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# Islands of inversion and other challenges to the no-core shell model

Calvin W. Johnson, SDSU

+ Mark Caprio, Notre Dame

"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 "

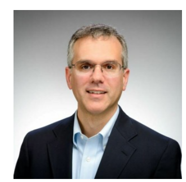
PAINT Workshop @ TRIUMF, Feb 27, 2024

# Islands of inversion and other challenges to the no-core shell model

See my talk after this!

Calvin W. Johnson, SDSU

+ Mark Caprio, Notre Dame



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And then mine!

See my talk after this!

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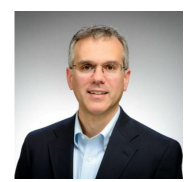

Anna McCoy

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PAINT Workshop @ TRIUMF, Feb 27, 2024

# Configuration-interaction shell model

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 functions allows for detailed analysis**

# Outline of talk

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- How to x-ray a wave function
- The challenge of intruders
- $^{11}$Li & $^{29}$F as case studies

- Possible paths forward

# 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

# The NCSM has been a triumph!

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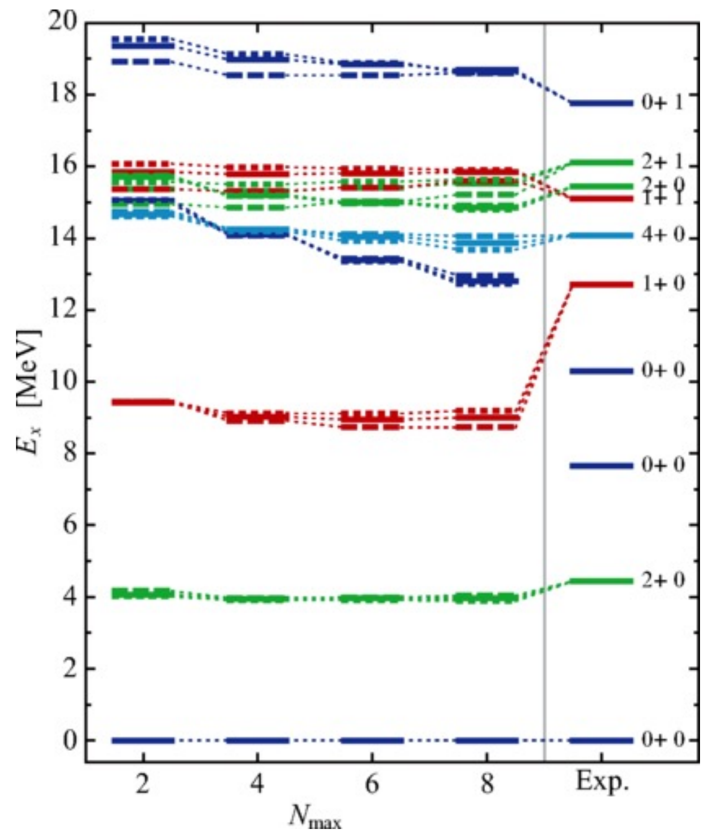
Maris *et al* PRC **90**, 014314 (2014)

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




We can reproduce experimental data! such as the g.s. band of $^{12}$C

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But M-scheme dimensions are huge—into the tens of billions*!
How can we possibly 'understand' them?

*See Anna McCoy's talk for a possible record, M-scheme dimension ~ 35 billion!

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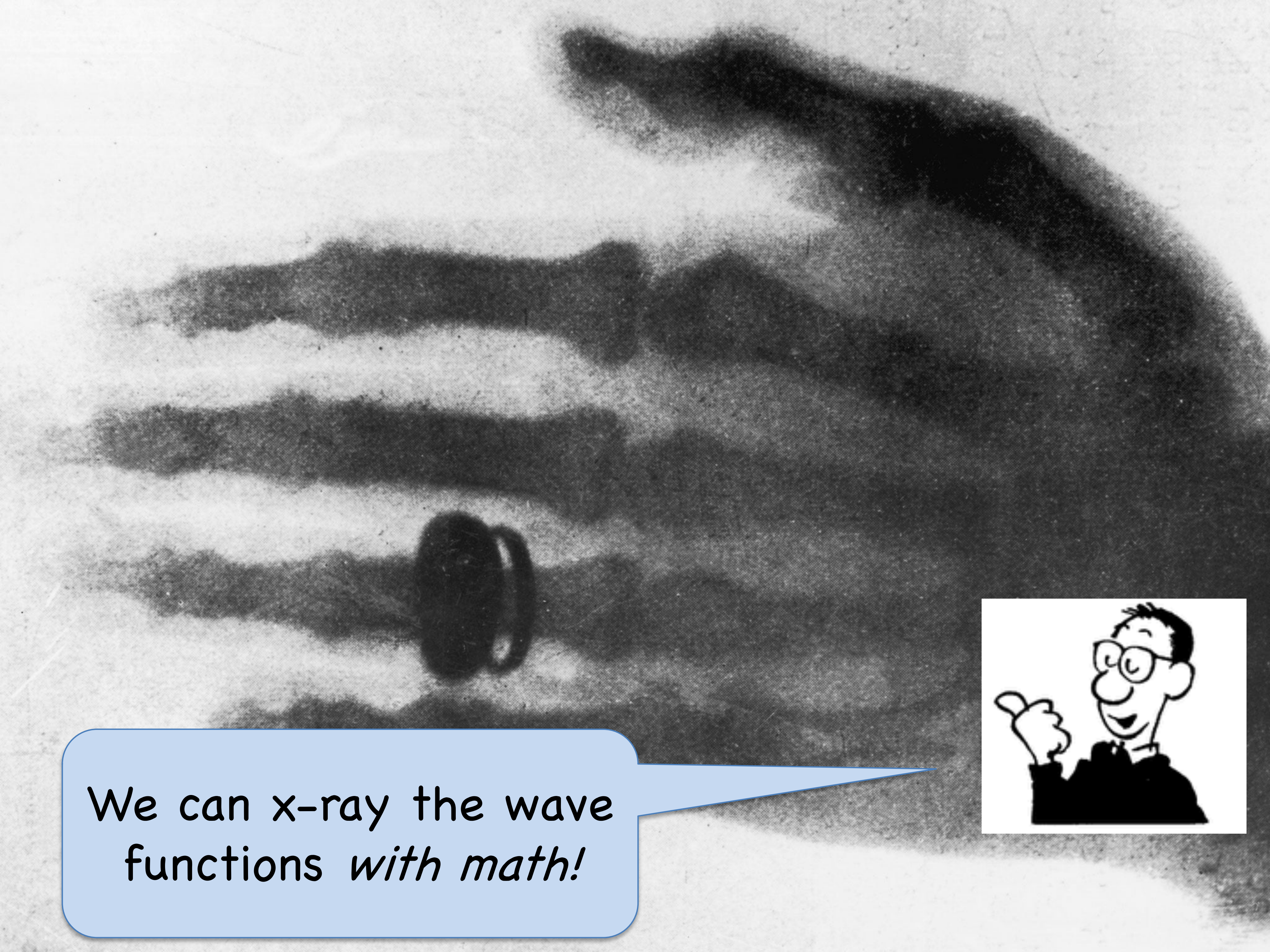
But M-scheme dimensions are huge—into the tens of billions*!
How can we possibly 'understand' them?

Richard Hamming:
*The purpose of computing is **insight**, not numbers.*

*See Anna McCoy's talk for a possible record, M-scheme dimension ~ 35 billion!


We can x-ray the wave functions *with math!*

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Use eigenvalues
of Casimir operators to label
subspaces (“irreps”)

See also talks by Caprio and McCoy, up next!

