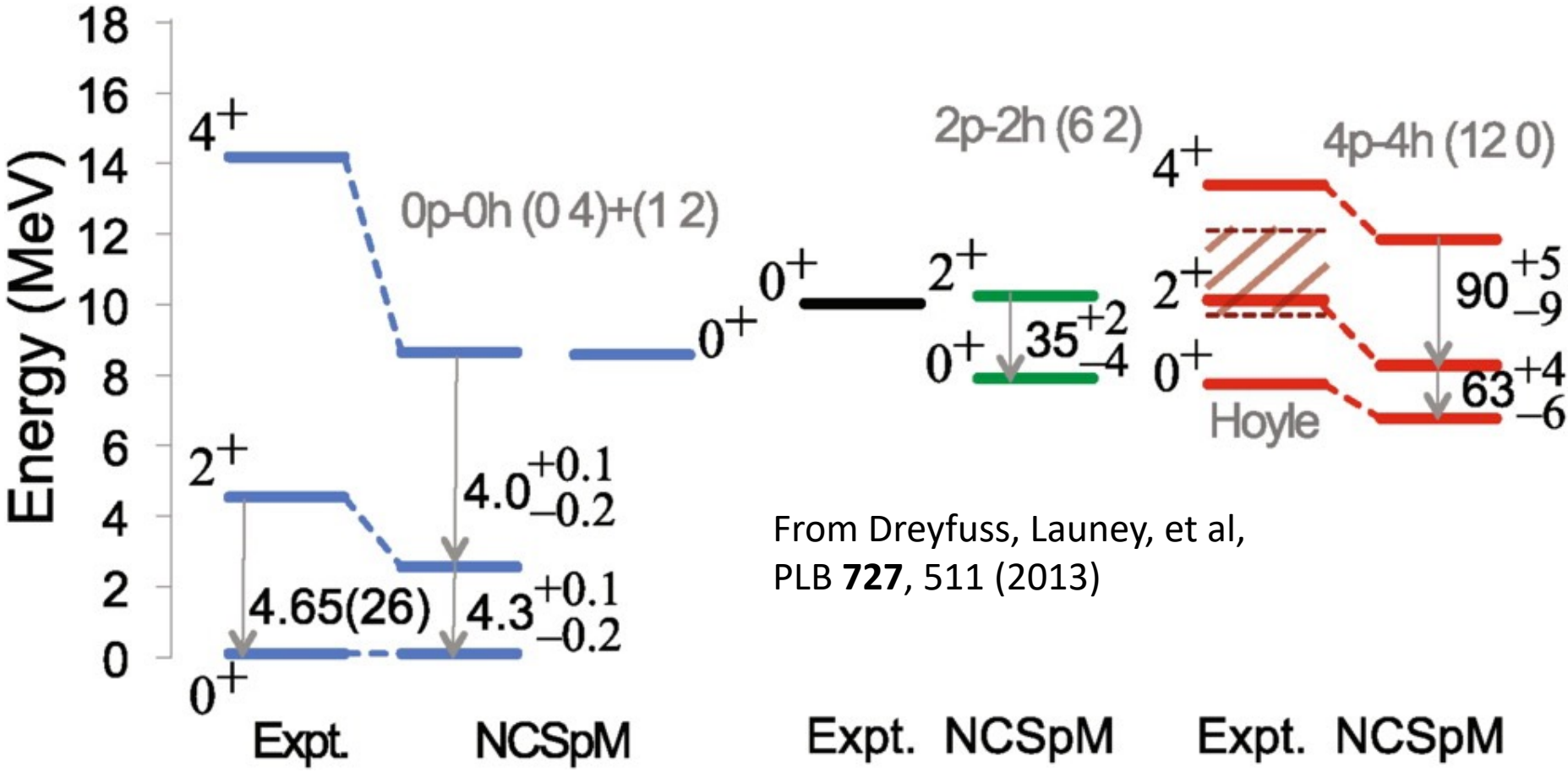
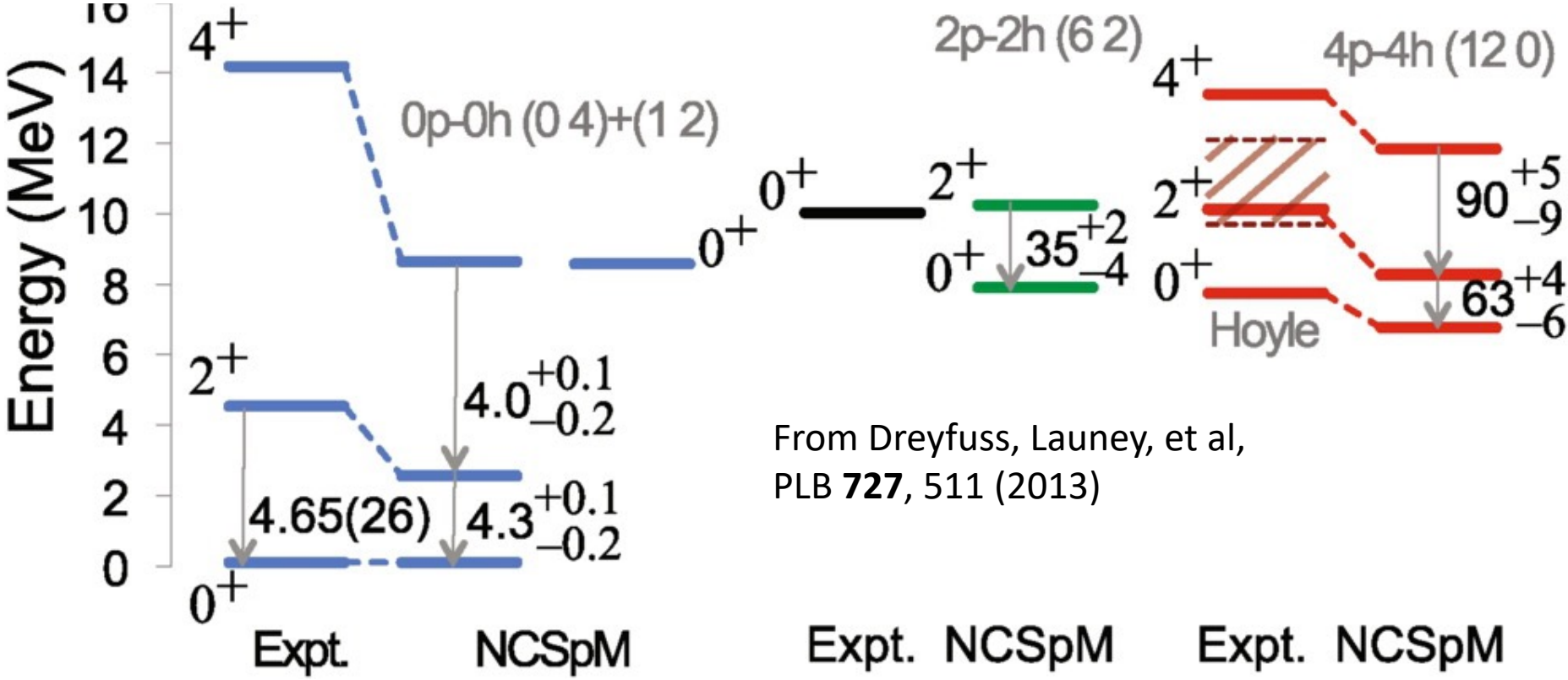
One can phenomenologically reproduce spectra or by adjusting the strength of an SU(3) Casimir



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

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

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

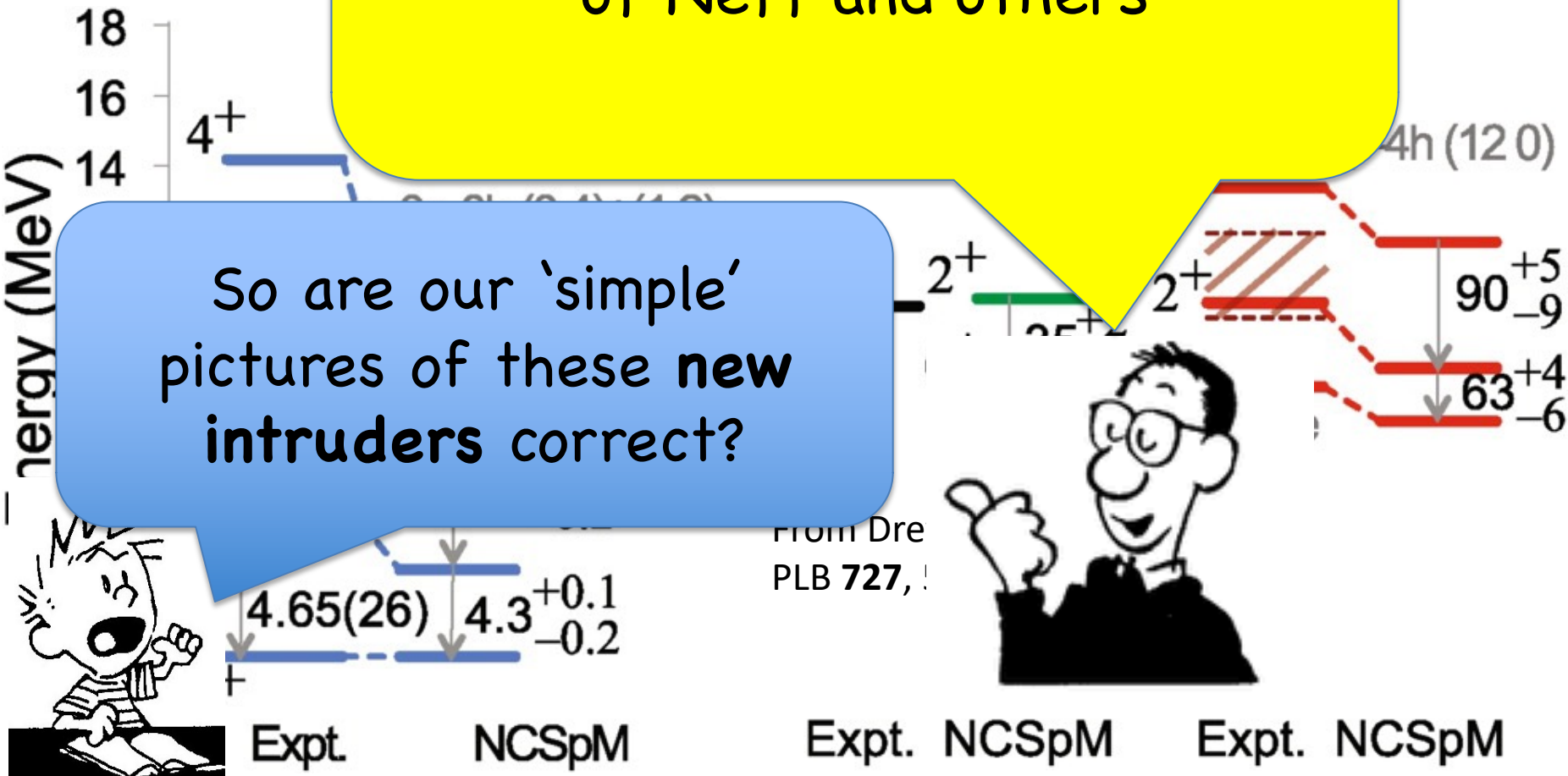


From Dreyfuss, Launey, et al,
PLB **727**, 511 (2013)

One can pher
or by adjustir

But this is a 4hω calculation, at variance with the 30+ hω of Neff and others

So are our 'simple' pictures of these **new intruders** correct?



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

Case study: ^{11}Li

San Diego State University

^{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

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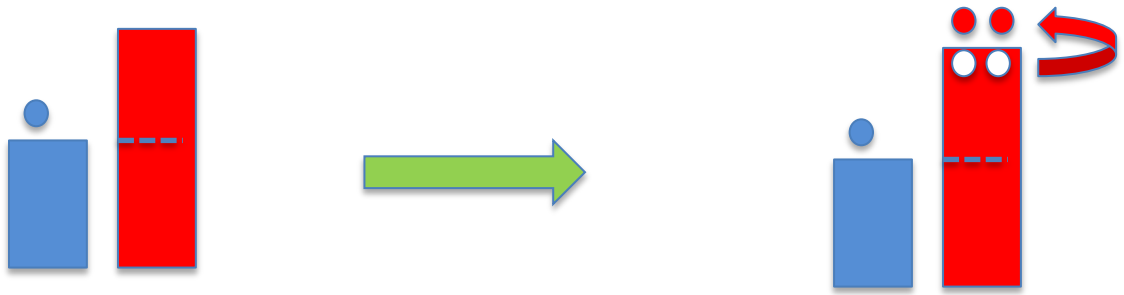


One proton outside a filled shell
+ filled neutron shell

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

"island of inversion"

CASE STUDY: ^{11}LI

SAN DIEGO STATE UNIVERSITY

^{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

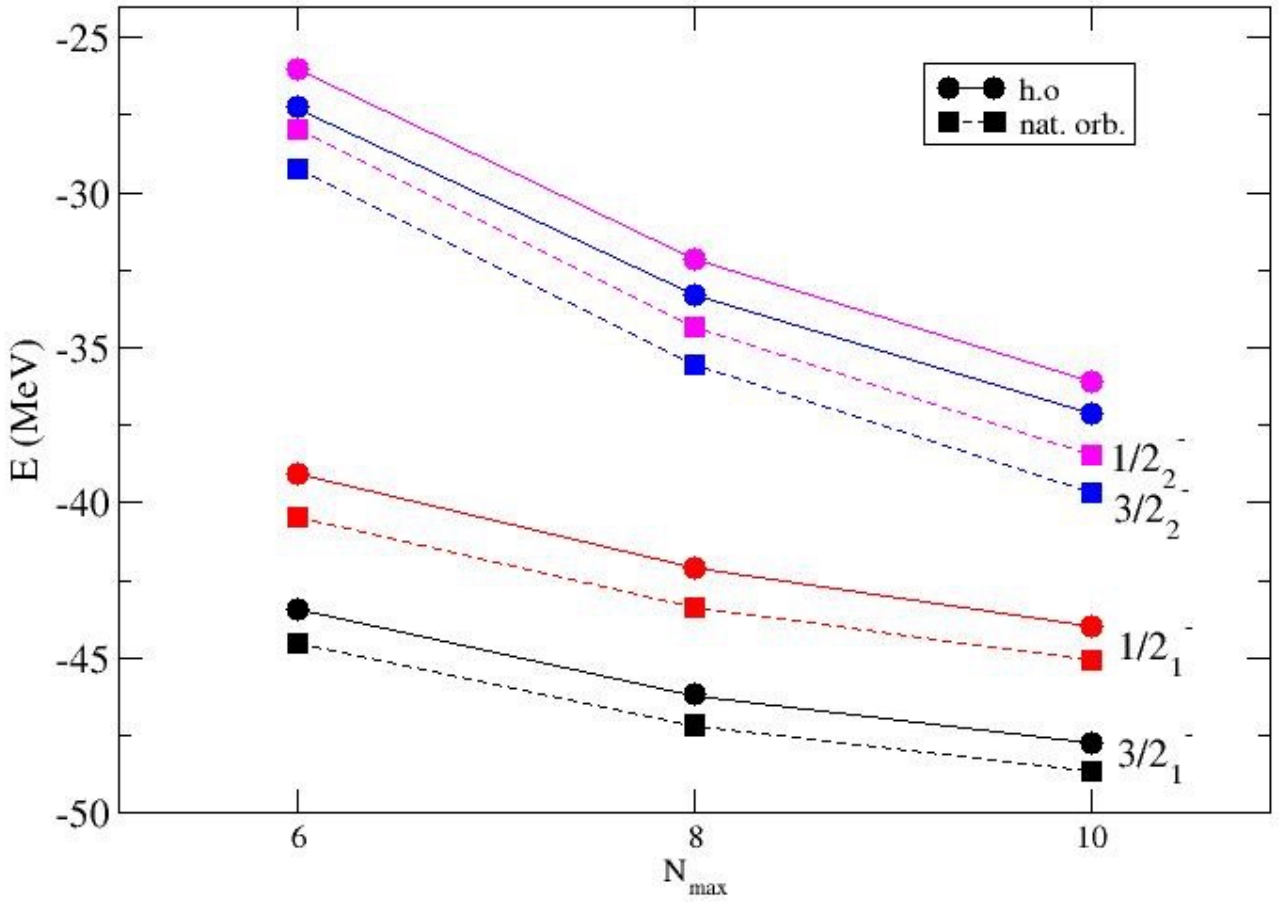
San Diego State University

^{11}Li makes for an excellent case study

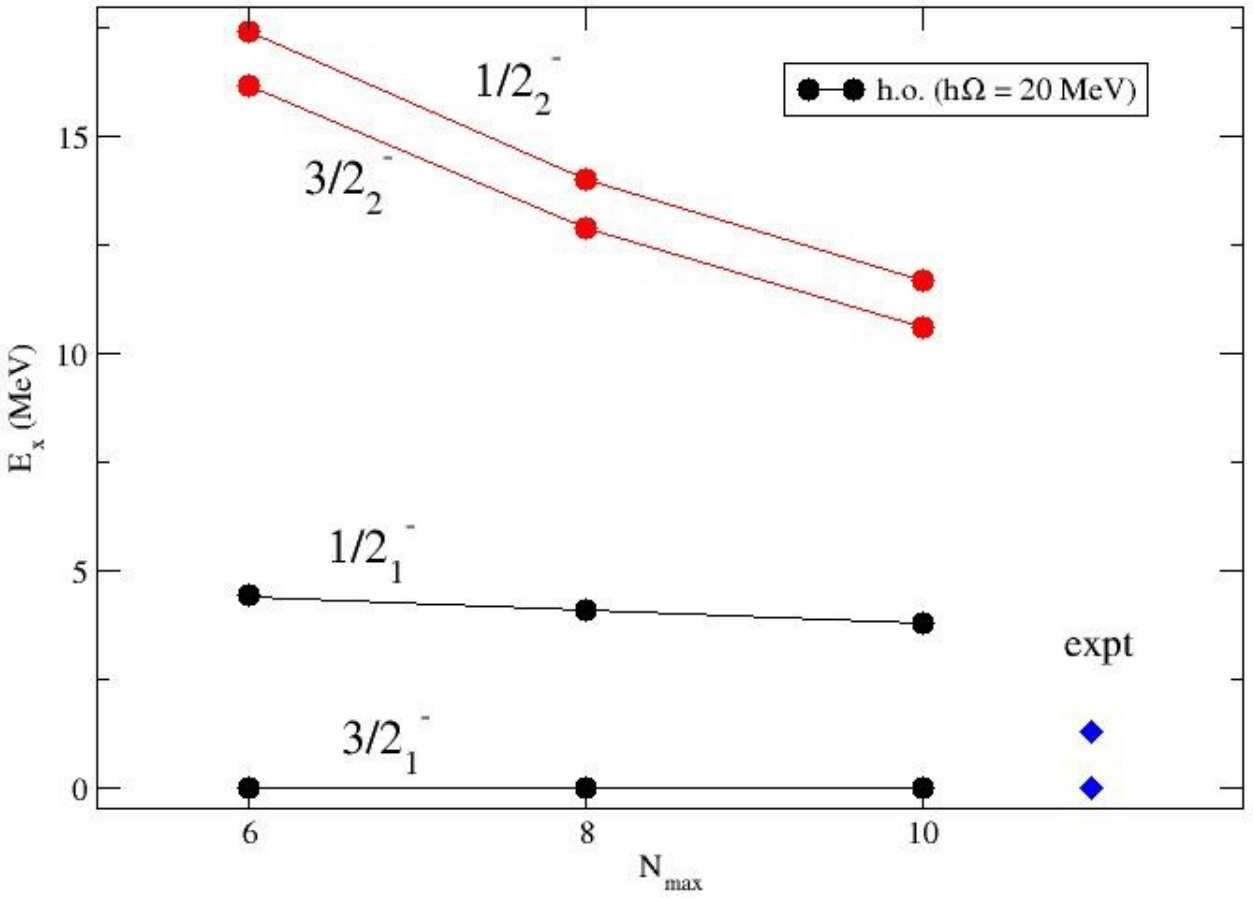
Calculations with Entem-Machleidt N3LO chiral (no 3-body) at $h\Omega$ = 20 MeV.

Also computed with natural orbitals

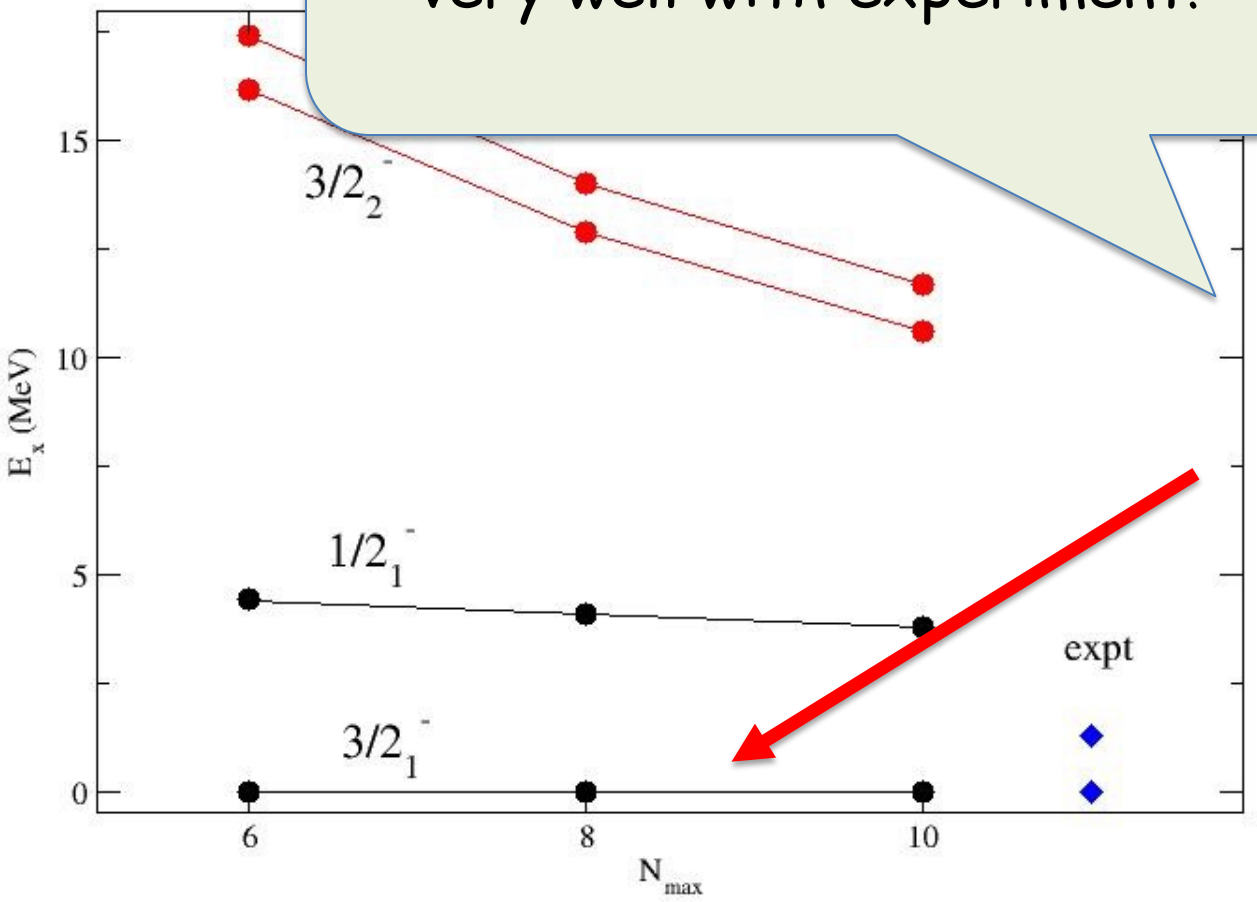
CASE STUDY: ^{11}LI



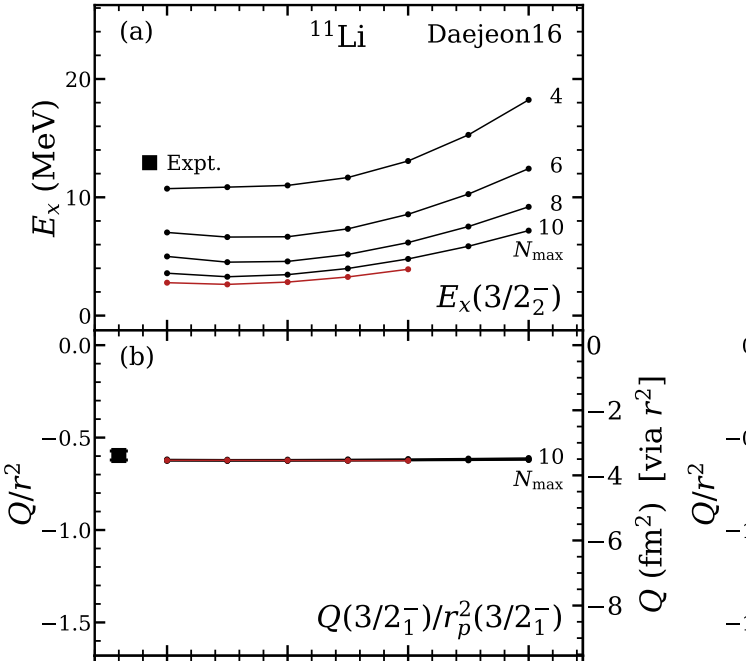
CASE STUDY: ^{11}LI



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

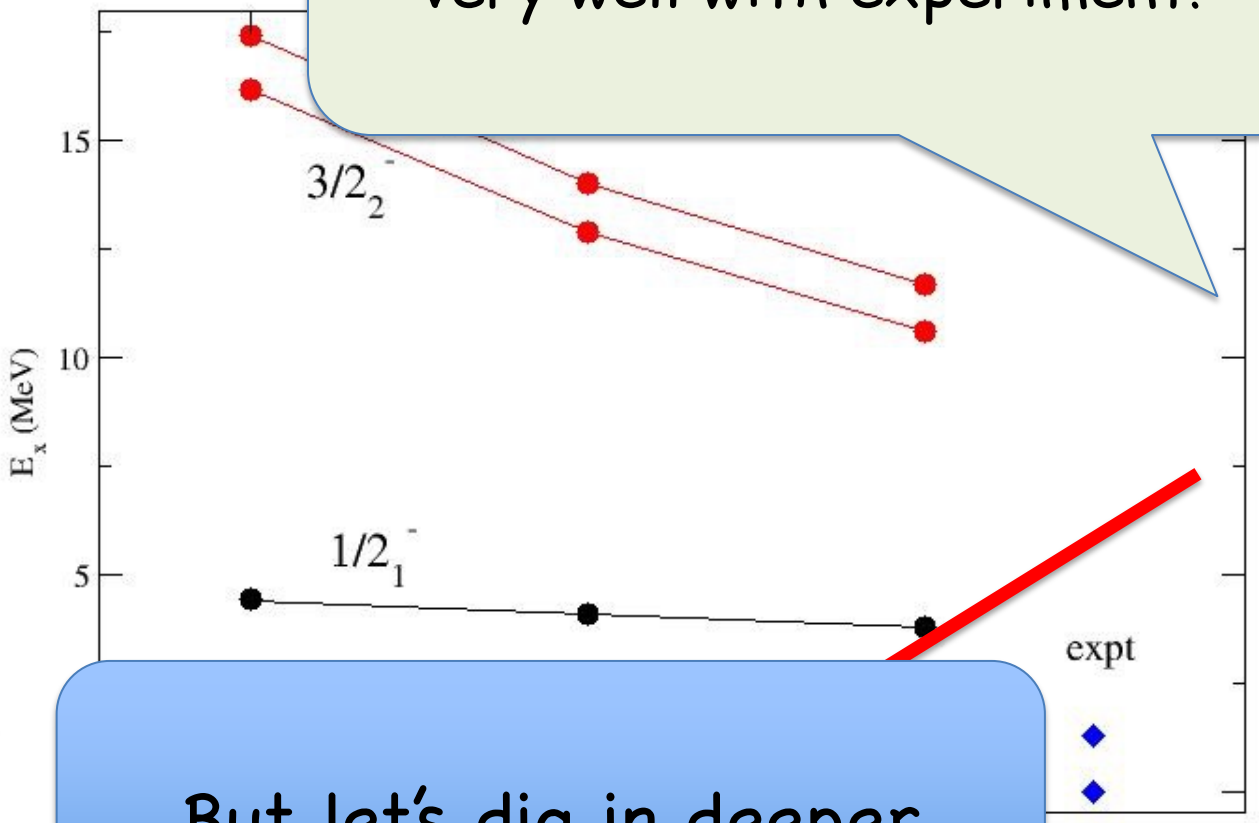


Mark Caprio


(a)
^{11}Li
Daejeon16
E_x (MeV)
Expt.
4
6
8
10
N_{max}
$E_x(3/2^-_2)$
(b)
Q/r^2
Q (fm^2) [via r^2]
$Q(3/2^-_1)/r^2_p(3/2^-_1)$

Mark Caprio

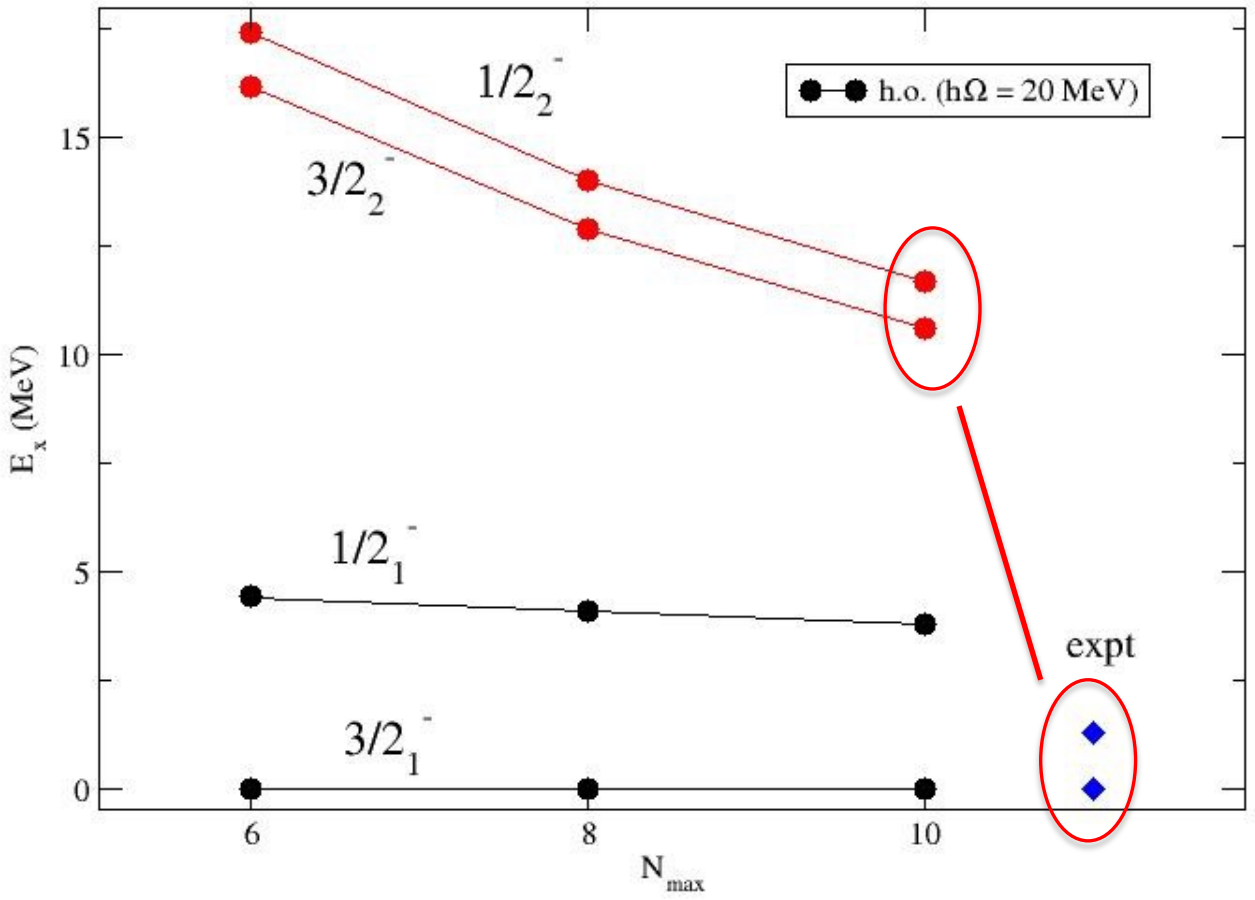
"The ratio Q_p/r^2_p agrees very well with experiment!"