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Casimir

$$\hat{C}\left|z,\alpha\right\rangle = z\left|z,\alpha\right\rangle$$

z (eigenvalue) labels the subspace

$\alpha$ indexes all the states in the subspace (same value of z)

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Casimir

$$\hat{C}\left|z,\alpha\right\rangle = z\left|z,\alpha\right\rangle$$

The best known Casimir is $\mathbf{J}^2$, which has eigenvalues $j(j+1)$

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Casimir

$$\hat{C}\left|z,\alpha\right\rangle = z\left|z,\alpha\right\rangle$$

Another is Elliott's representation of an SU(3) Casimir:

$$\hat{C}_{SU(3)} = \vec{Q}\cdot\vec{Q} - \frac{1}{4}\vec{L}^2$$

For this 2-body SU(3) Casimir,
the eigenvalue z = $\lambda^2+\lambda\mu+\mu^2+3(\lambda+\mu)$,
where $\lambda$, $\mu$ label the irreps

Casimir

$$\hat{C}\left|z,\alpha\right\rangle = z\left|z,\alpha\right\rangle$$

If the Casimir(s) commute(s) with the Hamiltonian, $\left[\hat{H},\hat{C}\right]=0$

then the Hamiltonian is block-diagonal in the *irreps* (irreducible representation)

This is known as *dynamical symmetry*

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A key idea: A Casimir can be used
to divide up a Hilbert space into subspaces,
labeled by eigenvalues

*even if the Casimir does not commute with the Hamiltonian*

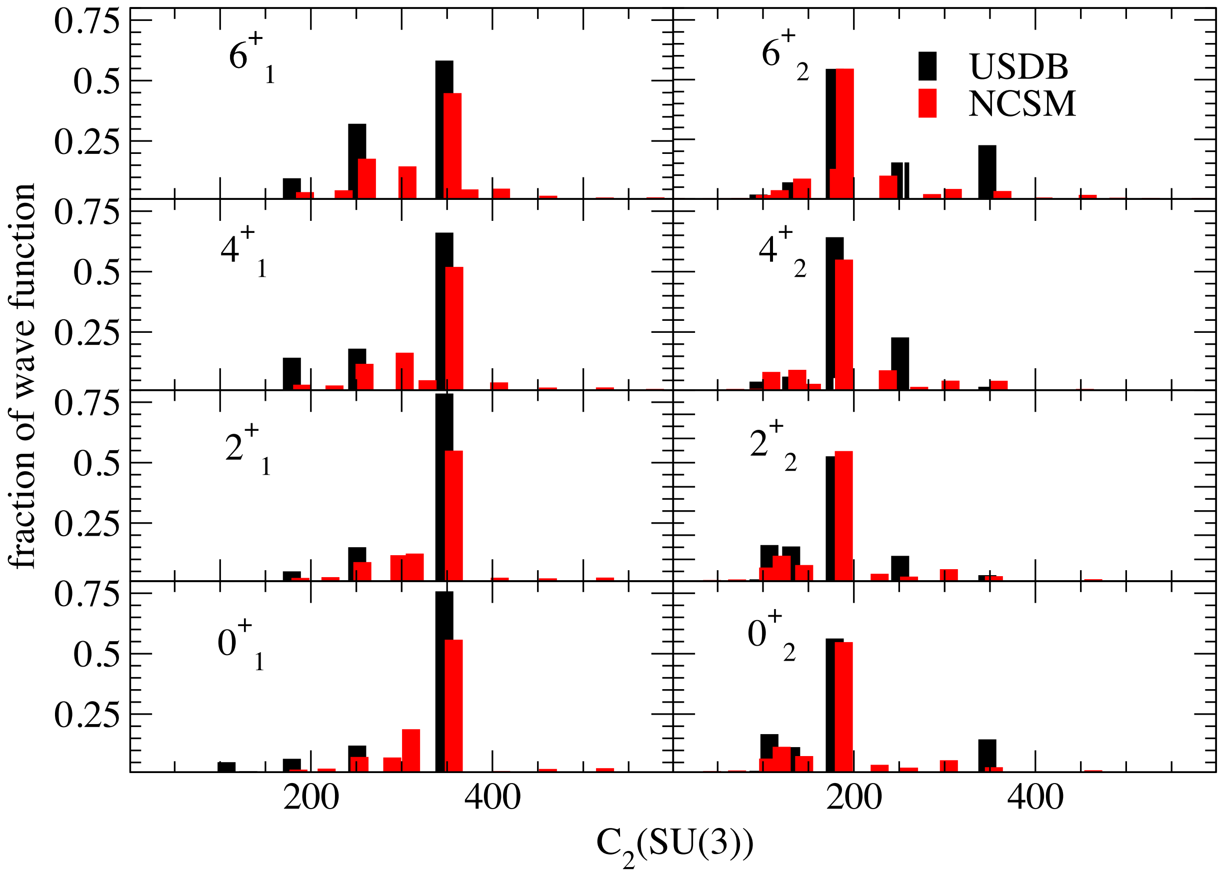
Casimir

$$\hat{C}\left|z,\alpha\right\rangle = z\left|z,\alpha\right\rangle$$

For some wavefunction | Ψ >, we define the *fraction of the wavefunction in an irrep*

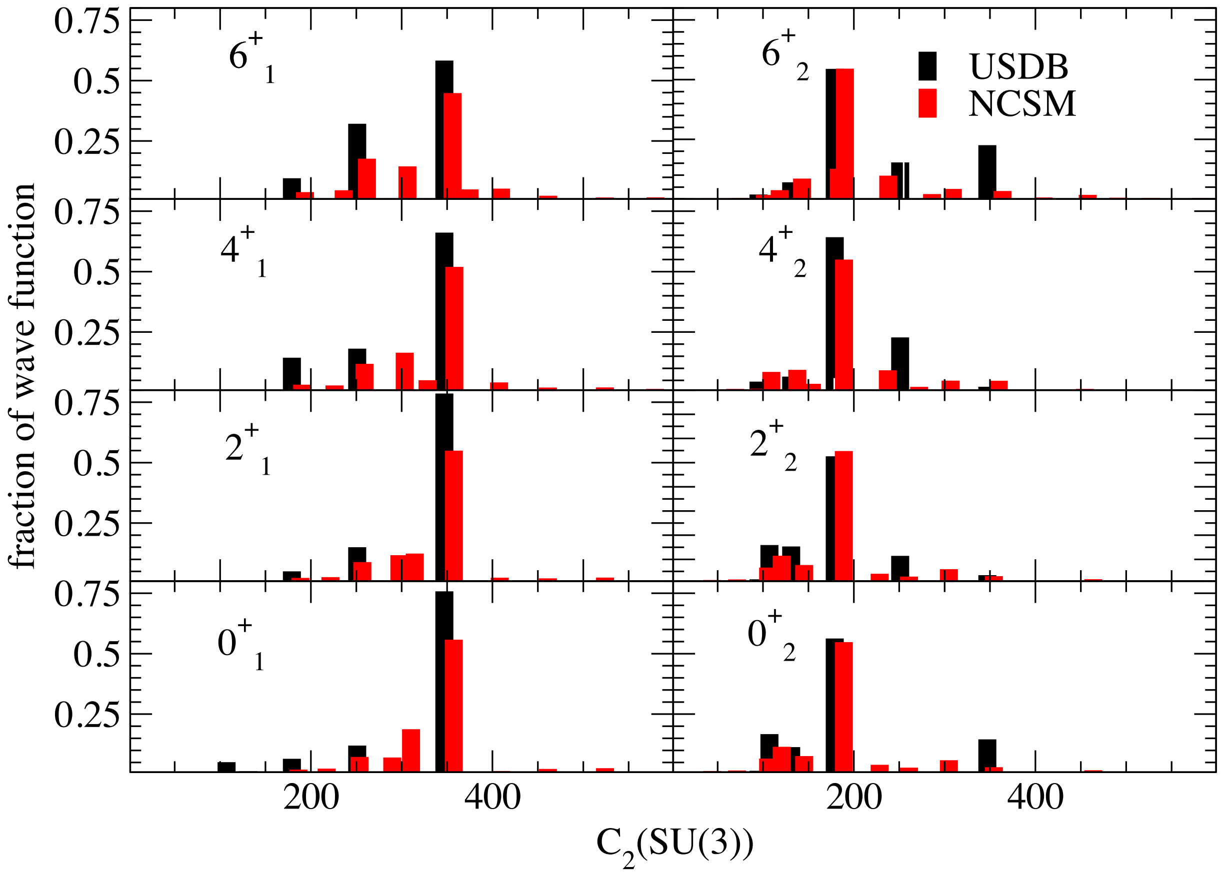
$$F(z) = \sum_{\alpha}\left|\left\langle z,\alpha\middle|\Psi\right\rangle\right|^2$$