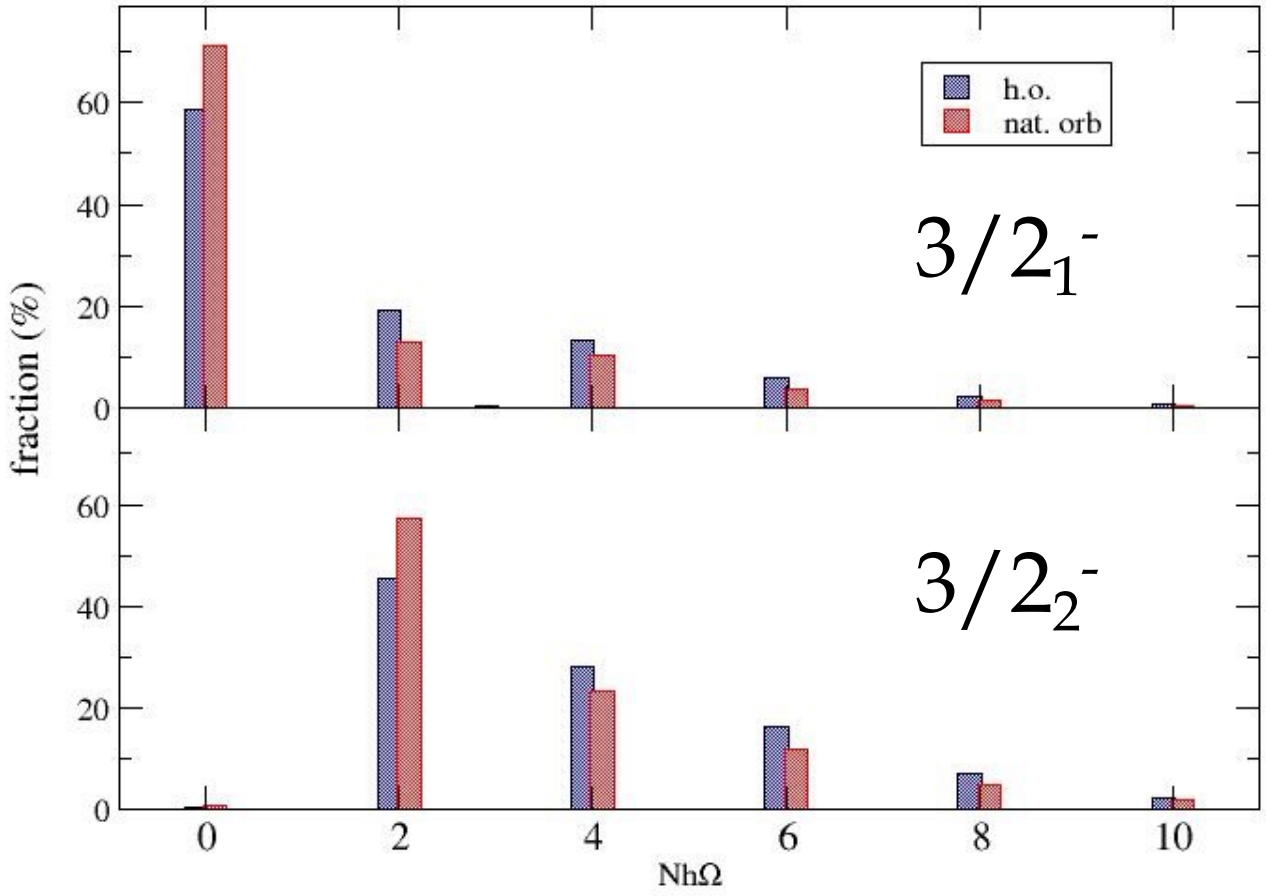
Mark Caprio

But let's dig in deeper

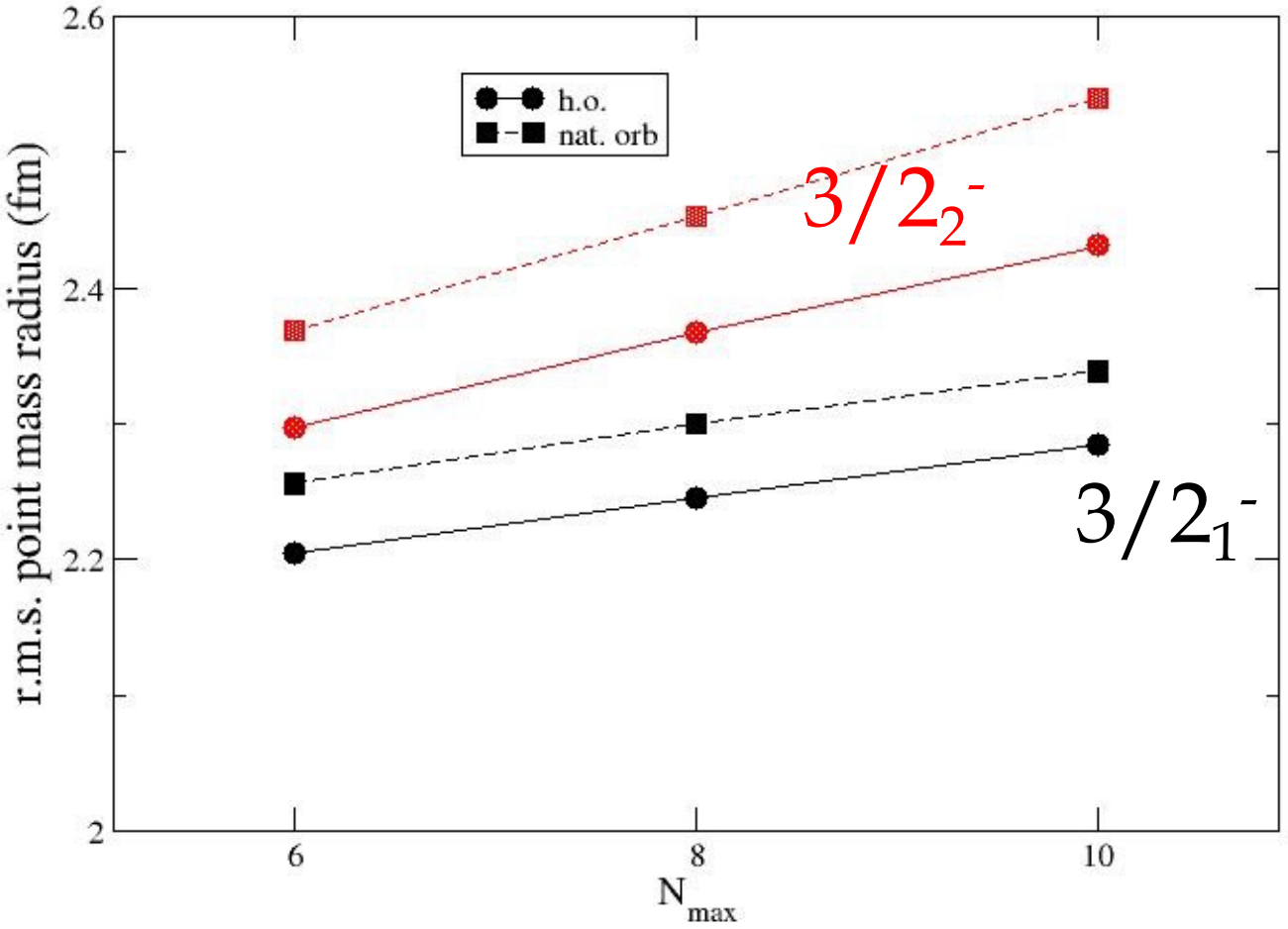
CASE STUDY: ^{11}LI



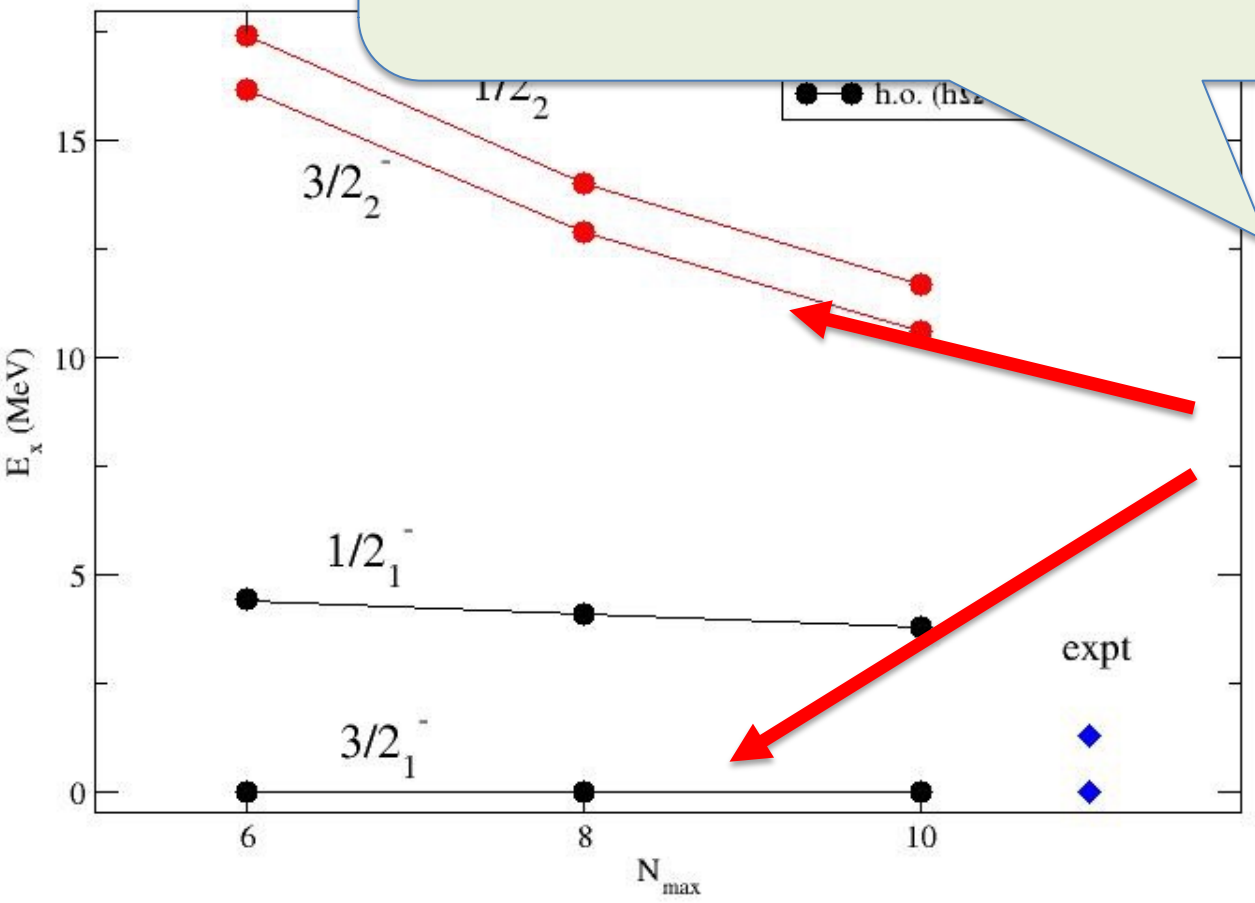
CASE STUDY: ^{11}LI



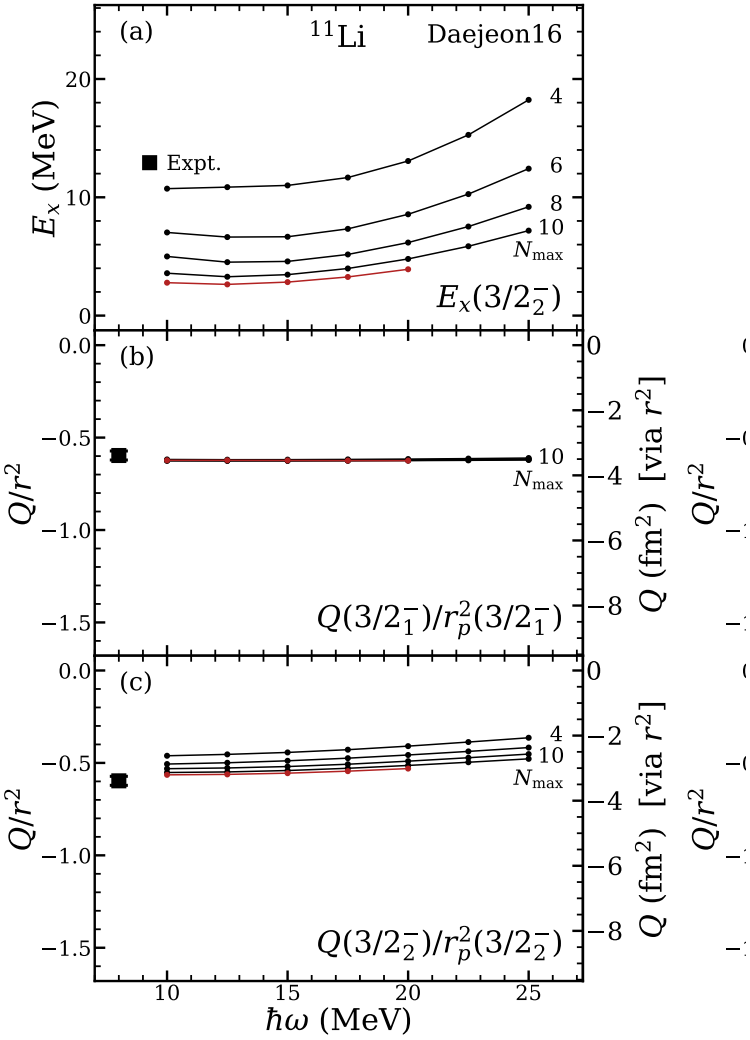
CASE STUDY: ^{11}LI



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

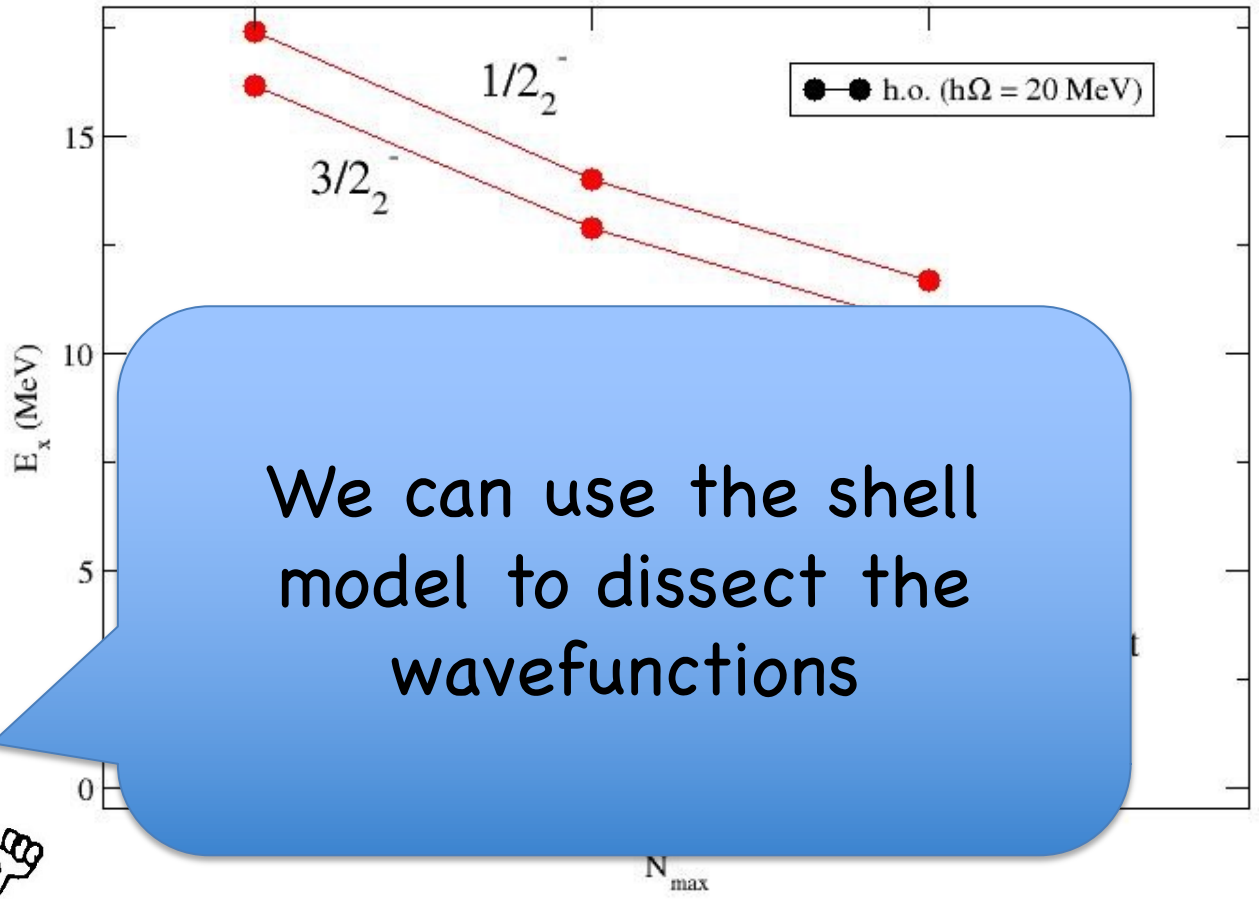


Mark Caprio


(a)
^{11}Li
Daejeon16
E_x (MeV)
Expt.
4
6
8
10
$N_{\max}$
$E_x(3/2_2^-)$
(b)
Q/r^2
$Q(3/2_1^-)/r_p^2(3/2_1^-)$
Q (fm^2) [via r^2]
(c)
$Q(3/2_2^-)/r_p^2(3/2_2^-)$
$\hbar\omega$ (MeV)

Mark Caprio

CASE STUDY: ^{11}LI



We can use the shell model to dissect the wavefunctions

CASE STUDY: ^{11}LI

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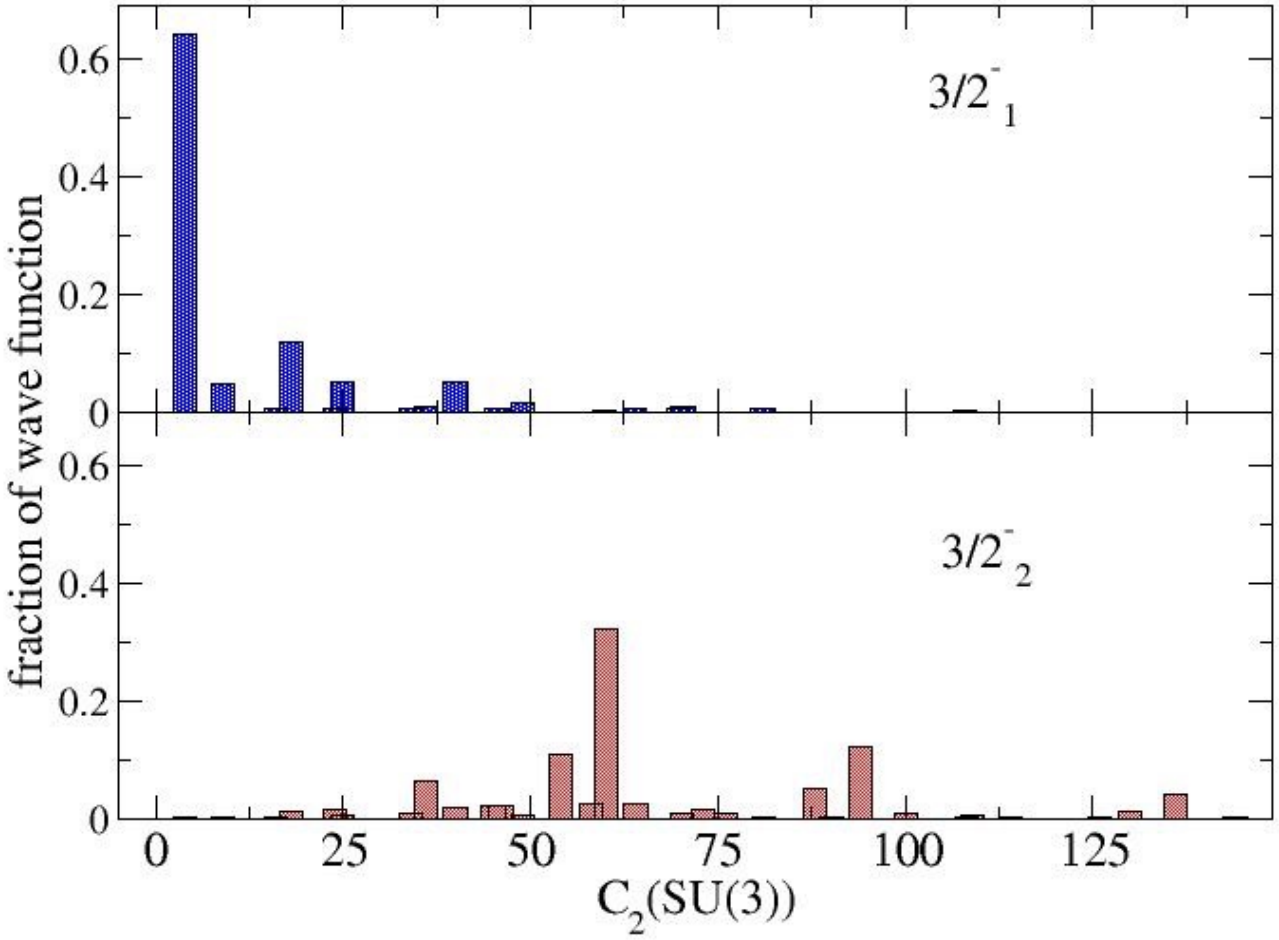

Group-theoretical Decomposition

Elliot SU(3)

CASE STUDY: ^{11}LI

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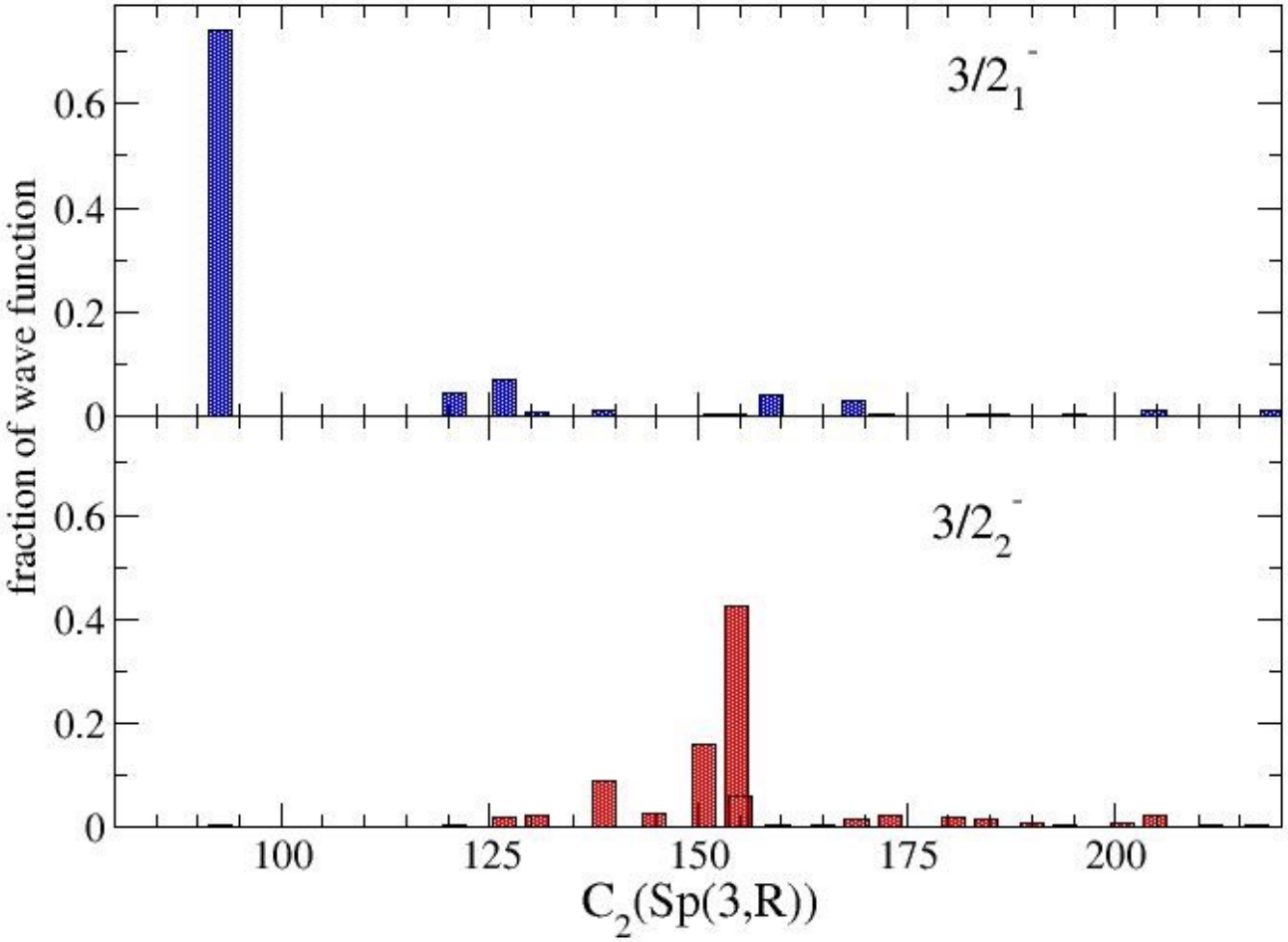

Group-theoretical Decomposition

Symplectic Sp(3,R)