# $^{20}$Ne



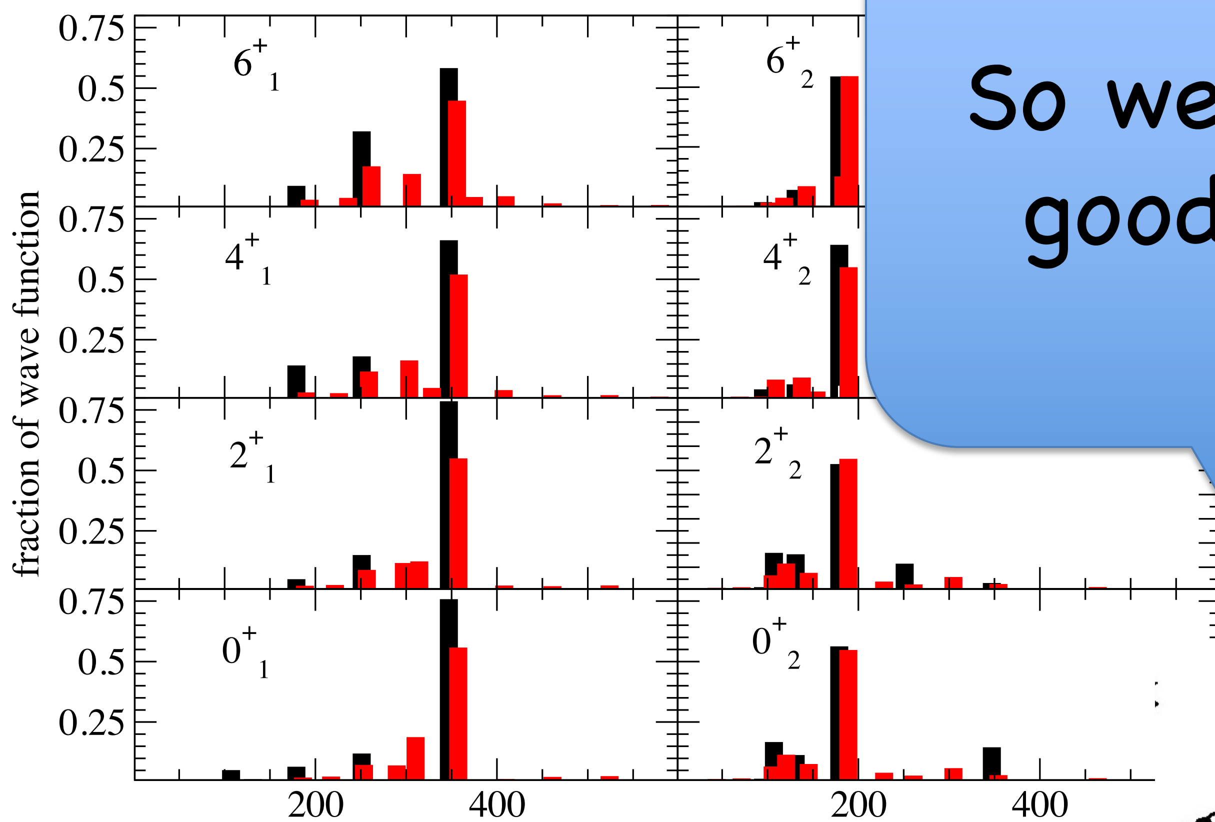

This can be done efficiently using a variant of the Lanczos algorithm:
CWJ, PRC **91**, 034313 (2015)

# $^{20}$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!

# $^{20}Ne$

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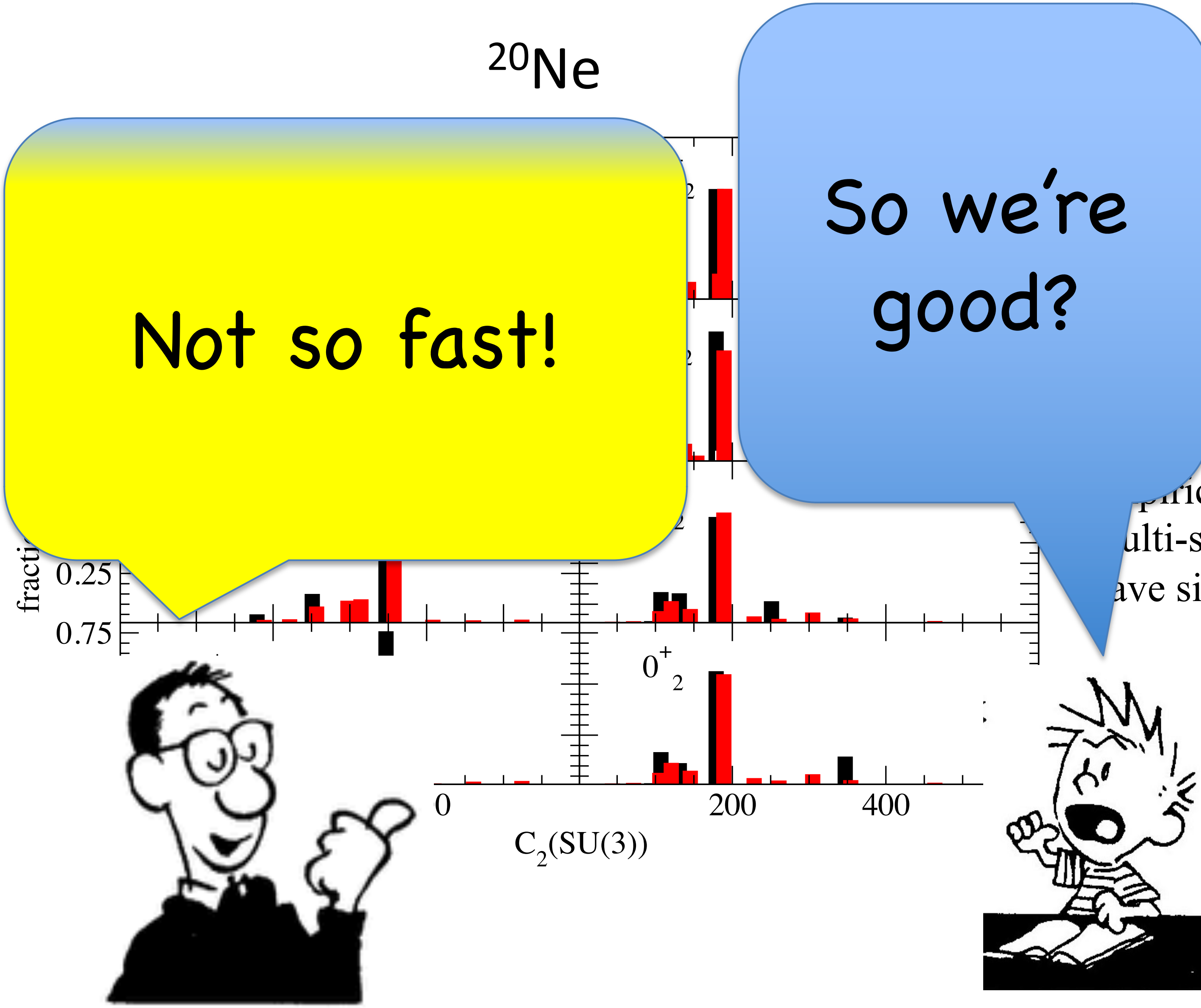
…king at the group-
…cal decomposition,
…even show that
…ence-space
…pirical and *ab initio*
…ulti-shell wave functions
…ave similar structure!

So we're good?

We can reproduce expt *and* have insight!

# $^{20}$Ne

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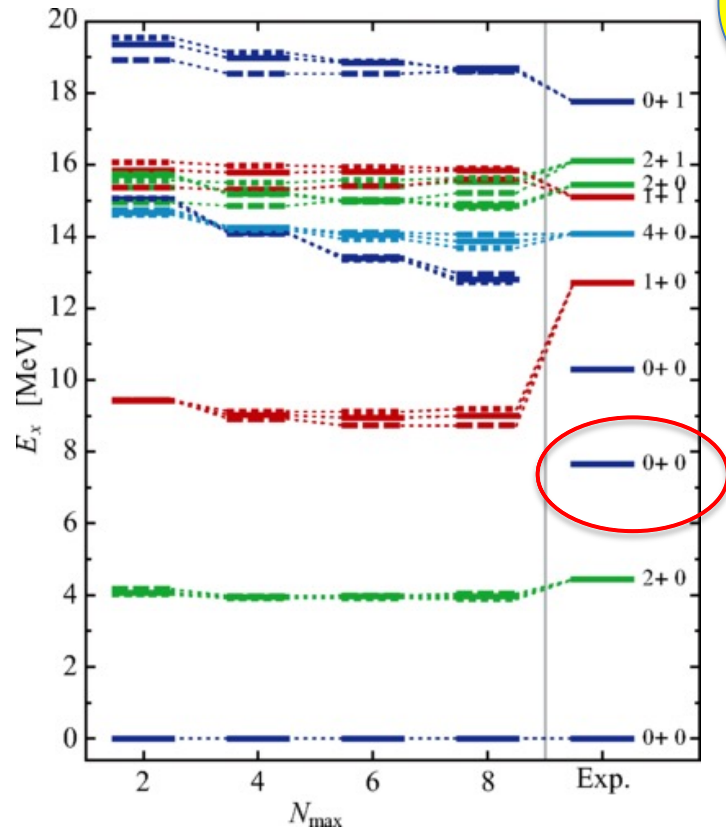
…ave similar structure!

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

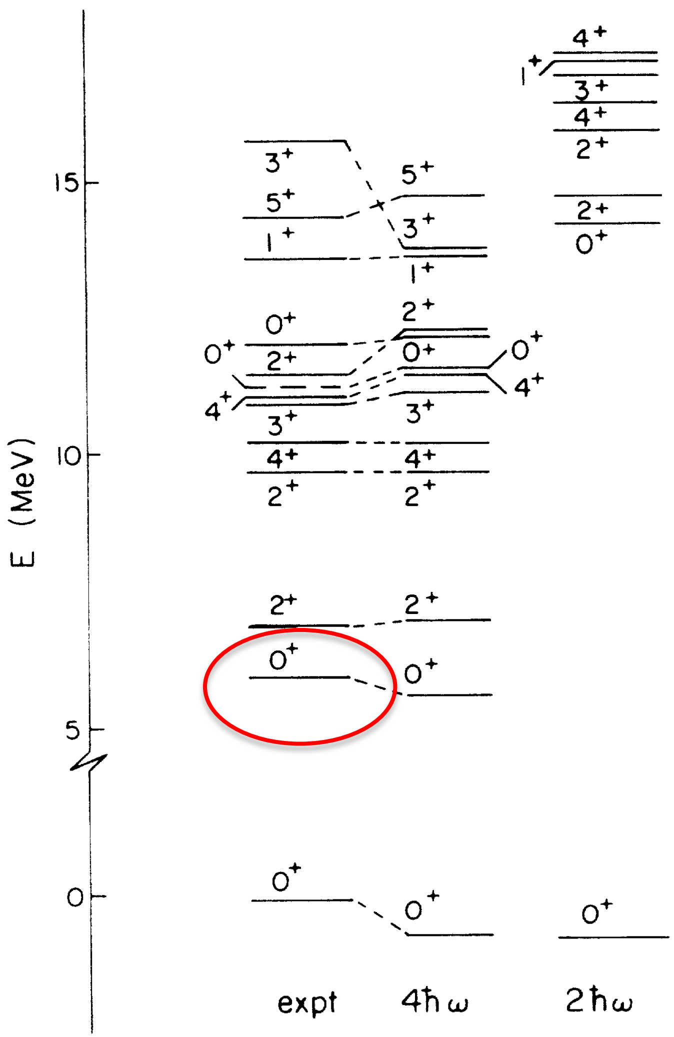
$^{12}C$ with chiral 2+3 body forces

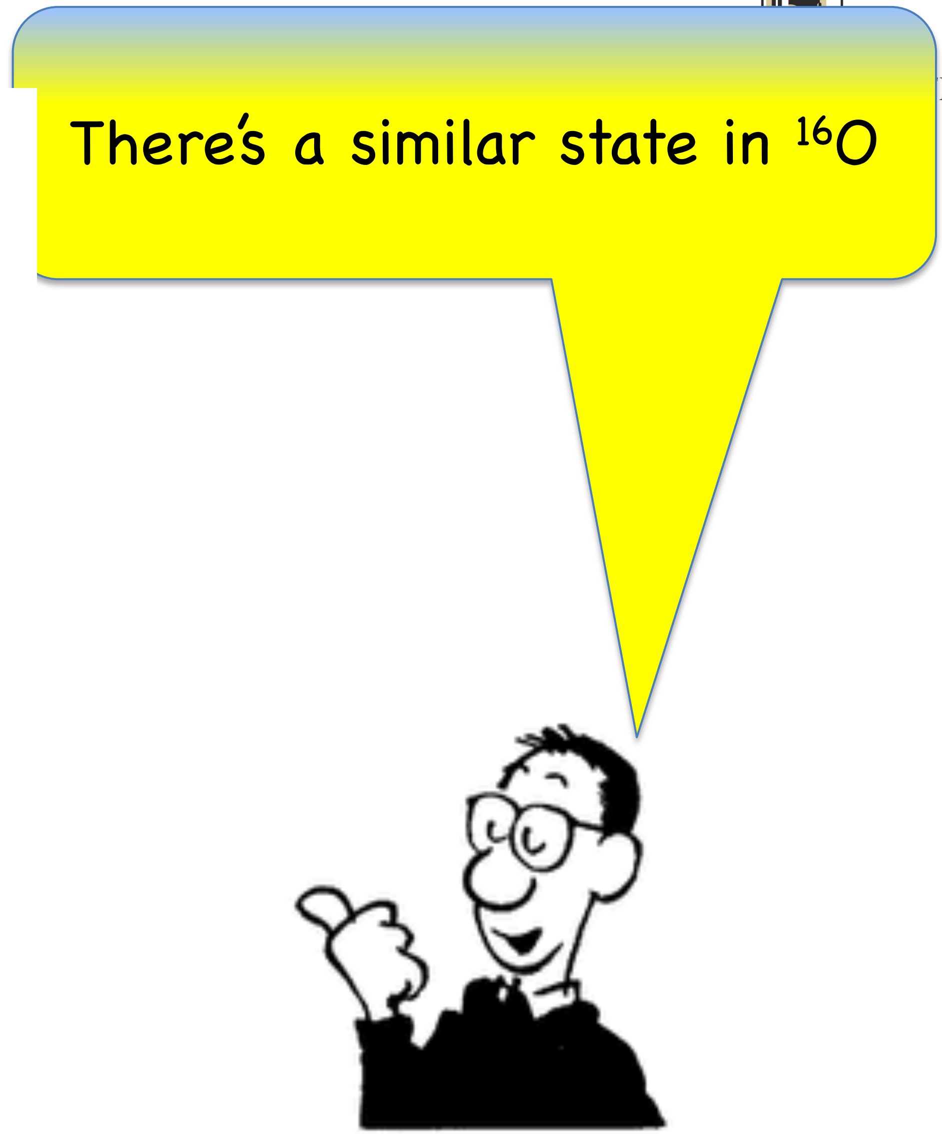
The Hoyle state in $^{12}C$ is a problem!