CASE STUDY: ^{11}LI

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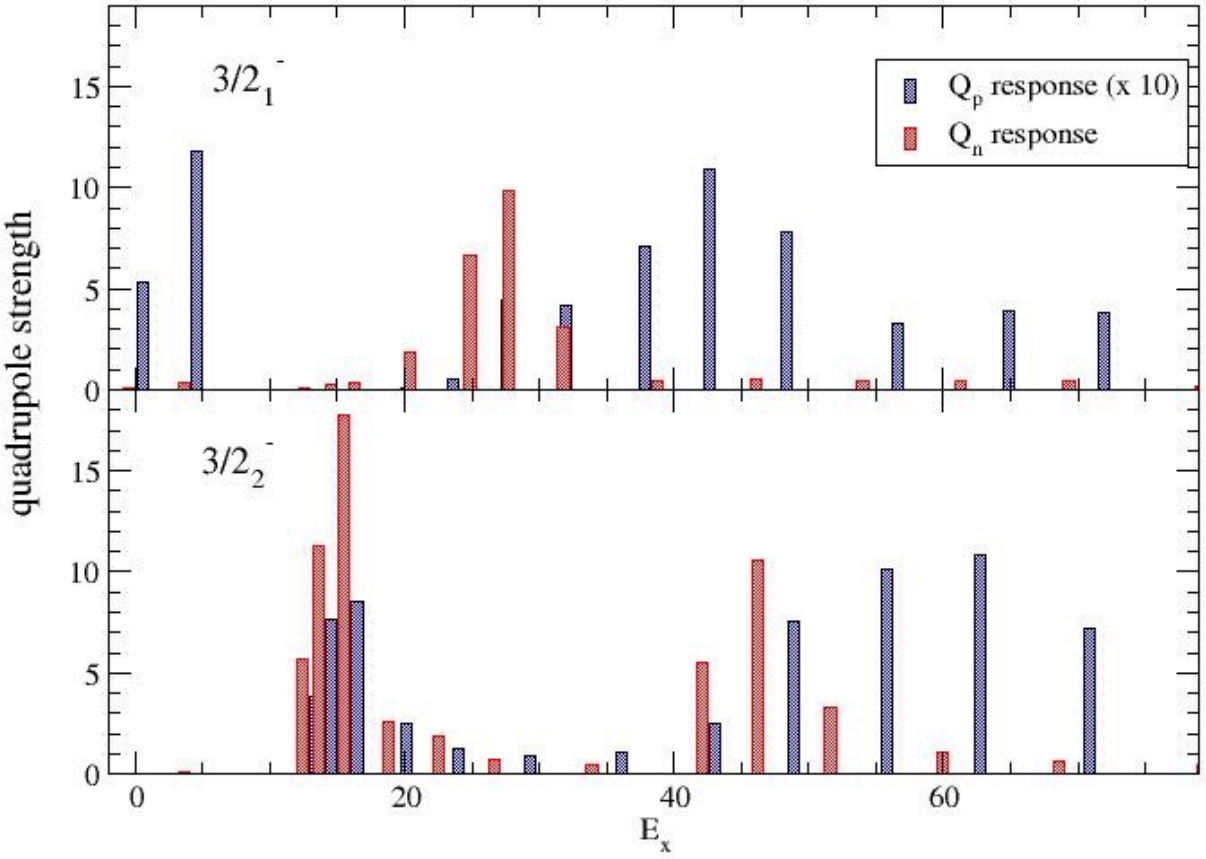

"E2" response

Probably not expt measurable, but double-hump illuminates deformation

CASE STUDY: ^{29}F

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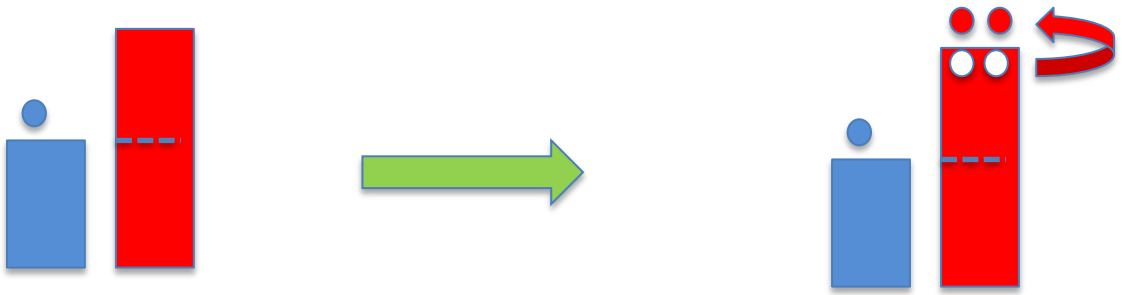
^{29}F is an analog of ^{11}Li



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

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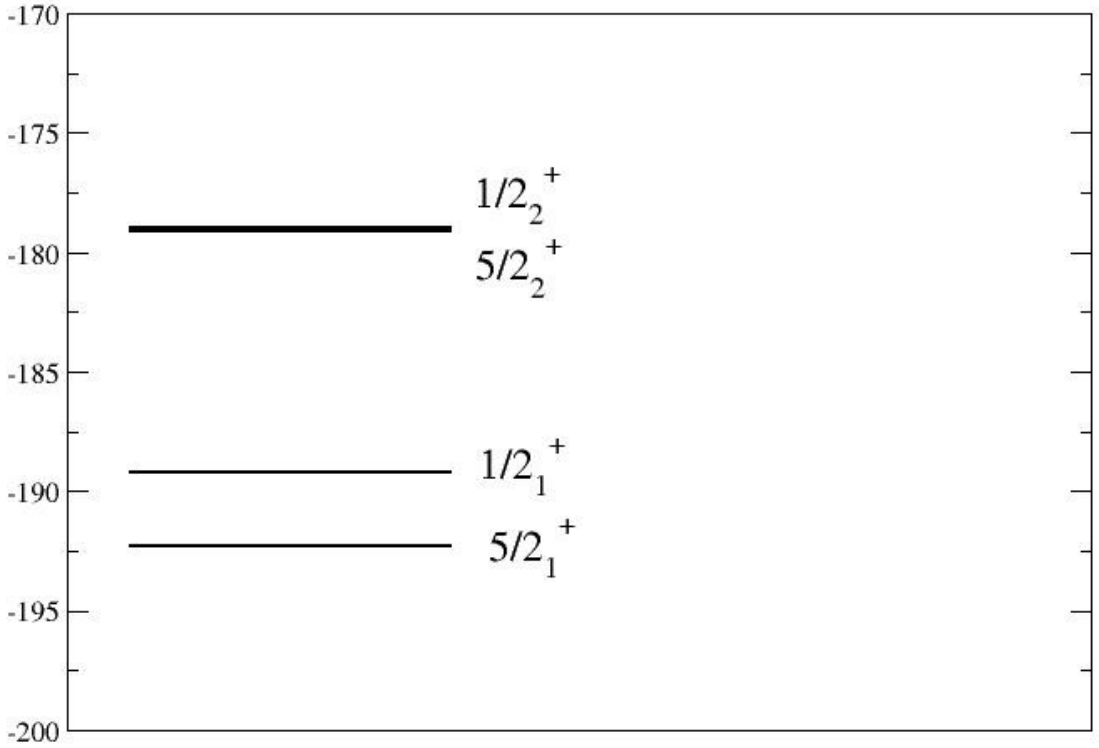
^{29}F is an analog of ^{11}Li (calculations done this week!)



N_{max} = 4, natural orbitals

CASE STUDY: ^{29}F

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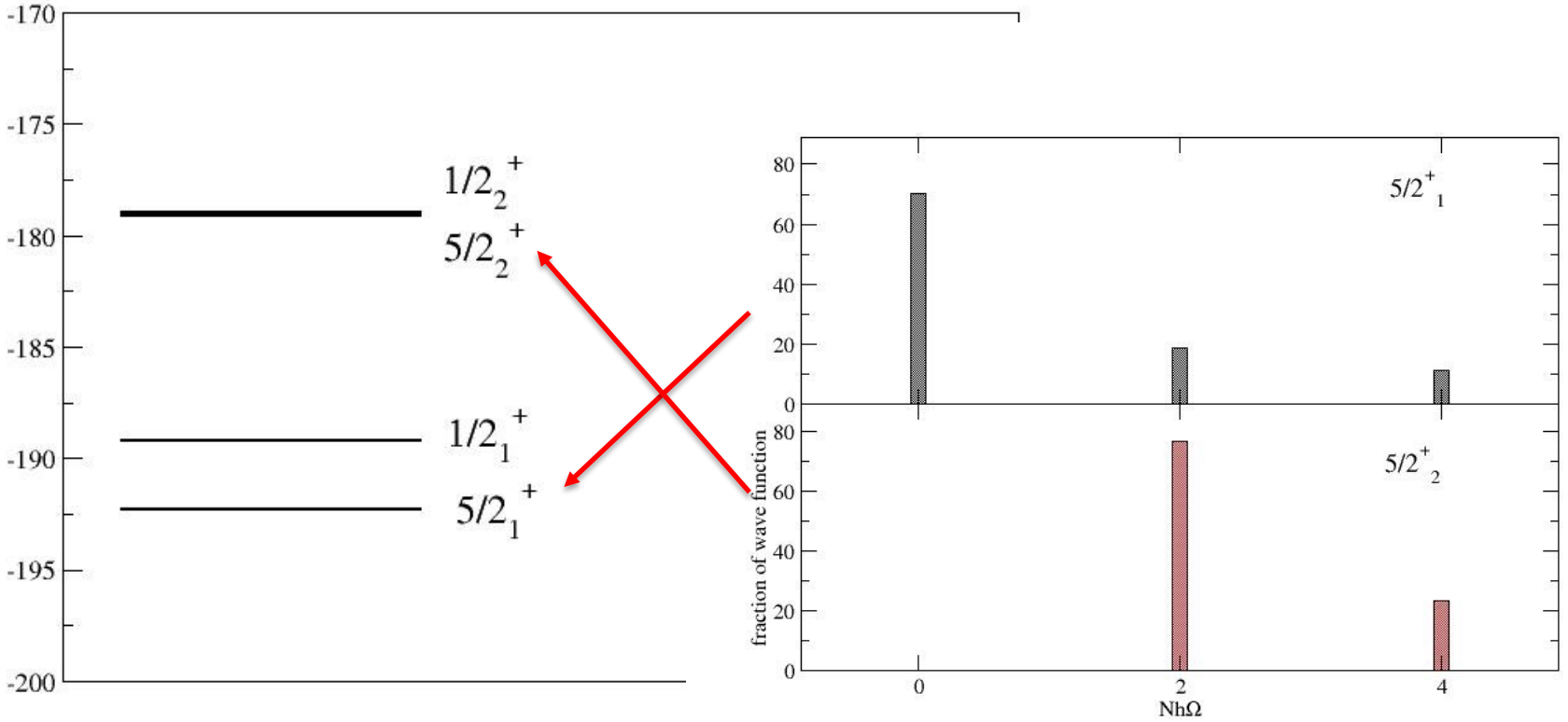
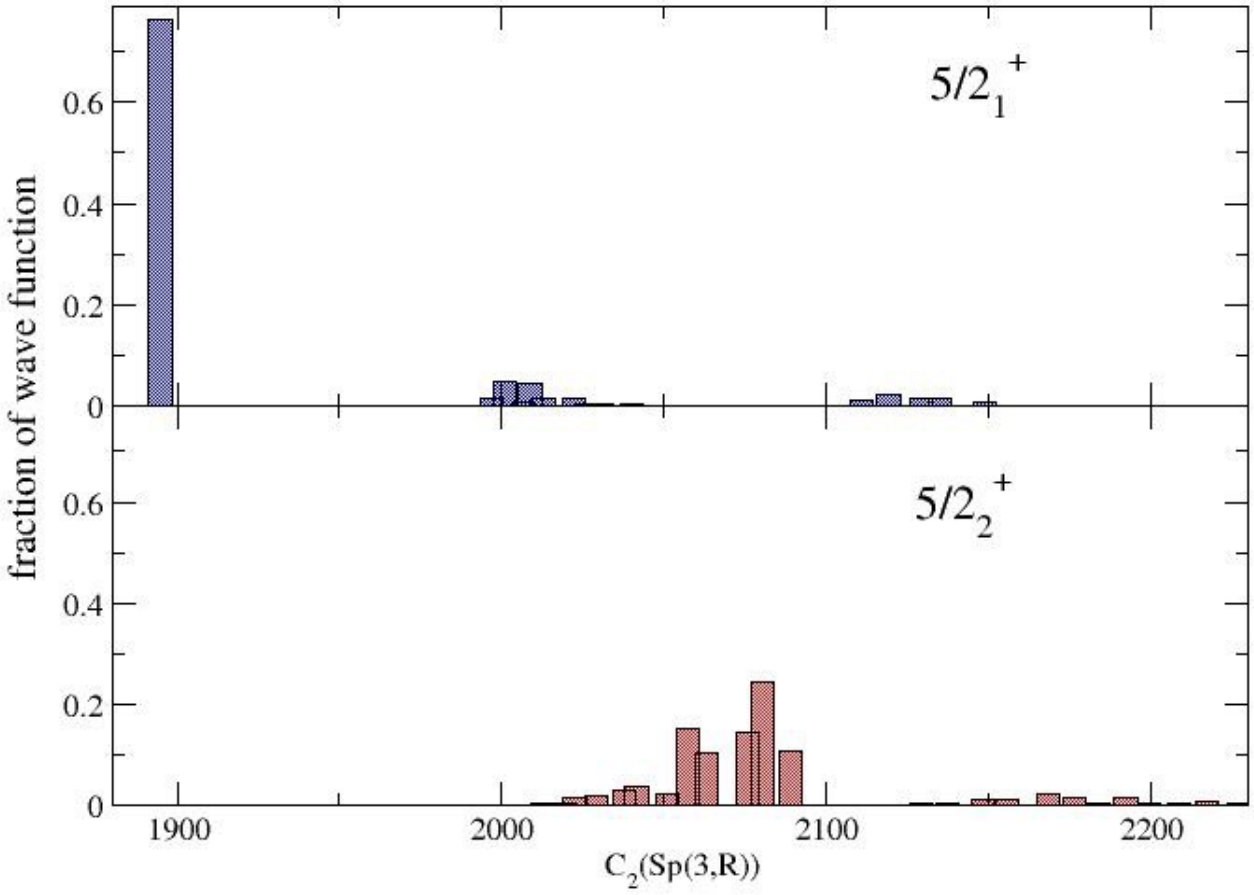
^{29}F is an analog of ^{11}Li (calculations done this week!)



N_{max} = 4, natural orbitals

CASE STUDY: ^{29}F

SAN DIEGO STATE UNIVERSITY



N_{max} = 4, natural orbitals

Group-theoretical Decomposition

Symplectic Sp(3,R)

CASE STUDY: ^{29}F

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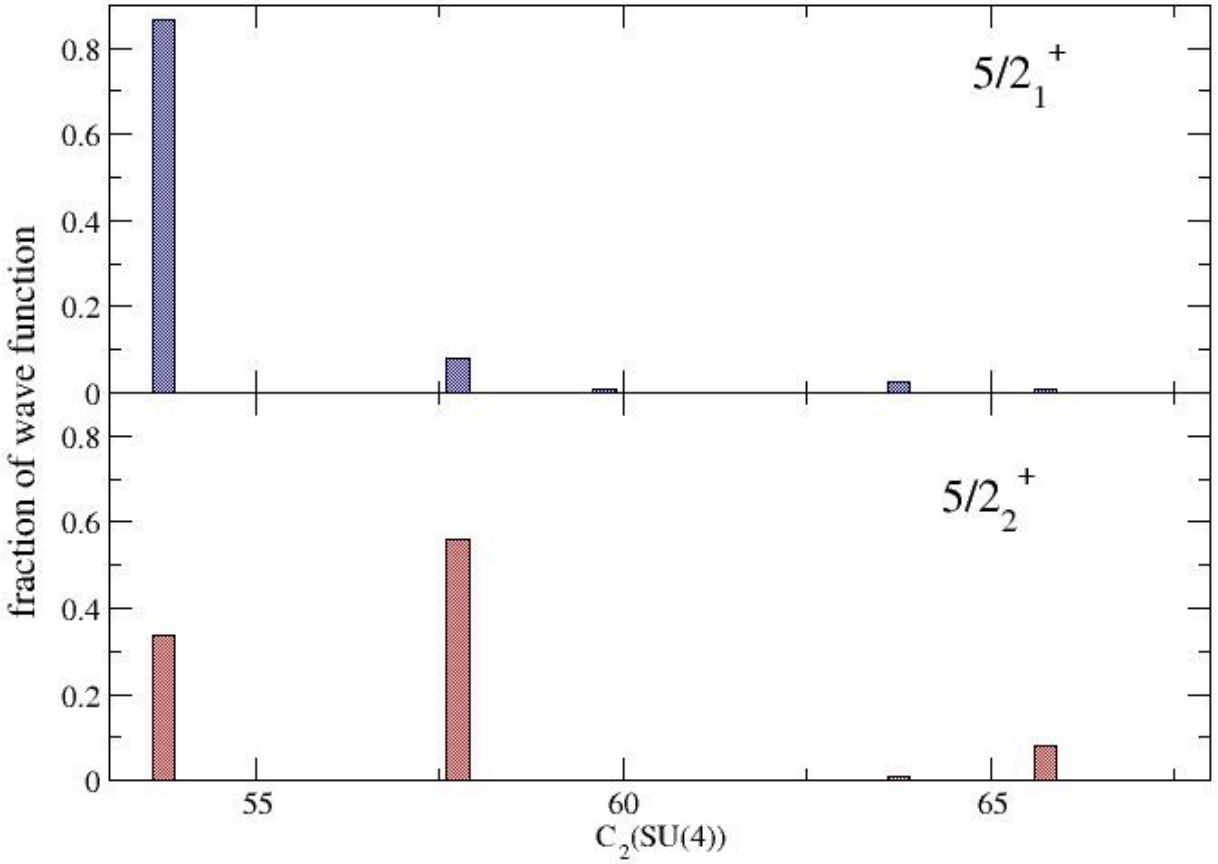

N_{max} = 4, natural orbitals

Group-theoretical decomposition

SU(4)

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.).

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**!

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These calculations were performed with an M-scheme (fixed-Jz) on-the-fly code.