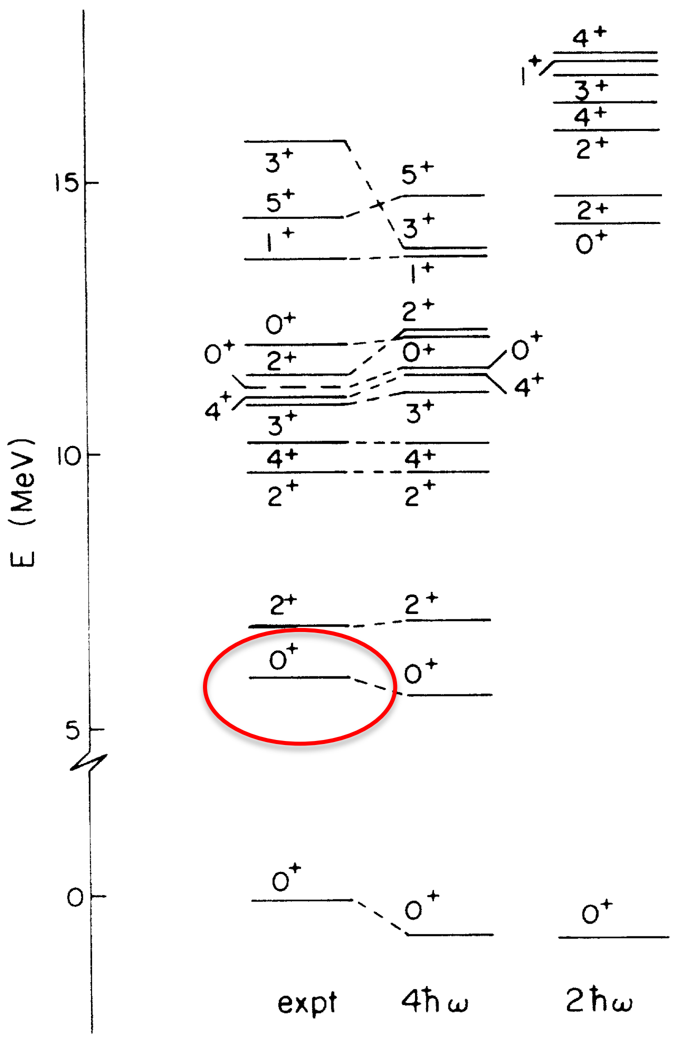

Hoyle state

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



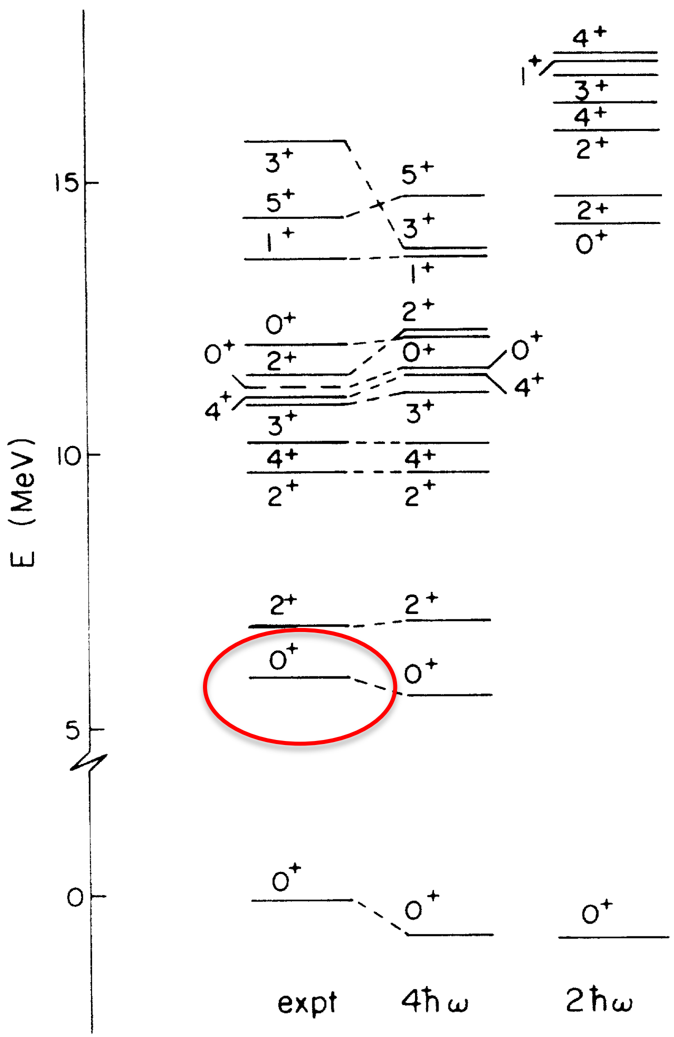
Haxton and Johnson, PRL **65**, 1325 (1990)




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

One can think of these as alpha-cluster states

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

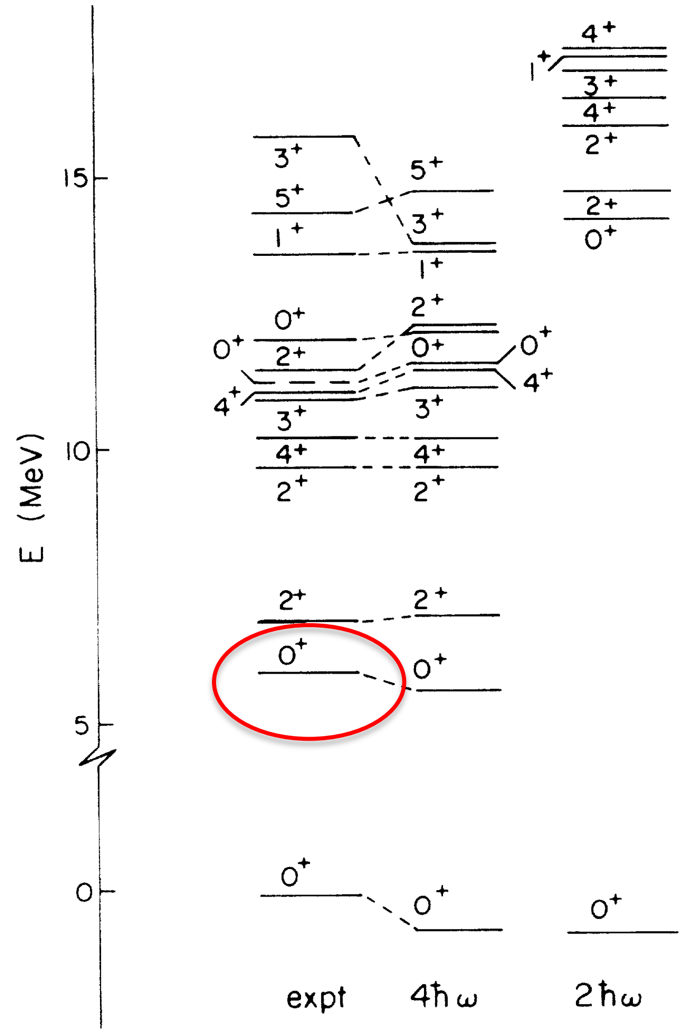



There's a similar state in $^{16}O$

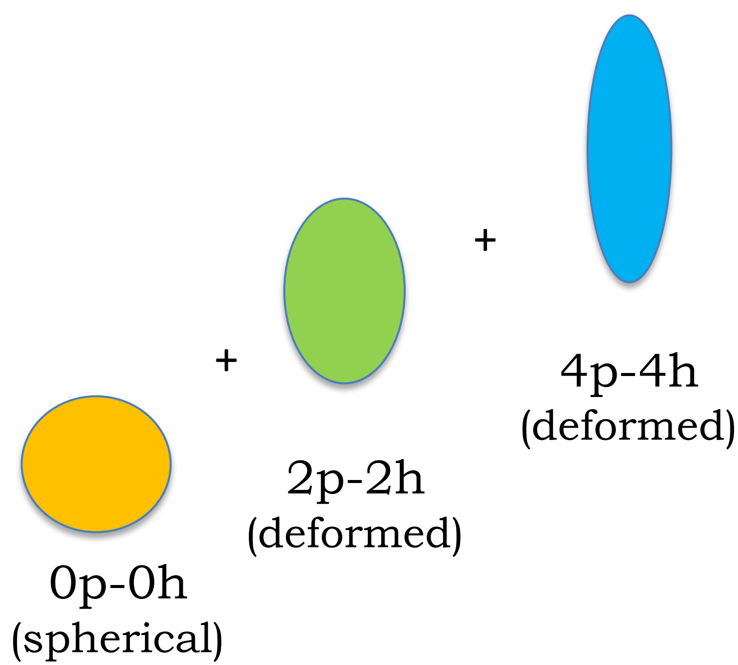
One can think of these as alpha-cluster states