Such on-the-fly codes (ANTOINE, BIGSTICK, etc) are extremely efficient (CWJ et al, Comp. Phys.Comm. 184, 2761(2013))

But even those codes have their limits

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

Strategies for moving forward

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- Many-body bases: algebraic and other cluster bases (see talks by (Caprio?) McCoy, Volya)

- Many-body bases from single-particle: projected Hartree-Fock + GCM (see talk by Nowacki)

- Proton-neutron truncated basis

- Energy-truncation of shell-model basis

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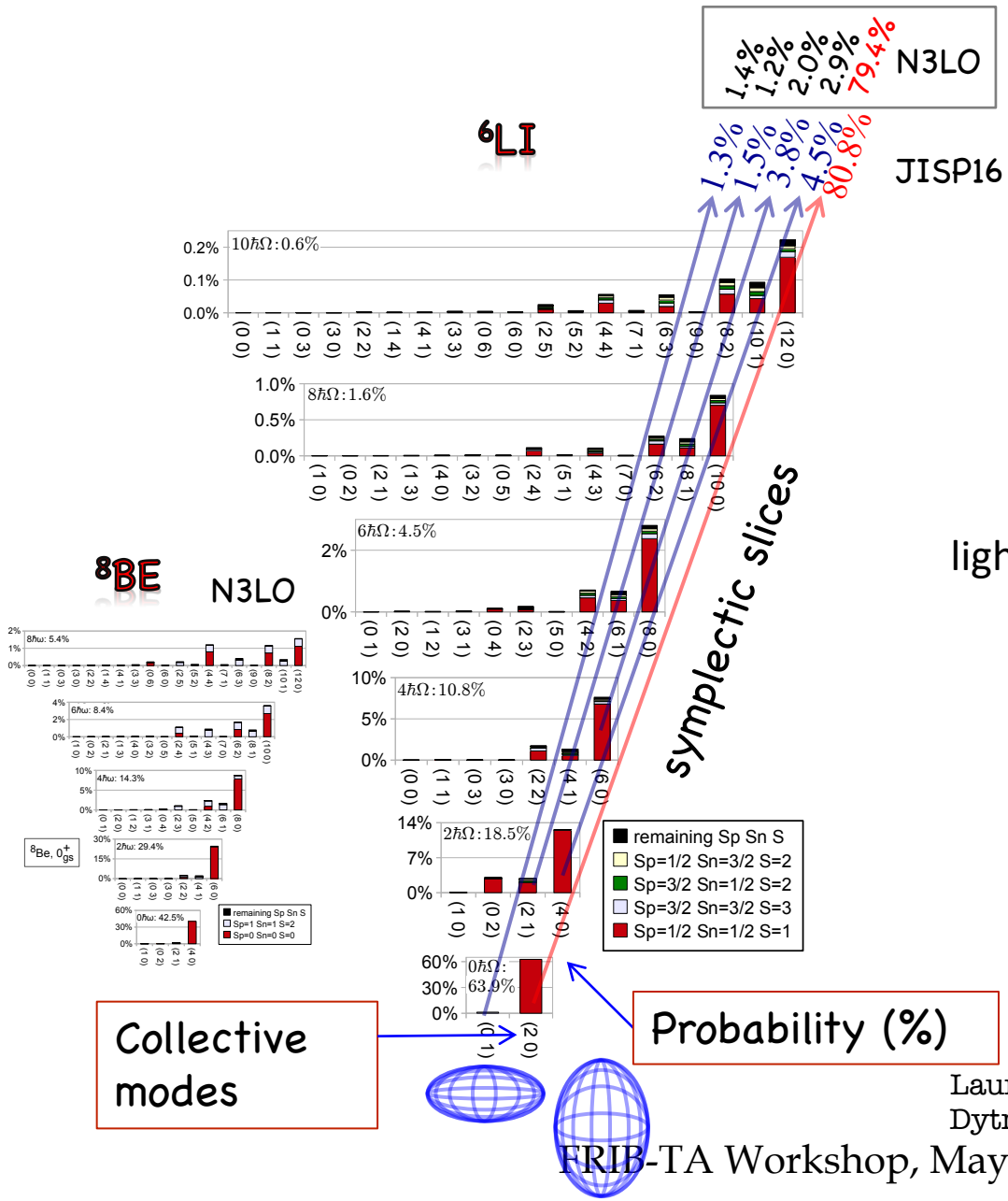
Symplectic Sp(3,R) Symmetry



(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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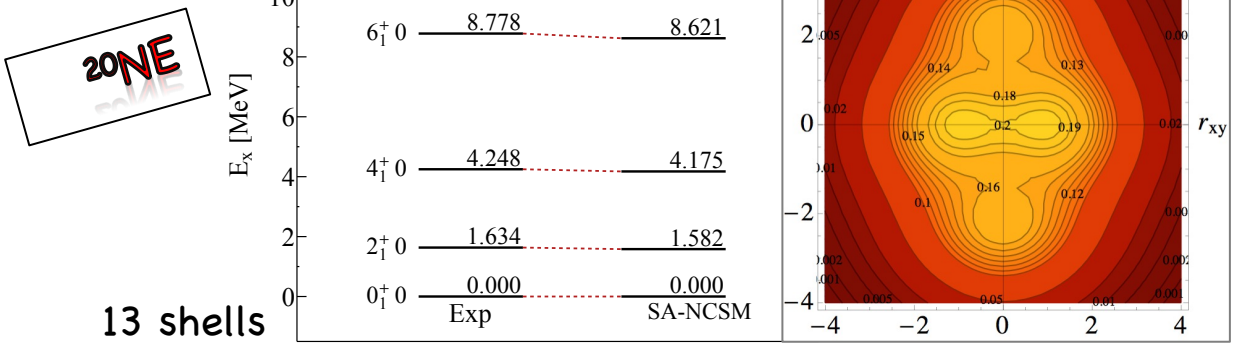


13 shells

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

Complete model space: 1000 billion states

^{18}Ne, B(E2: $2^+ \to 0^+$)

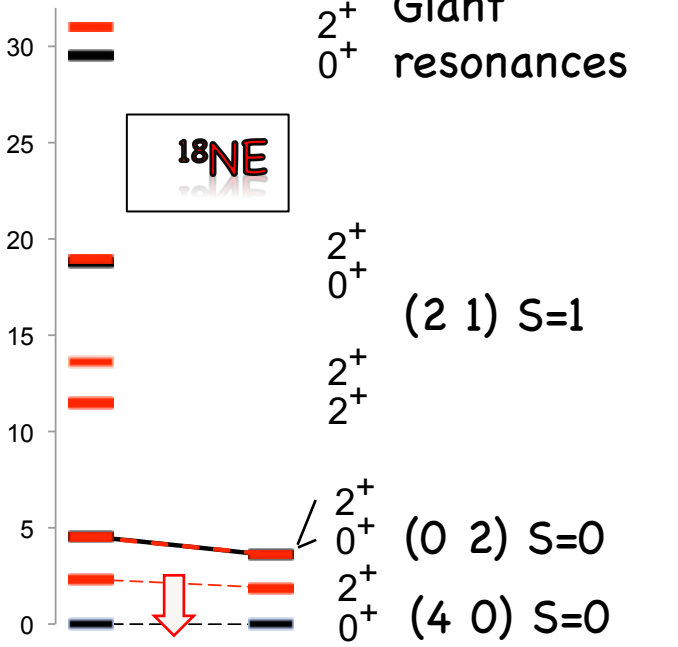
Experiment…… 17.7(18) W.u.

9 shells …… 1.13 W.u.

33 shells ……. 13.0(7) W.u.

(no effective charges)

Ne & Mg isotopes



N2LOopt; 9 shells, ħω = 15 MeV

Grigor Sargsyan, PhD student, LSU

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Group theory may be a natural framework for cluster physics

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

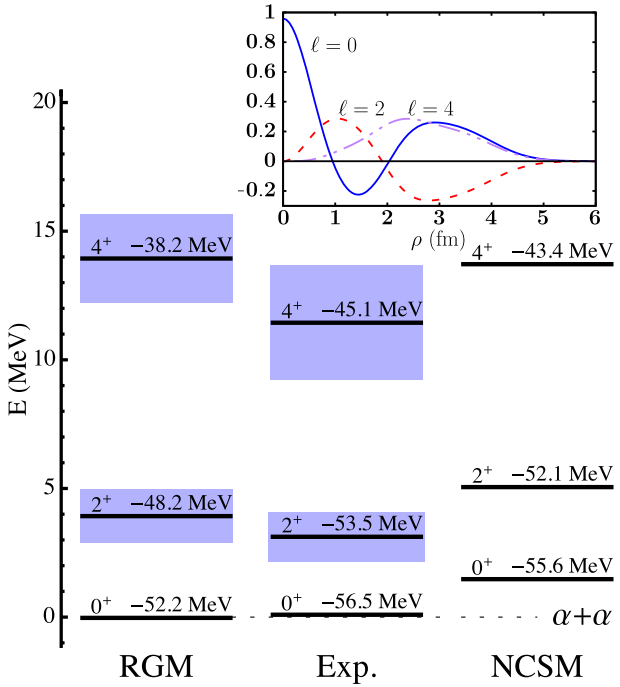

FIG. 1. Spectrum of RGM Hamiltonian with the SRG softened N3LO interaction ($\lambda = 1.5$ fm^{-1}) and $\hbar\Omega = 25$ MeV for a 2α system. Zero on the energy scale is set by the $\alpha + \alpha$ breakup threshold of the corresponding model. Levels are marked by spin and parity and by an absolute 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.

Strategies for moving forward

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- Many-body bases: algebraic and other cluster bases (see talks by McCoy, Volya)

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- Energy-truncati

These alternatives are not without challenges!

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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

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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)	9×10^6	2×10^{12}

(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 $N_{max} = 8$

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

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

Choice of wave function basis

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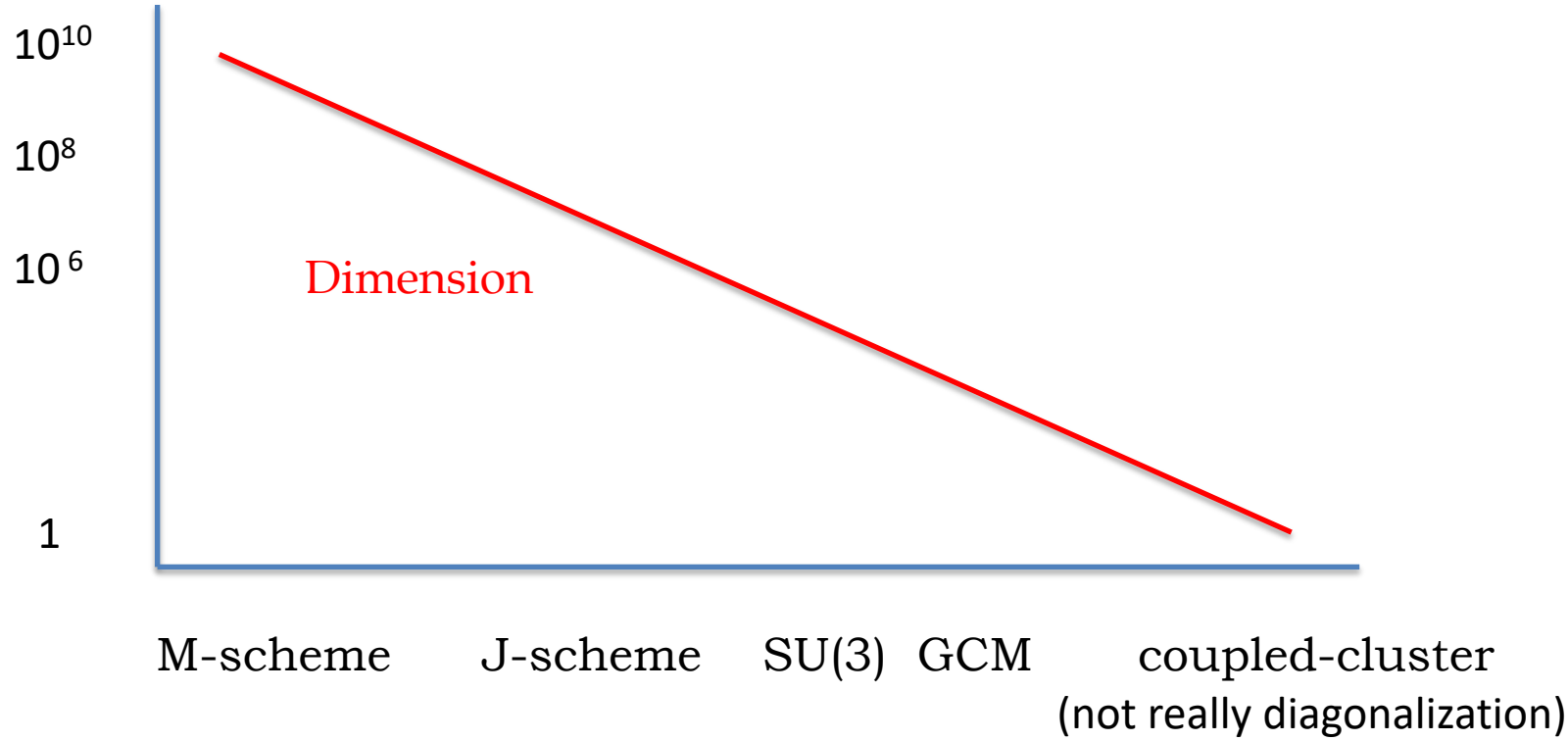
One chooses between *a few, complicated states*
or *many simple states*



Choice of wave function basis

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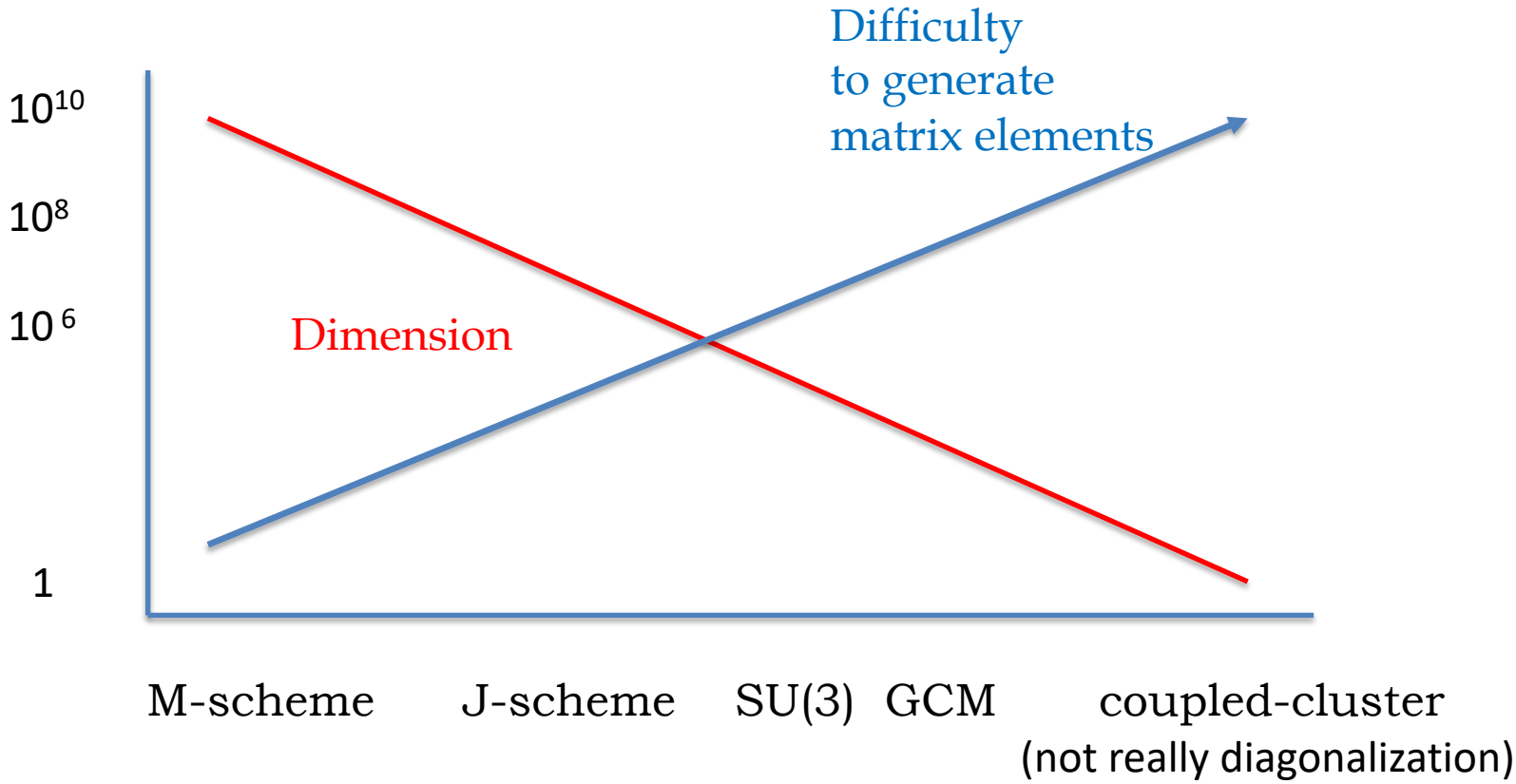
One chooses between *a few, complicated states*
or *many simple states*



Choice of wave function basis

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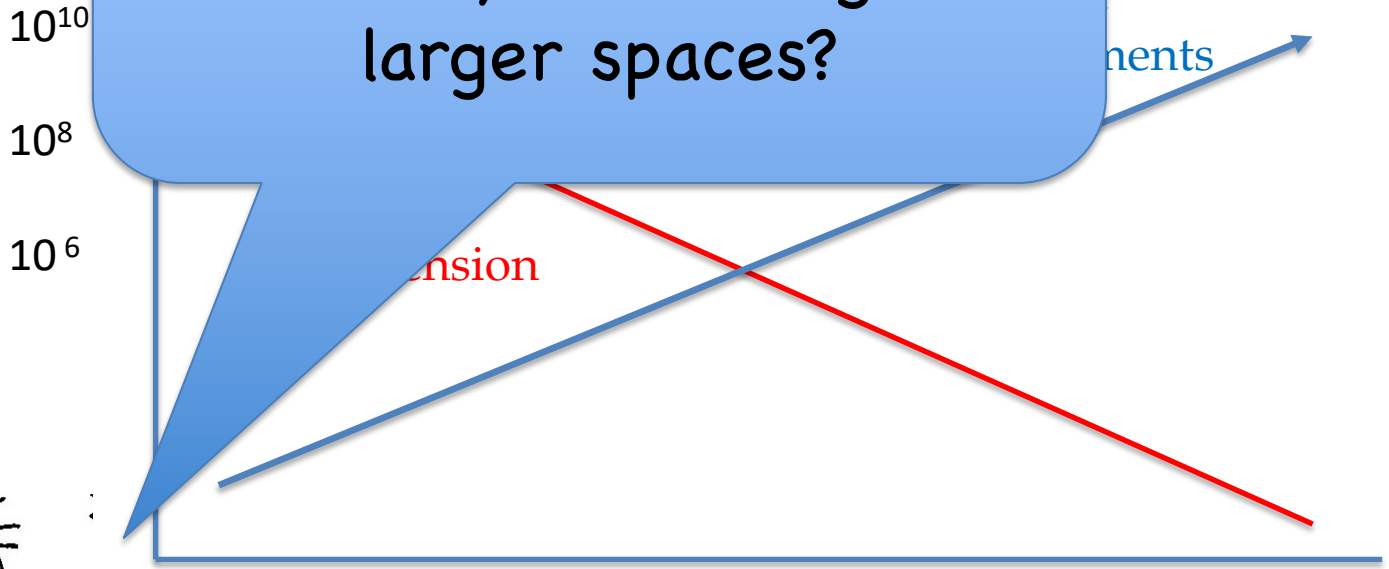
One ch ed states
or *ma*

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



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

Strategies for moving forward

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Alternate approach for medium/heavy nuclei: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Can we truncate to just a few components?

Gorton and CWJ, J. Phys. G **50**, 045110 (2023).

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Alternate approach for medium/heavy nuclei: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$\left(a_1\left|010110\ldots\right\rangle + a_2\left|110010\ldots\right\rangle + a_3\left|001011\ldots\right\rangle + \ldots..\right)$$

No longer single “Slater determinants” but linear combinations…

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Alternate approach for medium/heavy nuclei:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Can we truncate to just a few components?