Or as *n*p-*n*h states

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

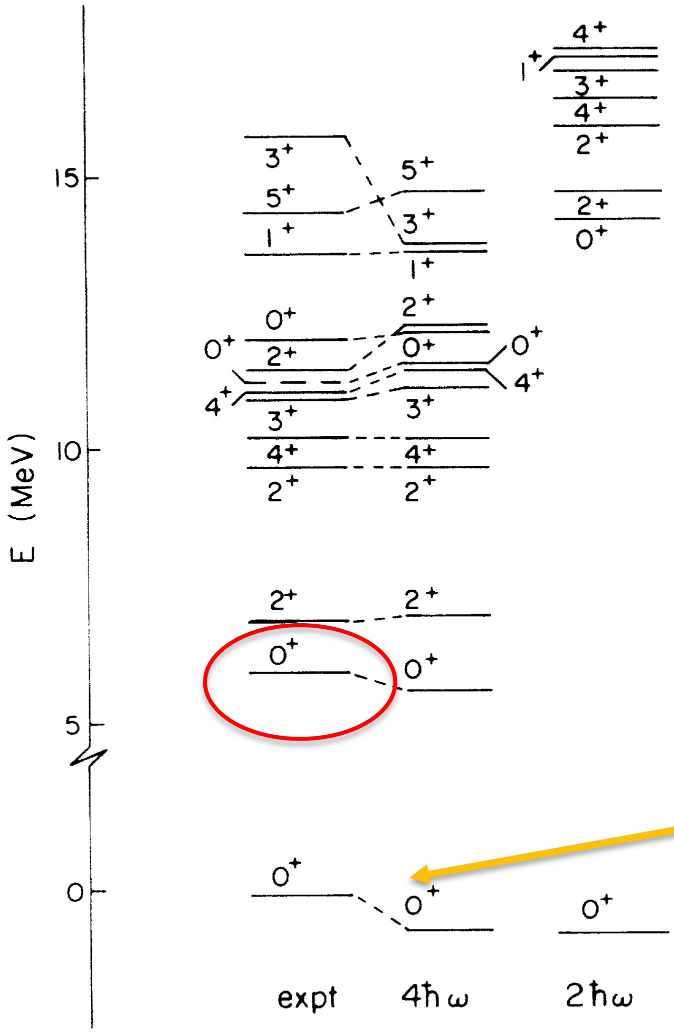


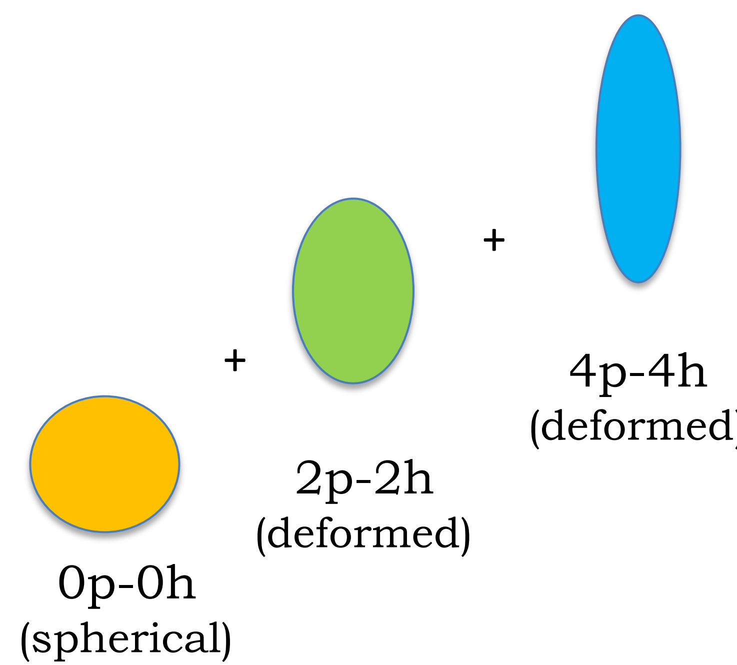

Brown and Green, Nucl. Phys. **75**, 401 (1966)



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

Brown and Green, Nucl. Phys. **75**, 401 (1966)



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

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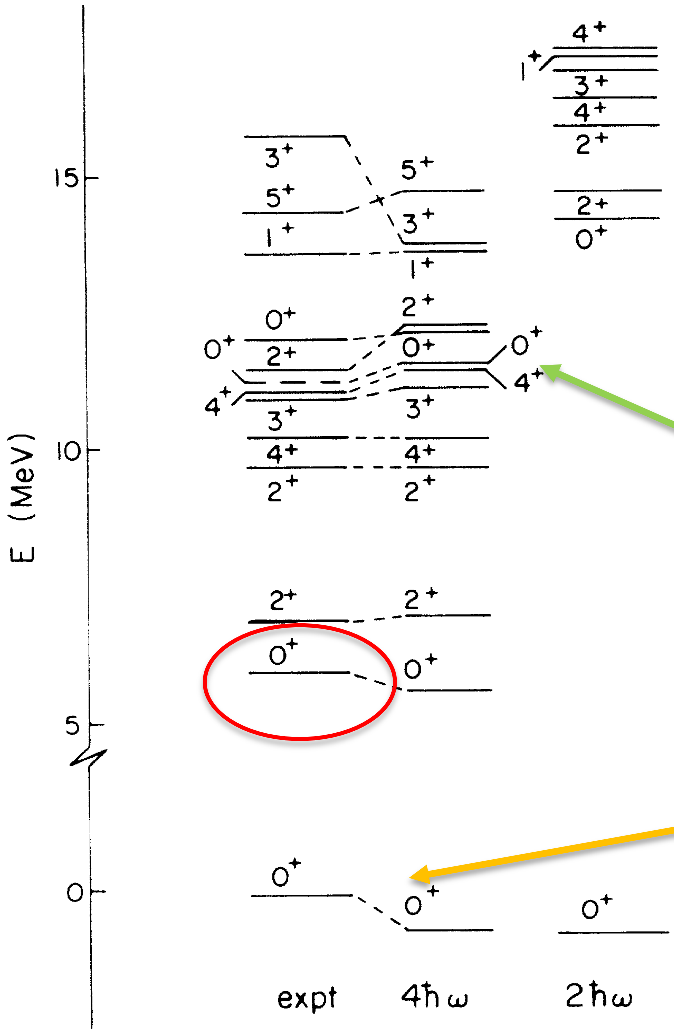
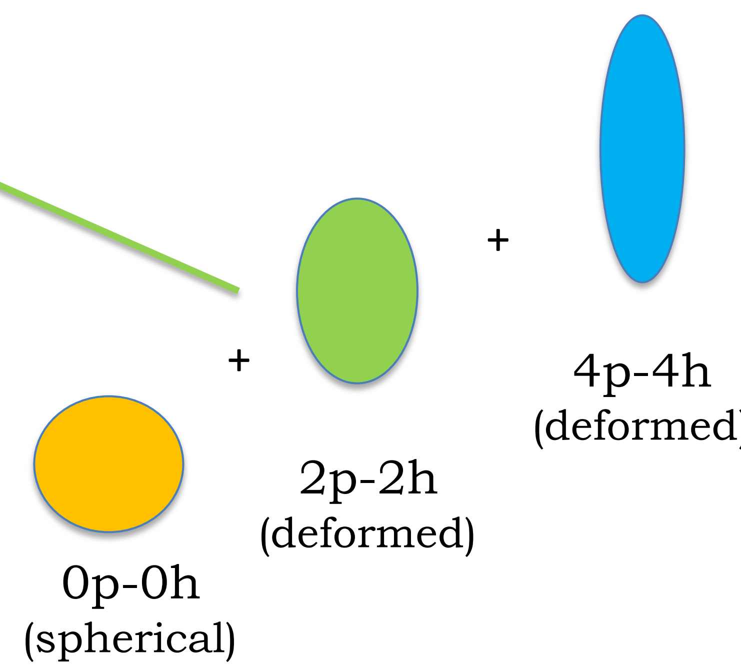



Brown and Green, Nucl. Phys. **75**, 401 (1966)



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

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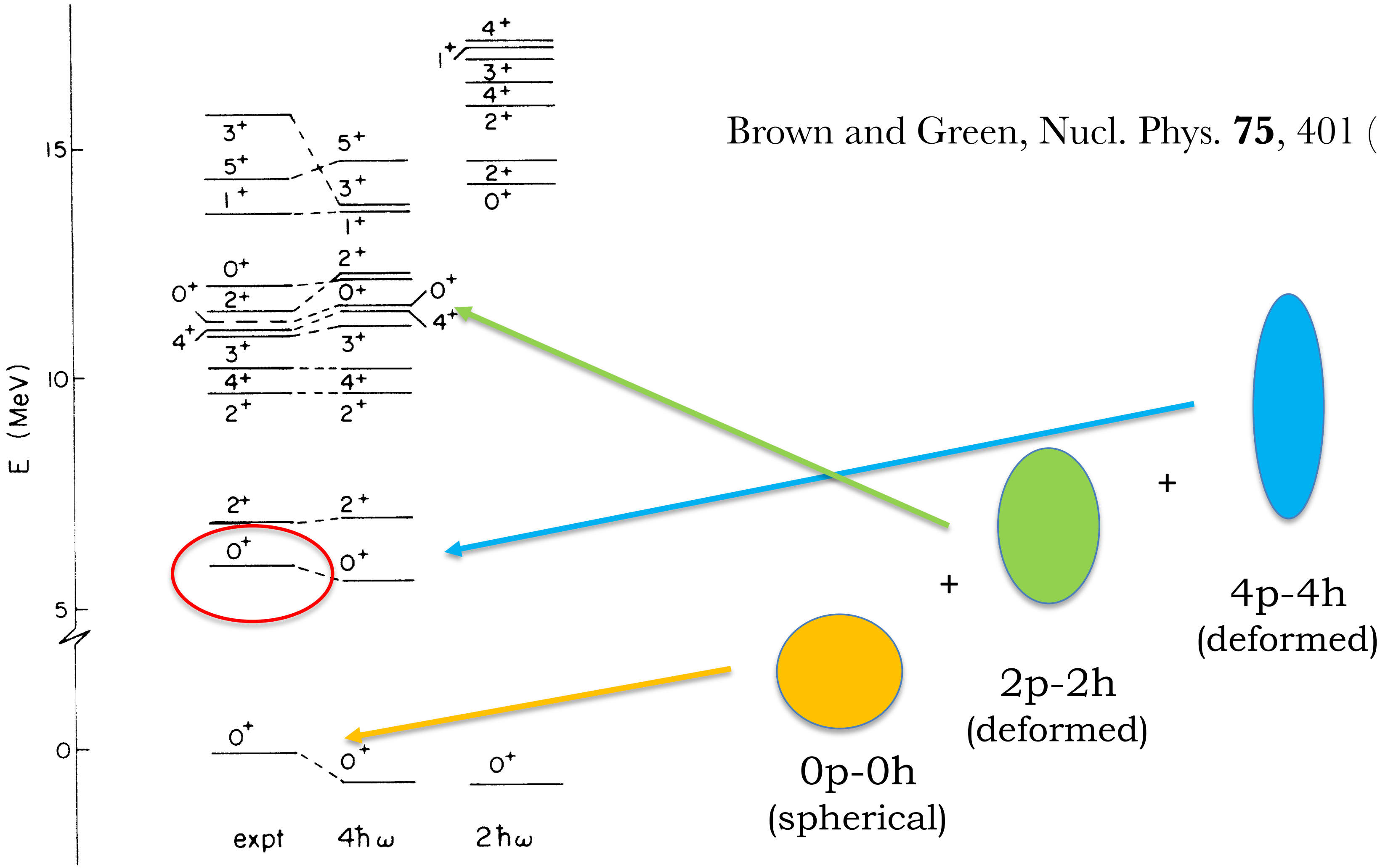
Brown and Green, Nucl. Phys. **75**, 401 (1966)



$^{16}O$ B(GT) experimentally measured via *(n,p)* at TRIUMF!
Hicks *et al* PRC **43**, 2554 (1991)

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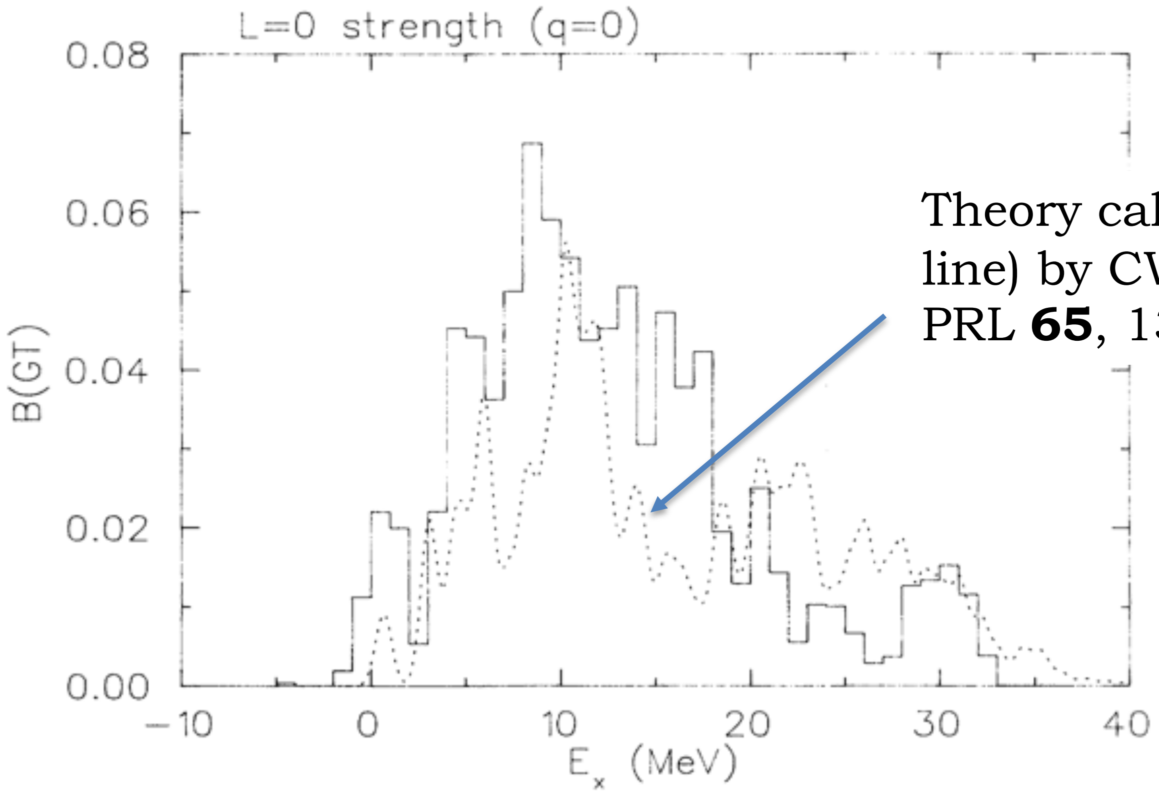
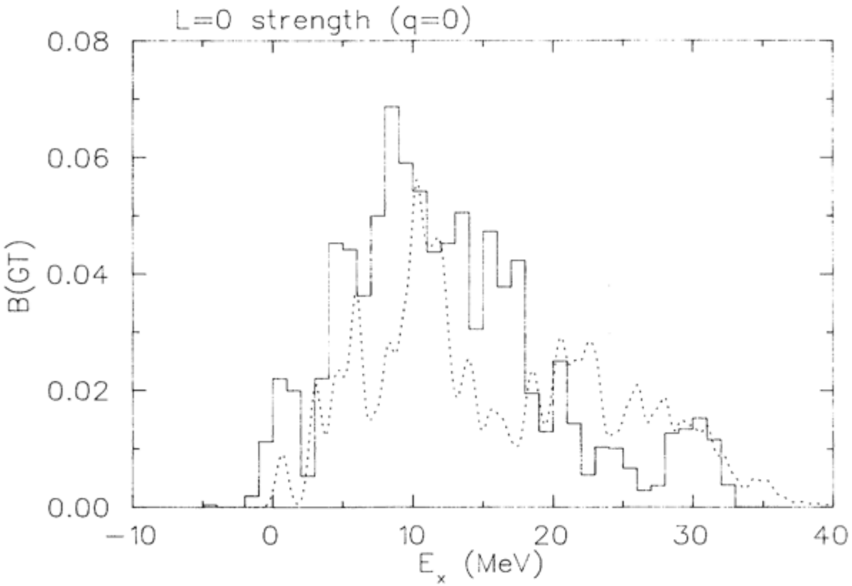
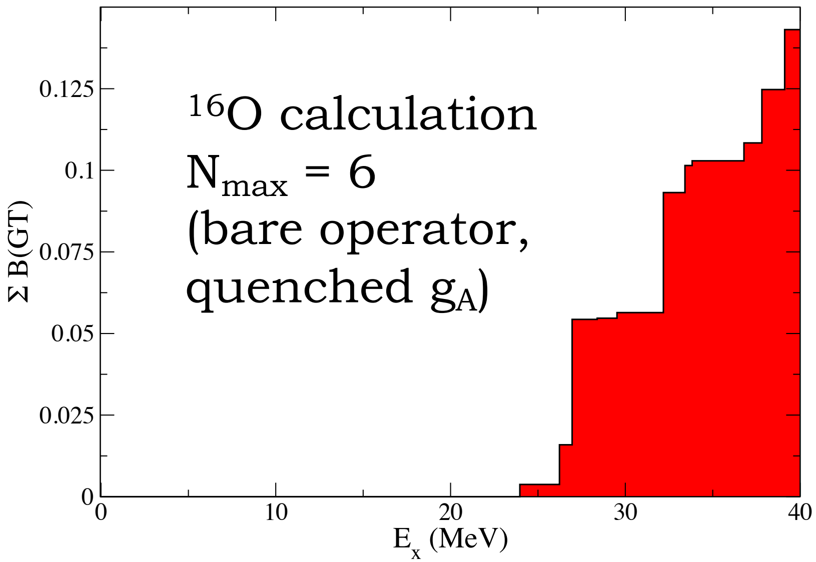