Priori work by Papenbrock, Juodagalvis, Dean,
Phys. Rev. C **69**, 024312 (2004), **focused on N =Z**

similar to DMRG (density-matrix renormalization group)
(but not exactly)

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Why we think this could work:

Decompose full wfn into proton, neutron components

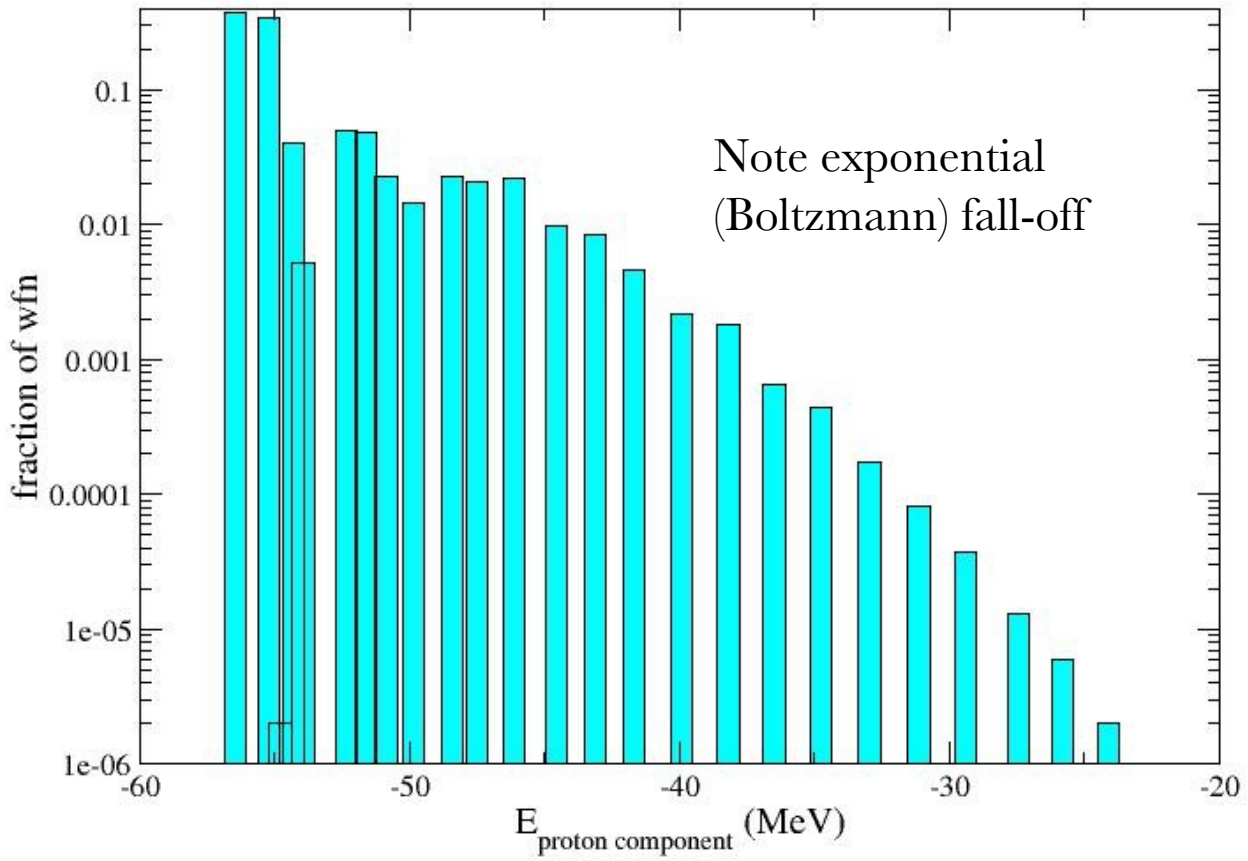
$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$frac_\mu = \sum_\nu \left|c_{\mu\nu}\right|^2$ = fraction of full wave function with *proton* (eigen)state μ

(one can compute this very efficiently with the Lanczos algorithm, using just the **proton part of the full Hamiltonian**)

^{52}Fe in *pf*-shell with GX1A interaction

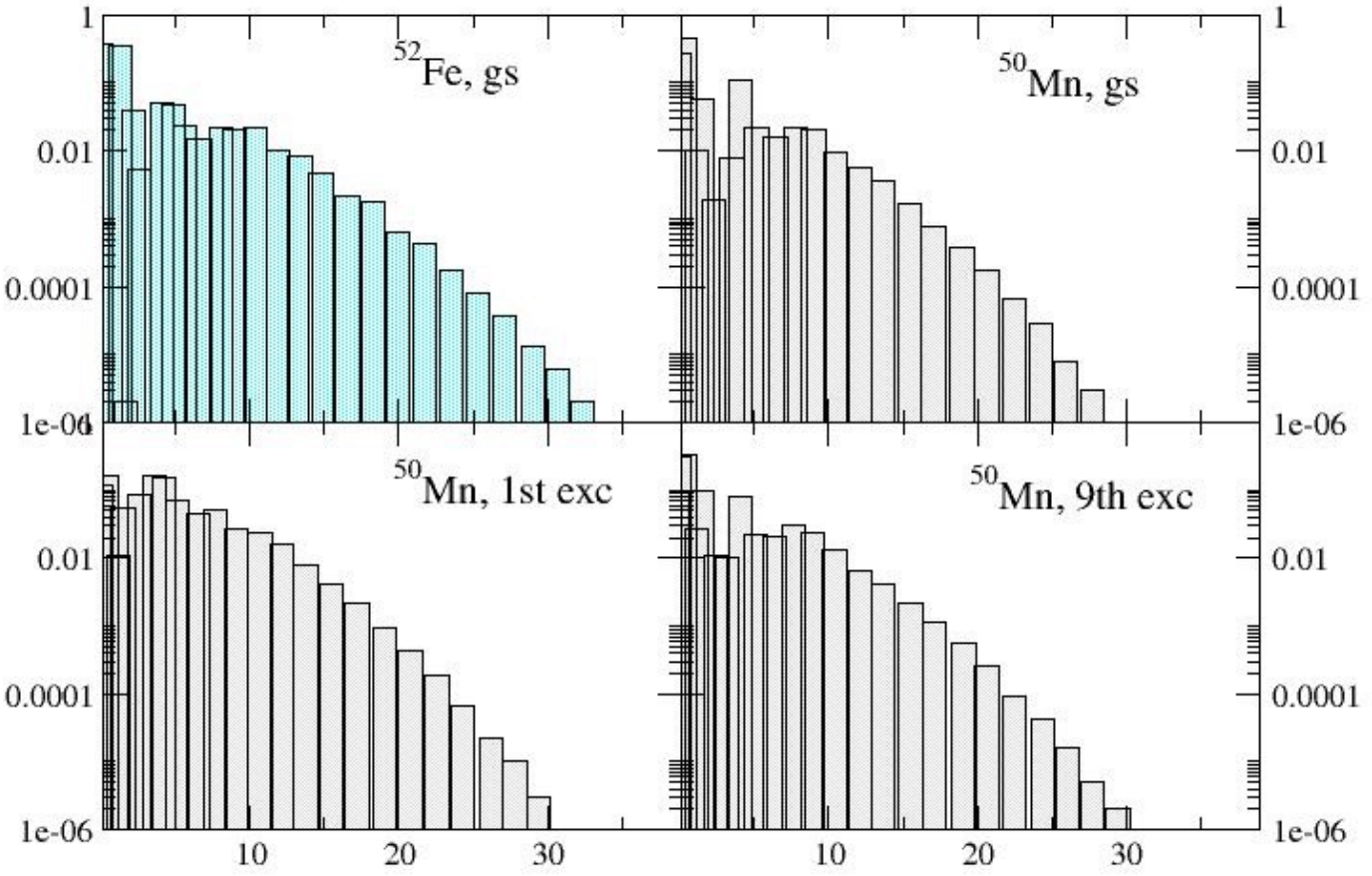
decomposition of g.s.



These energies are the eigenenergies of 6 valence protons in the *pf* shell

pf-shell with GX1A interaction

decomposition into proton components



Note exponential (Boltzmann) fall-off

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Example application:

shells between 50 and 82 ($0g_{7/2}$ 2s1d $0h_{11/2}$)

^{129}Cs: M-scheme dim 50 billion (haven't tried!)

Proton Slater determinant dimension: 14,677
Neutron Slater determinant dimension: 646,430

We have written a code (O. Gorton)

Proton And Neutron Approximate Shell model:

PANASh

We want to find solutions to

$$\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle \quad \text{where} \quad \hat{H} = \hat{H}_{pp} + \hat{H}_{nn} + \hat{H}_{pn}$$

We solve $\hat{H}_{pp}\left|\Psi_p\right\rangle = E_p\left|\Psi_p\right\rangle \qquad \hat{H}_{nn}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$

and choose certain $\left|\Psi_p\right\rangle\left|\Psi_n\right\rangle$ as basis for diagonalization;

Oliver Gorton

Using BIGSTICK we construct many-**proton** states of good J

$$\left|\Psi_p, J_p M\right\rangle = \sum_\mu c_\mu \left|p_\mu, M\right\rangle$$

and the same for many-**neutron** states; these we **couple** together in a *J-scheme* code with fixed *J* for basis:

$$\left|\Psi_J\right\rangle = \sum_{ab} c_{ab} \left[\left|\Psi_p a, J_p\right\rangle \otimes \left|\Psi_n b, J_n\right\rangle\right]_J$$

same here, only for neutrons

We don't take all possible of these, but choose those lowest in energy when solving the proton-only system

Oliver Gorton

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BIGSTICK (protons)

BIGSTICK (neutrons)

proton many-body energies + densities

neutron many-body energies + densities

PANASh couples through p-n interaction

proton+neutron energies and densities

FRIB-TA Workshop, May 26 2023

Oliver Gorton

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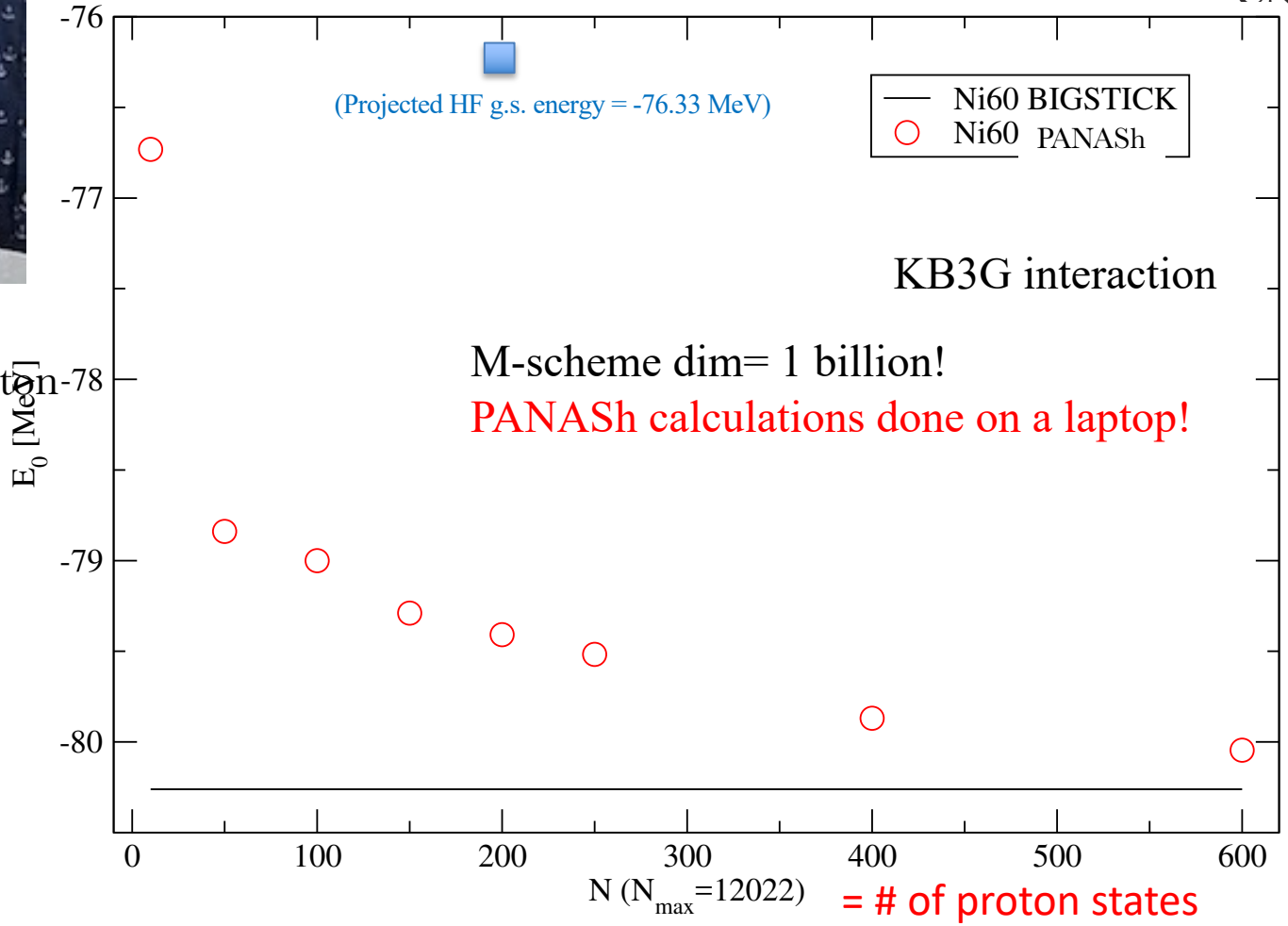
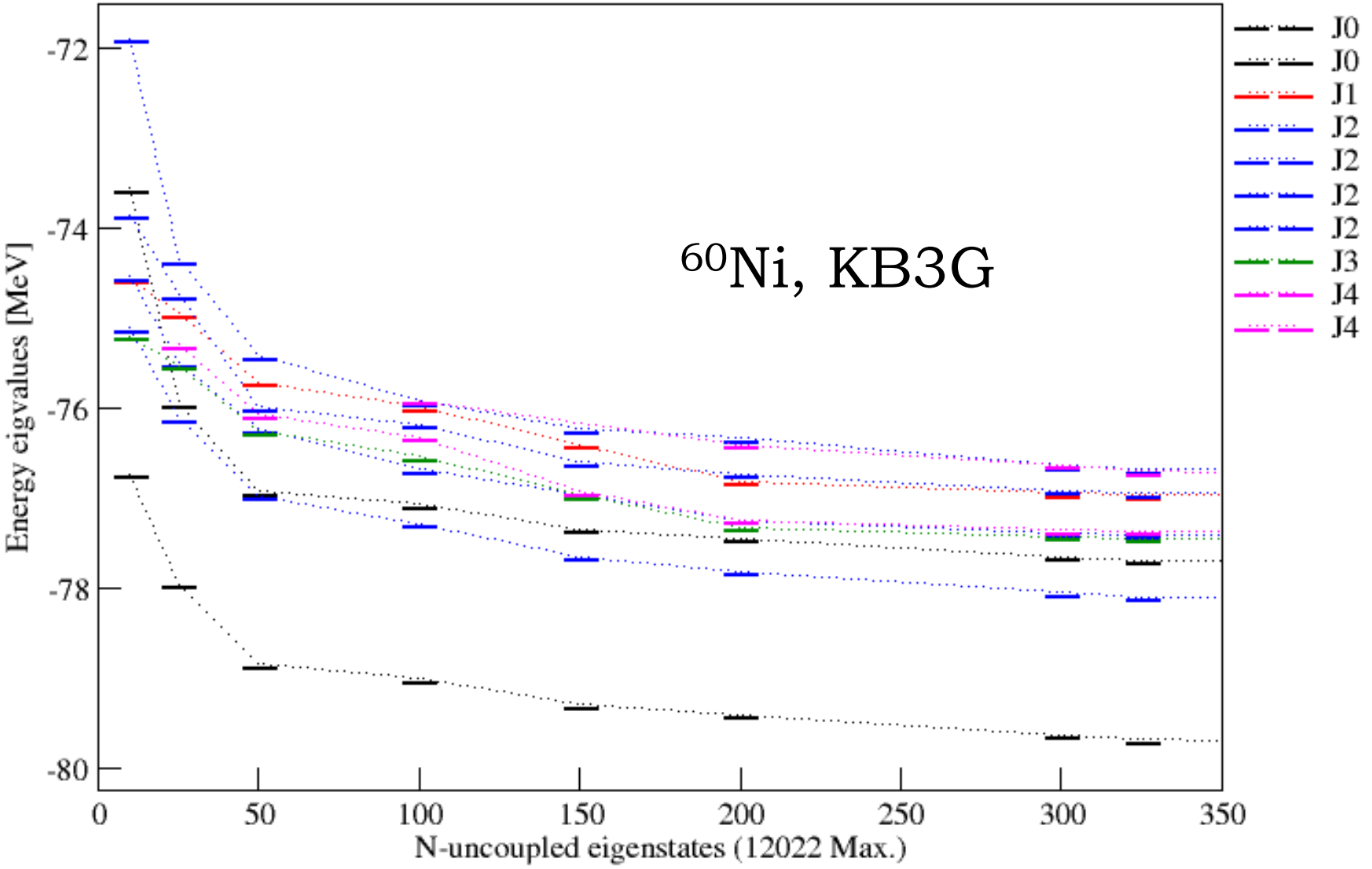
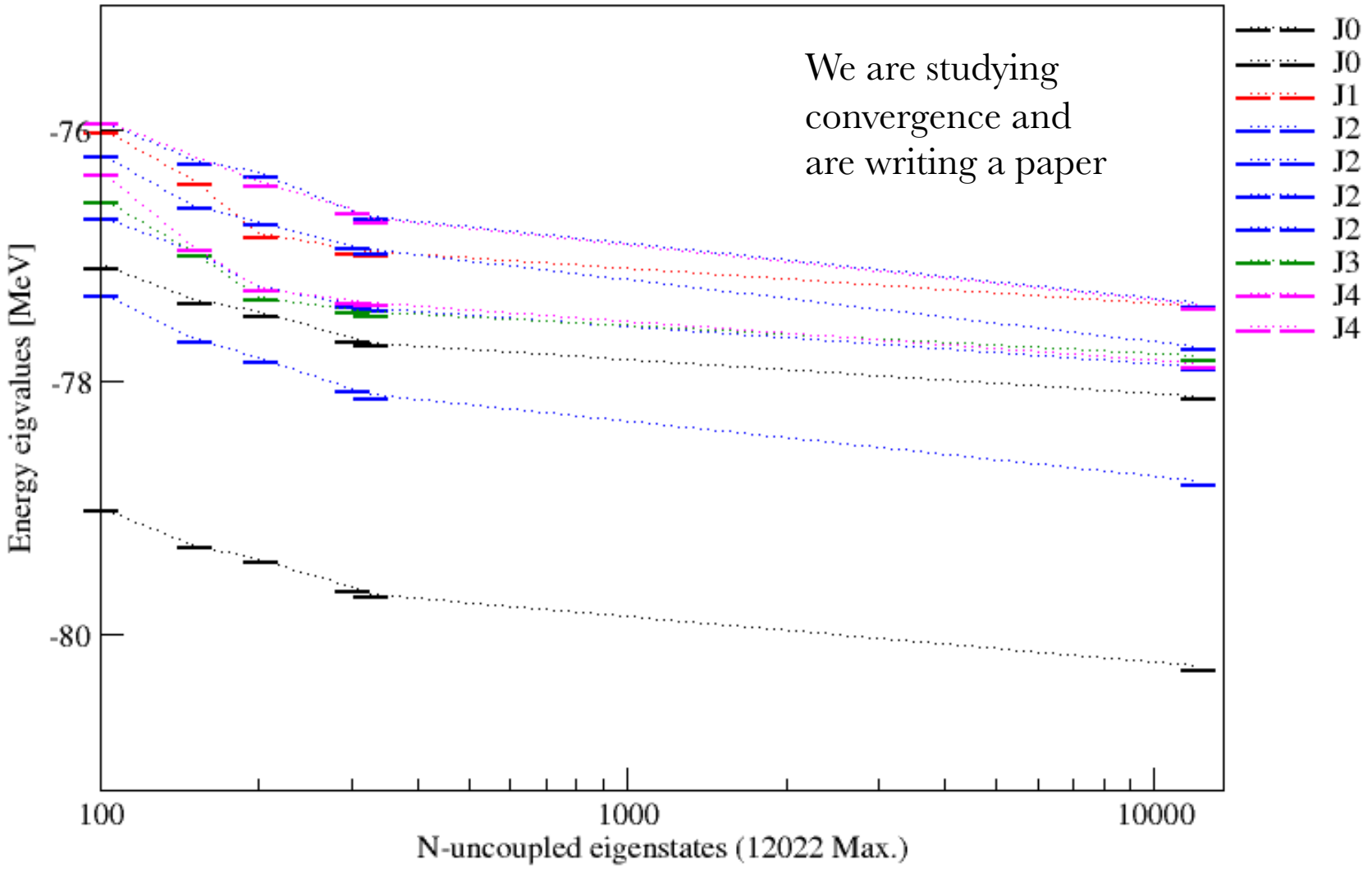
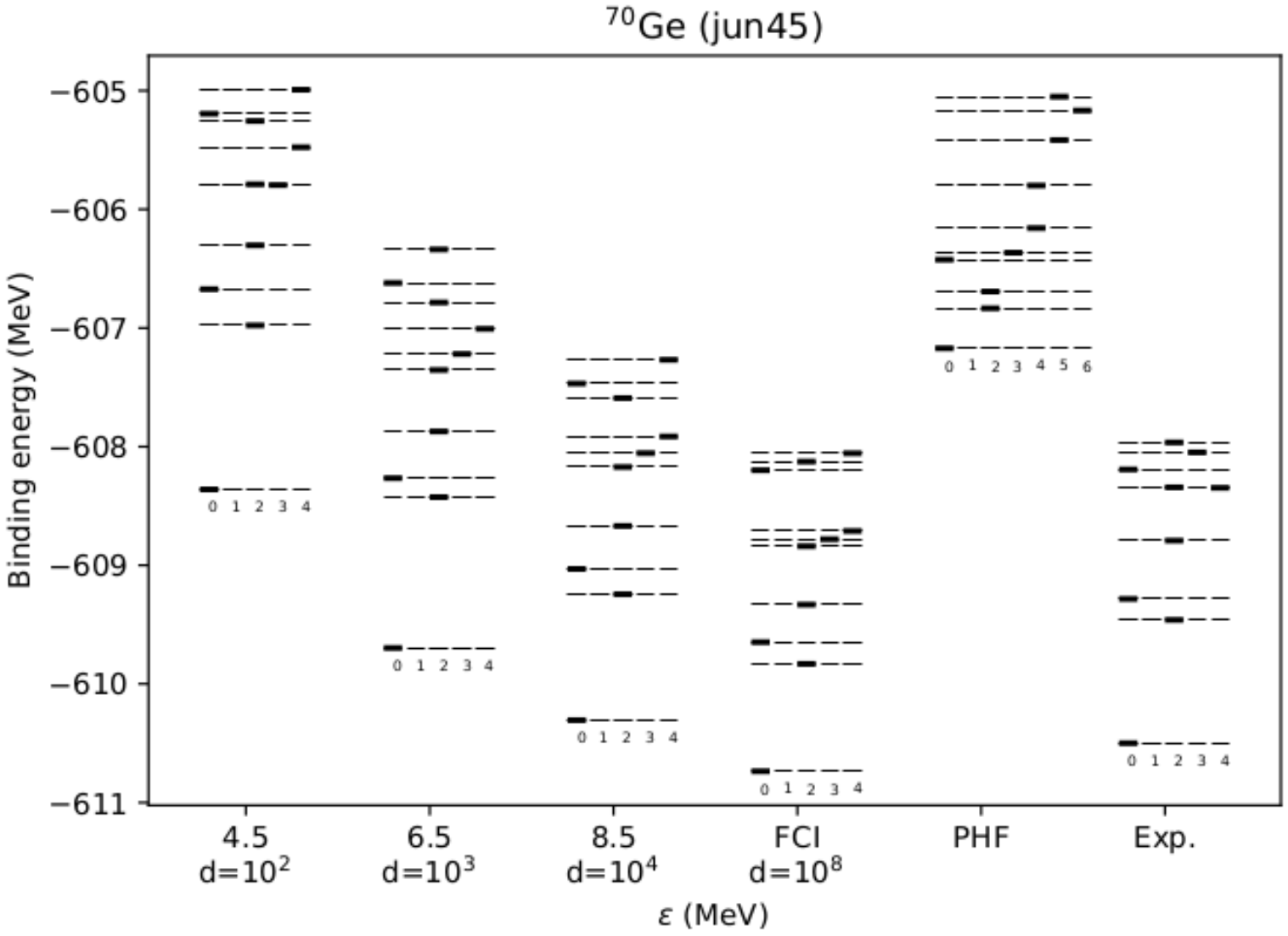
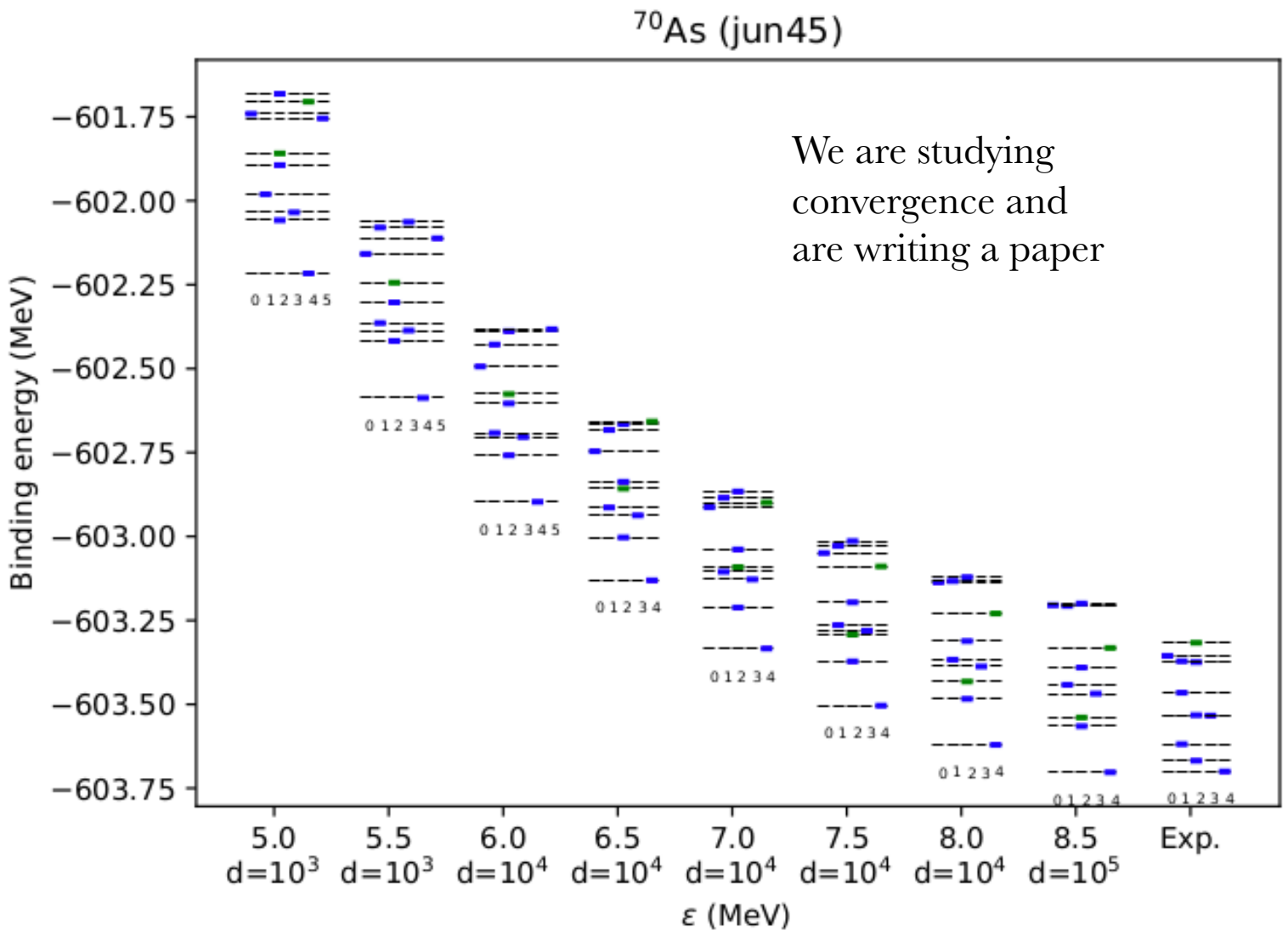



^{60}Ni, KB3G
Energy eigvalues [MeV]
-72
-74
-76
-78
-80
0
50
100
150
200
250
300
350
N-uncoupled eigenstates (12022 Max.)
J0
J0
J1
J2
J2
J2
J2
J3
J4
J4


We are studying
convergence and
are writing a paper
J0
J0
J1
J2
J2
J2
J2
J3
J4
J4
-76
-78
-80
Energy eigvalues [MeV]
100
1000
10000
N-uncoupled eigenstates (12022 Max.)


^{70}Ge (jun45)
Binding energy (MeV)
−605
−606
−607
−608
−609
−610
−611
0 1 2 3 4
0 1 2 3 4
0 1 2 3 4
0 1 2 3 4
0 1 2 3 4 5 6
0 1 2 3 4
4.5
d=10^2
6.5
d=10^3
8.5
d=10^4
FCI
d=10^8
PHF
Exp.
ε (MeV)



We are studying convergence and are writing a paper

We can also compute EM and weak transitions

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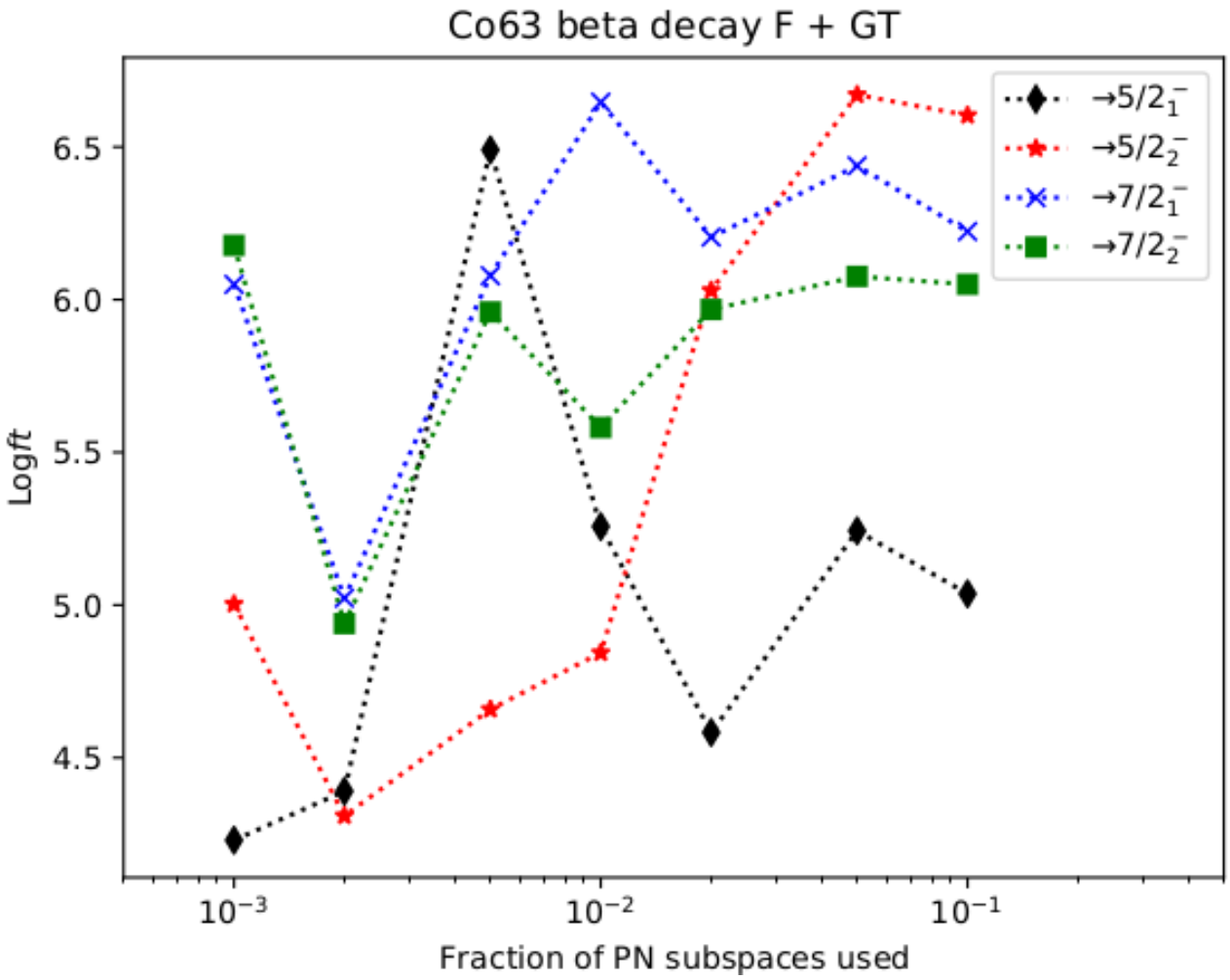

We can also compute EM and weak transitions

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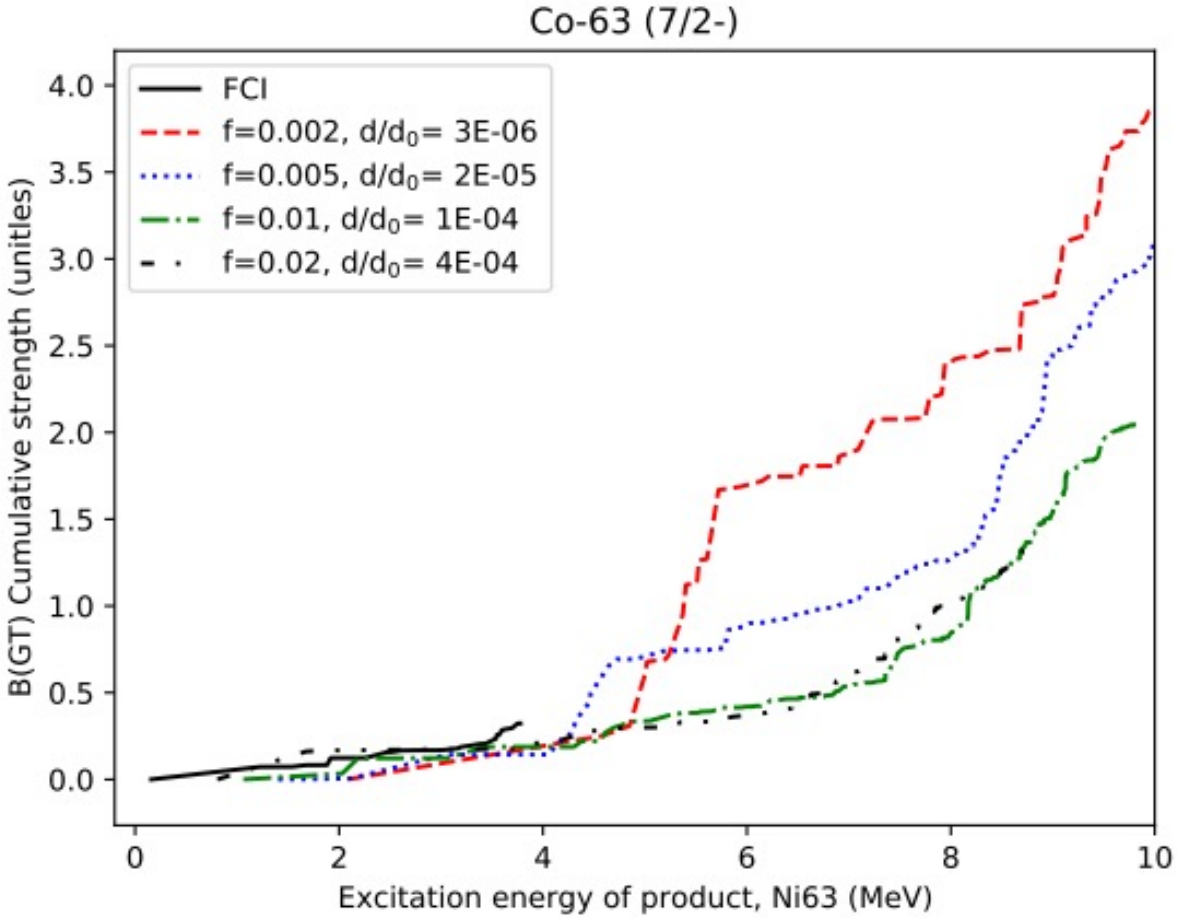

Moving forward

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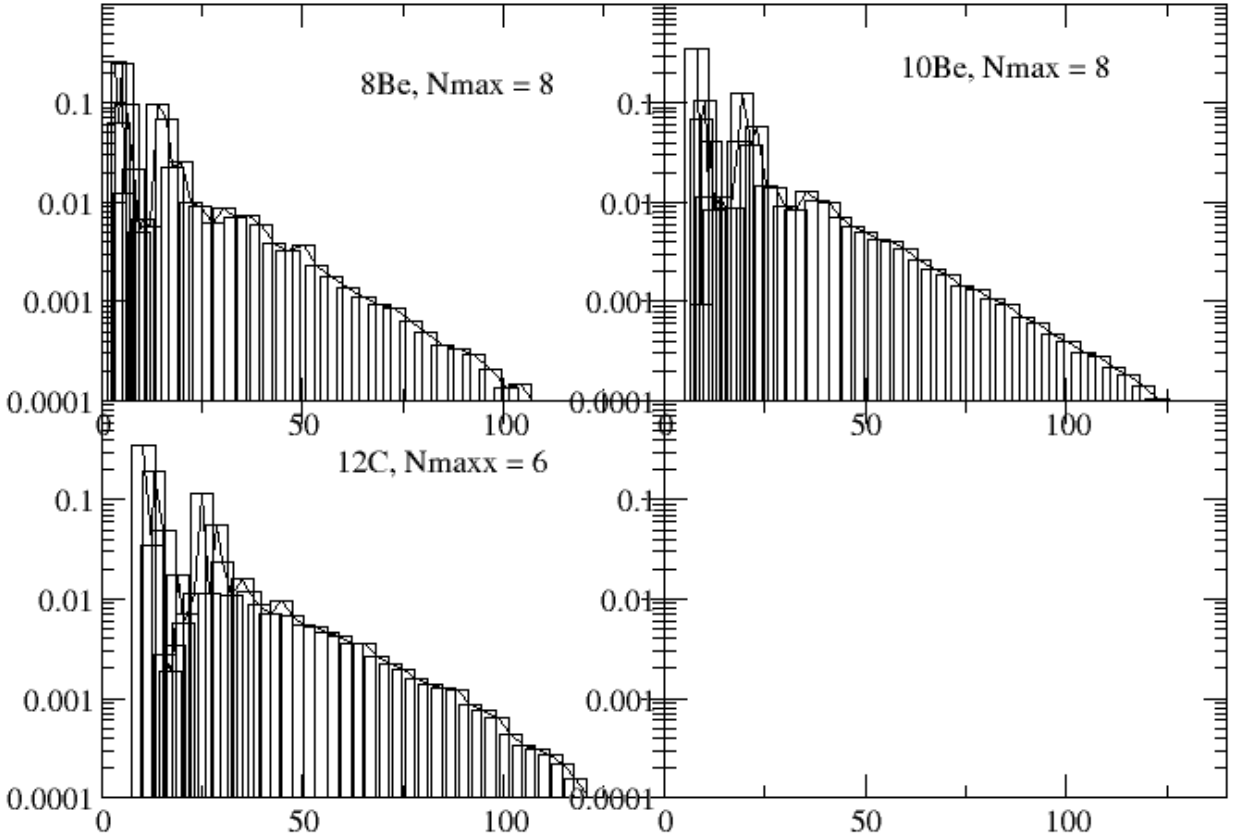
Can we apply to the no-core shell model?



Summary

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The configuration-interaction **shell model** remains useful despite its ups and downs.

The no-core shell model can describe **many** features naturally, but some 'intruder' states—such as halos, configuration inversion, the Hoyle state & analogs—are a challenge.

While M-scheme, on-the-fly codes are extremely efficient, alternative modalities—algebraic, GCM, proton-neutron—may be needed to **correctly** describe these 'intruder' states.

Extra slides

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Strategies for moving forward

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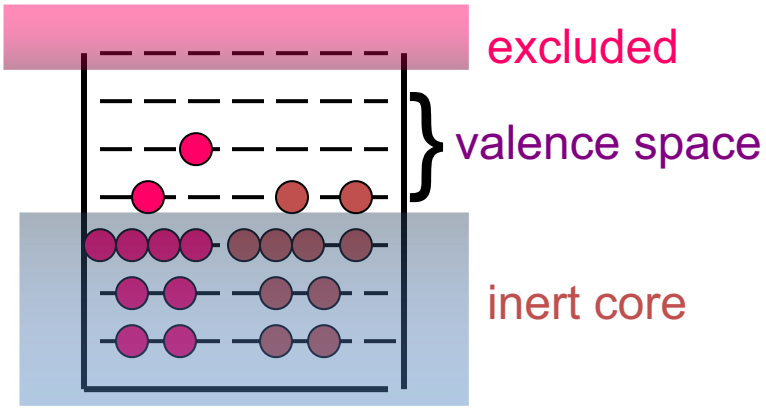
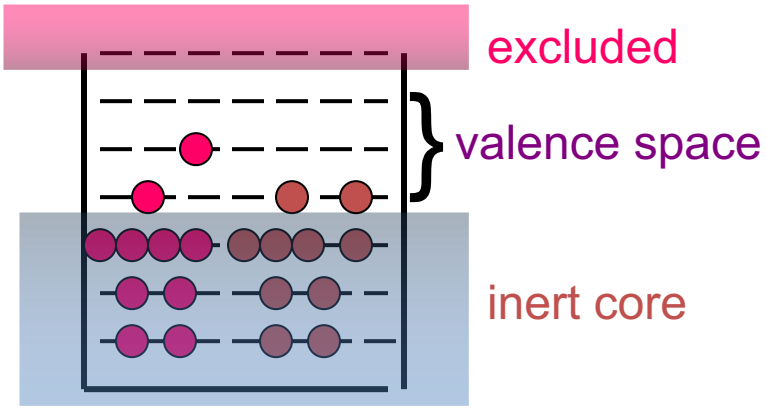
"Phenomenological" calculations work in a fixed space, usually with a core



However even valence space calculations can still become intractable

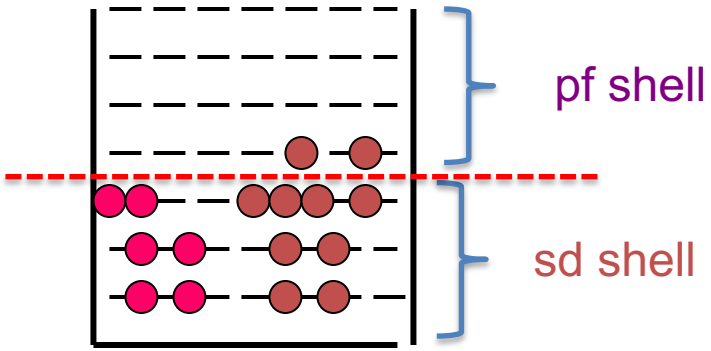


This is particularly true in calculations with two major shells, such as the *sd-pf* space

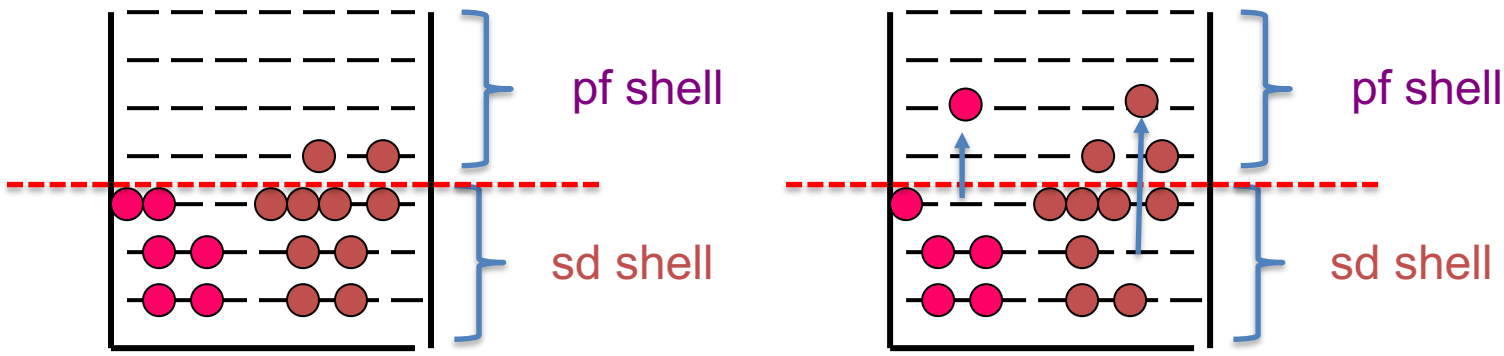
M-scheme dimension

^{40}Mg: 286 billion

^{40}Ar: 927 trillion!



Often we truncate by particle-hole excitations



2 particles, 2 holes

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M-scheme dimensions

	full space	0p-0h	2p-2h	4p-4h
^{40}Mg:	286 billion	5 million	1.3 billion	28 billion
^{40}Ar:	927 trillion!	1566	9 million	4.6 billion

But is this strategy optimal?

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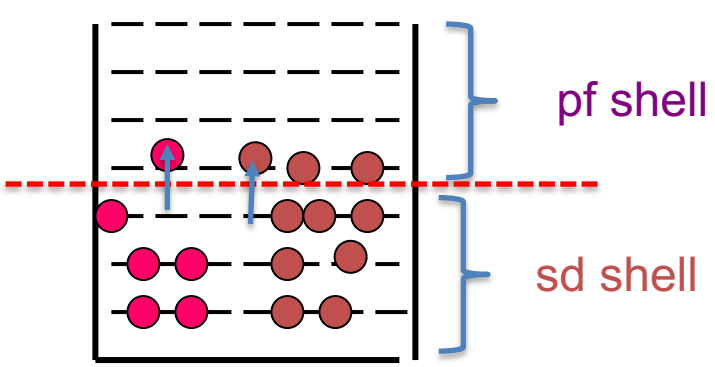
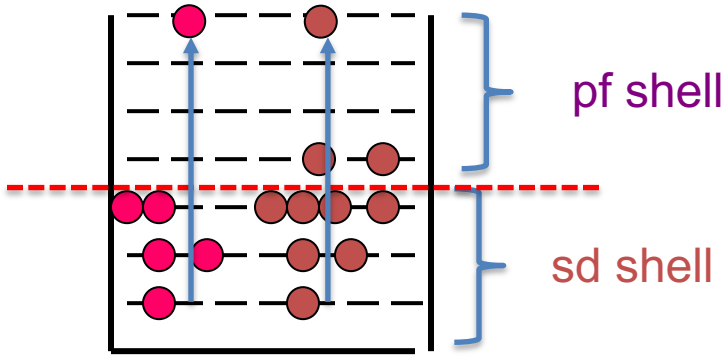
2p, 2h excitations





Not all single-particle energies are the same!
(and single-particle energies are not the whole story)

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Instead, we truncate based upon shell model 'configurations'

In particular, truncate on the **configuration centroid** (average)

(Horoi, Brown, and Zelevinsky, PRC 50, R2274(R) (1994))

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A *configuration* (or *partition*) is:

the set of all many-body states with a fixed occupation of shell model orbitals, i.e.,

$(0d_{5/2})^2(1s^{1/2})^1(0d_{3/2})^1$

$(0d_{5/2})^3(1s^{1/2})^1(0d_{3/2})^0$

etc.

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The *configuration centroid* is the average energy of all the states in a configuration

Duflo and Zuker,
PRC 59, R2347(R) (1999)

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A *configuration* (or *partition*) is:

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The configuration centroids depend only upon the single-particle energies and the monopoles, and can be easily computed *without* constructing the entire Hamiltonian matrix.

The *configuration centroid* is the average energy of all the states in a configuration

Duflo and Zuker,
PRC 59, R2347(R) (1999)

Example: ^{40}Ar in *sd-pf* space

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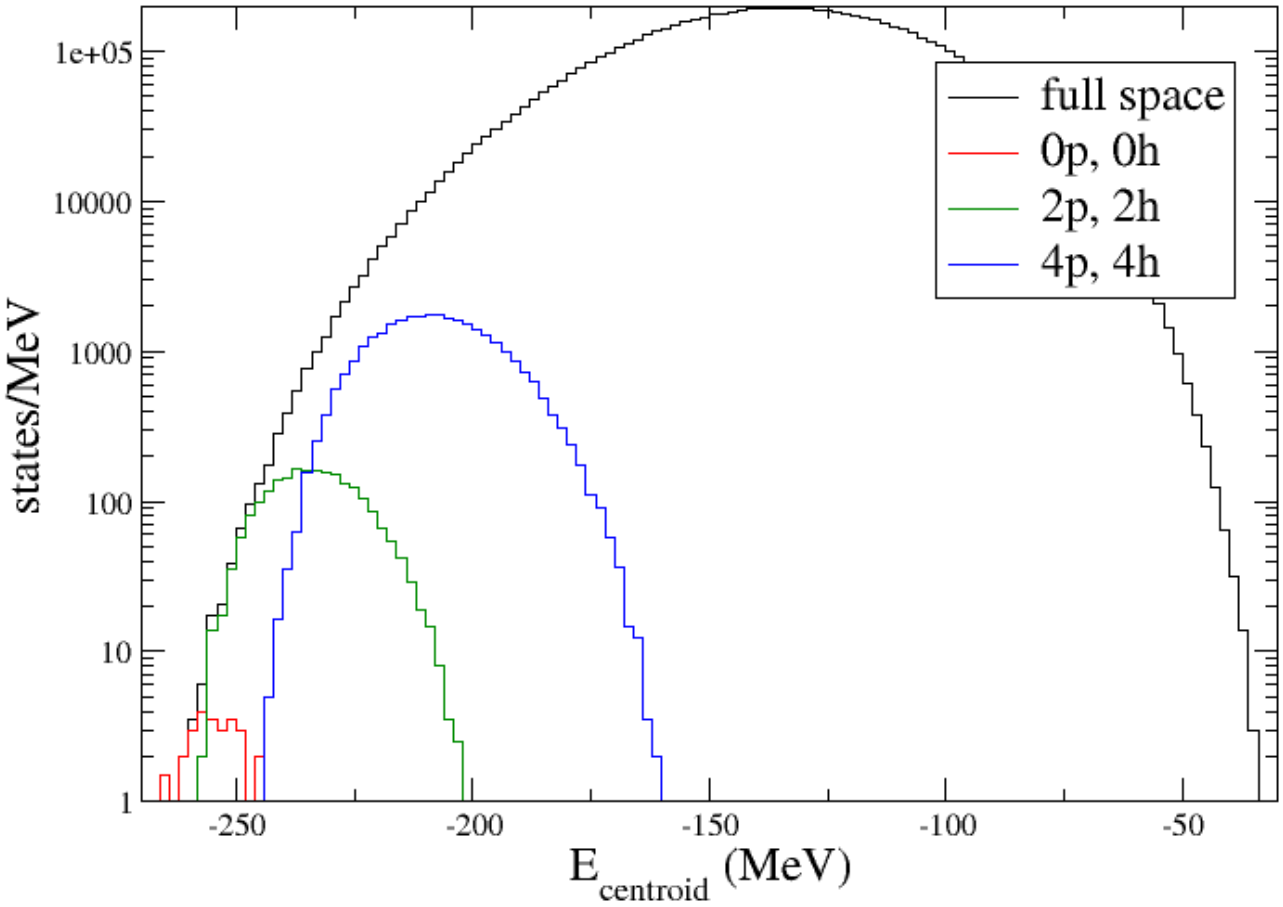

You can think of this as averages over blocks (configurations) of the diagonal of the Hamiltonian (but very fast!)

One can truncate the model space on the *configuration centroid*

Horoi, Brown, and Zelevinsky, PRC 50, R2274(R) (1994)

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This is a little nontrivial in `BIGSTICK`.

BIGSTICK is organized around quantum numbers, including a fake integer quantum number, '*w*' (or weight), assigned to each orbital. (For the no-core shell model, this is then principal quantum number N).

BIGSTICK truncates by restricting to a maximum total *W*. This is very fast!

But BIGSTICK's truncation is *linear* in the orbitals,

while configuration centroids are *quadratic*

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Nonetheless I had a master's student (A. Keller) write a code using simulated annealing to optimize the single-particle weights, based upon some targeted cutoff in centroids

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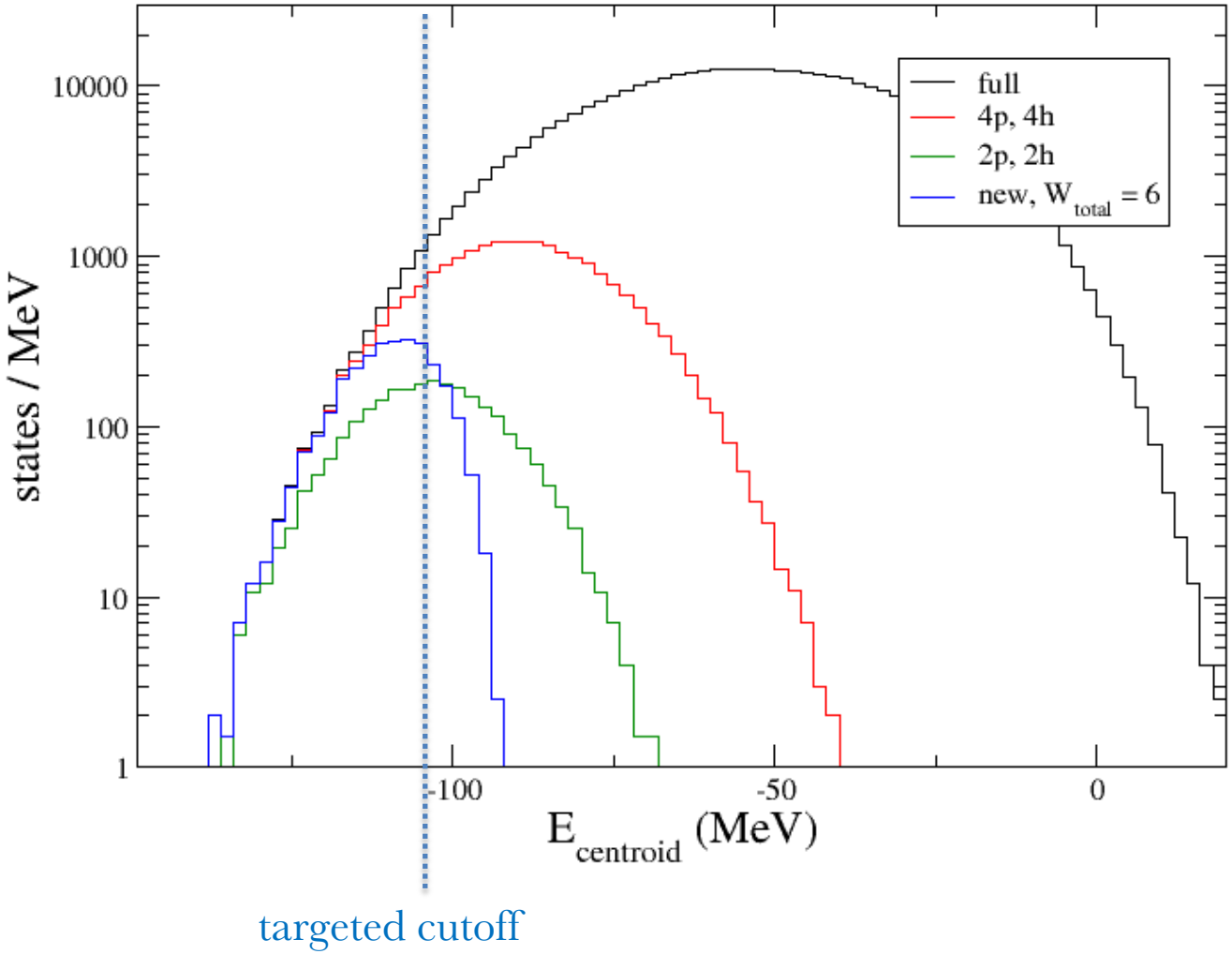

^{34}Mg in *sd-pf*

Full space: 587 billion!
2p,2h : 19.6 million
4p,4p: 2.3 billion

New : 146 million

New weights:

$1p_{1/2}$: 4
$0f_{5/2}$: 4
$1p_{3/2}$: 3
$0f_{7/2}$: 3
$0d_{3/2}$: 3
$1s_{1/2}$: 2
$0d_{5/2}$: 1

Nonetheless I had a master's student (A. Keller) write a code using simulated annealing to optimize the single-particle weights.

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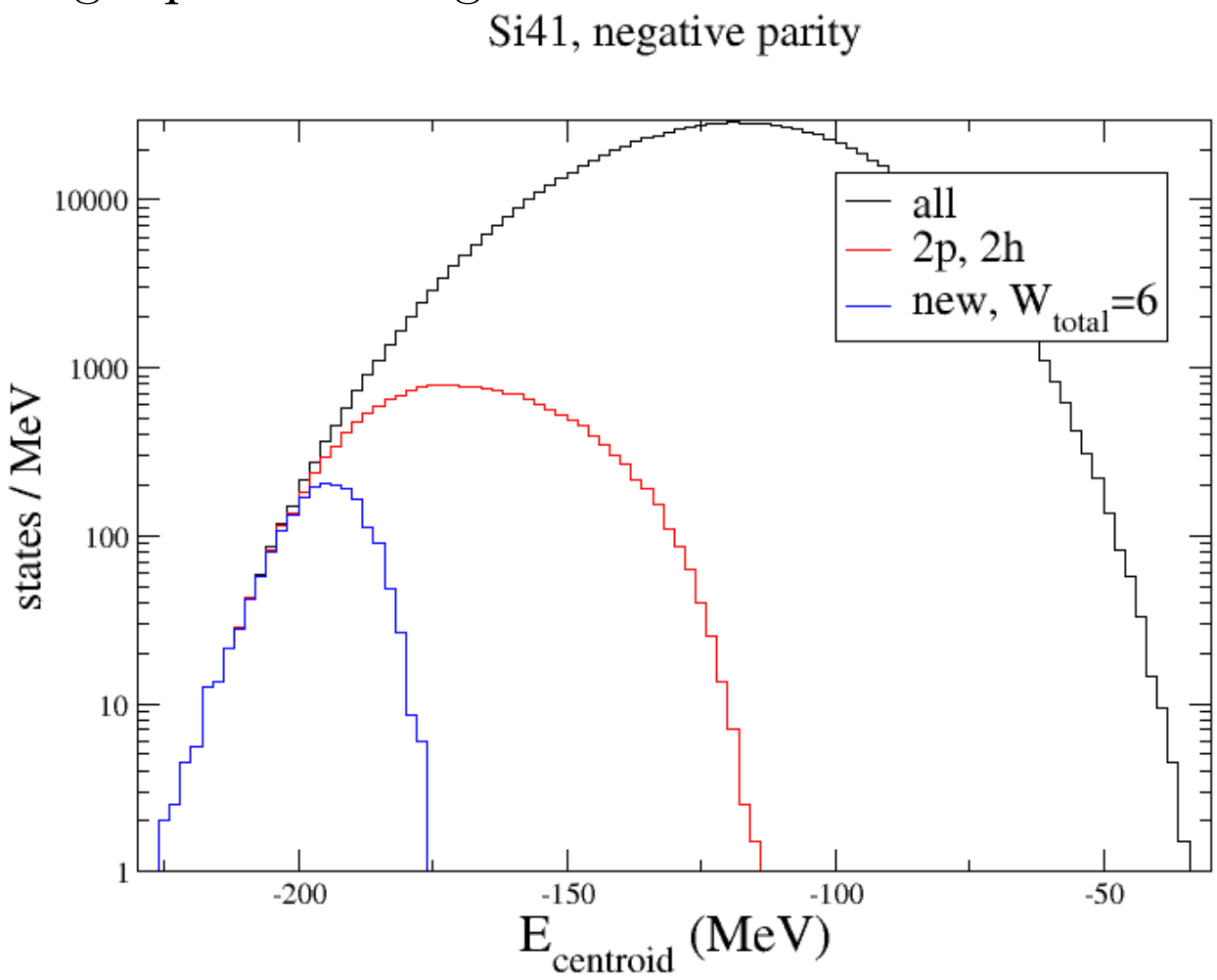

^{41}Si in *sd-pf*

Full space: 10.3 trillion!
2p,2h : 3.1 billion!

New : 136 million

New weights:

$1p_{1/2}$: 4
$0f_{5/2}$: 4
$1p_{3/2}$: 3
$0f_{7/2}$: 3
$0d_{3/2}$: 3
$1s_{1/2}$: 2
$0d_{5/2}$: 1

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This is work in progress!

- To reduce spurious center-of-mass motion, can add $+ \lambda H_{cm}$ (Lawson method)—reduces to < 1%.
- Still have yet to study convergence with basis dimension