Theory calculation (dotted line) by CWJ & Haxton, PRL **65**, 1325 (1990)

One can probe the mixing of np-nh in $^{16}O$ through Gamow-Teller

$^{16}$O B(GT) experimentally measured via *(n,p)* at TRIUMF!
Hicks *et al* PRC **43**, 2554 (1991)




One can probe the mixing of np-nh in $^{16}$O through Gamow-Teller

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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

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

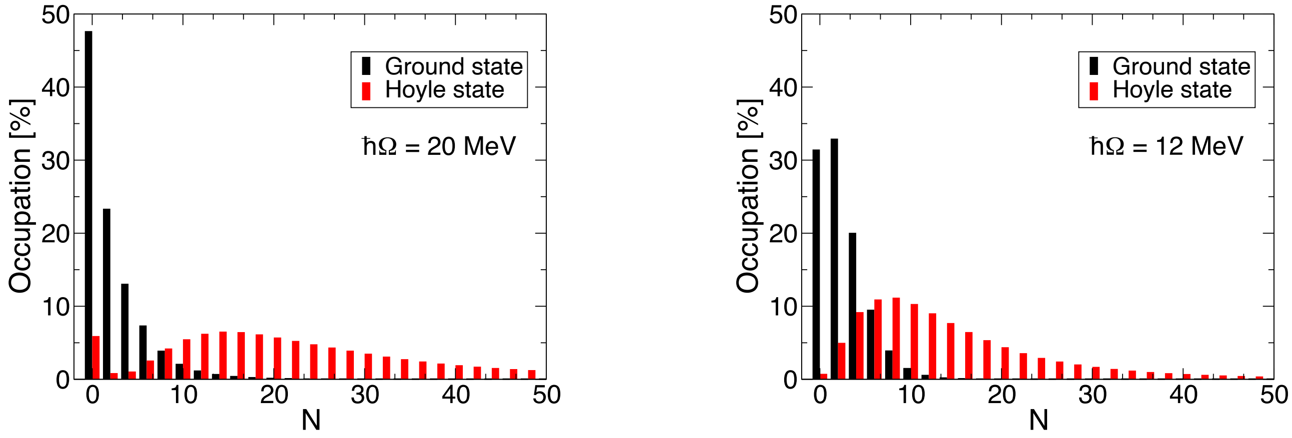


**Figure 6.** Decomposition of the $^{12}$C ground state and the Hoyle state into $N\hbar\Omega$ components for oscillator constants of 20 MeV (left) and 12 MeV (right).

Fermionic molecular dynamics calculation with Argonne V18 potential

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

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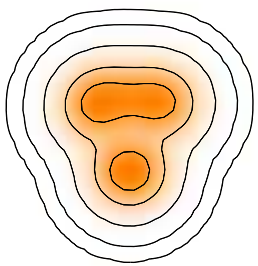
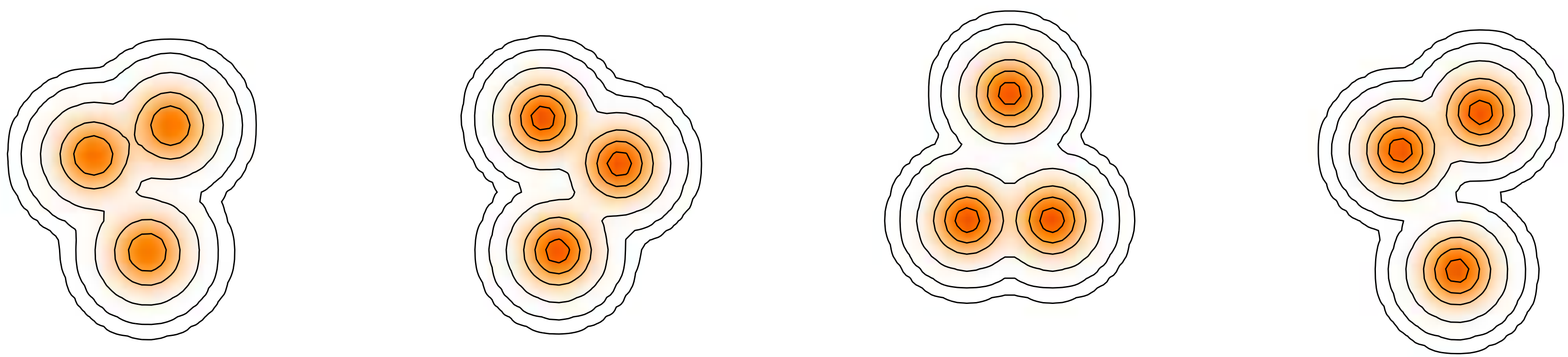


$^{12}$C g.s. (fermionic molecular dynamics FMD calculation)



$^{12}$C Hoyle state main FMD configurations.

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

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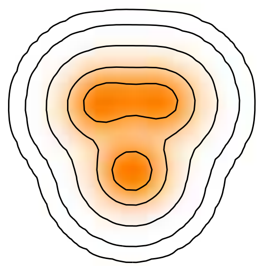
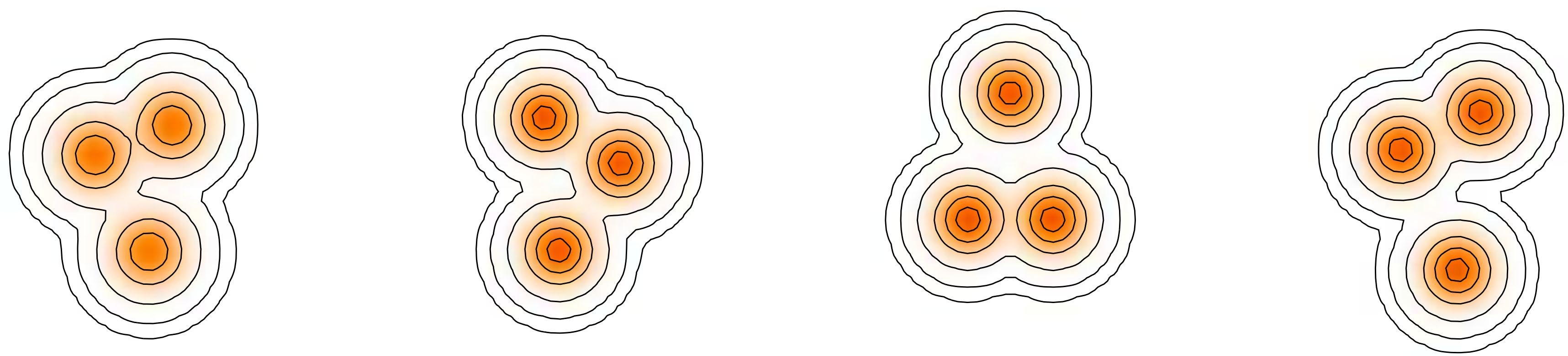


See also: S. Shen, D. Lee, et al, Nat. Commun. 14 (2023) 2777 (arXiv:2202.13596 ) for similar results on the lattice



$^{12}$C Hoyle state main FMD configurations.

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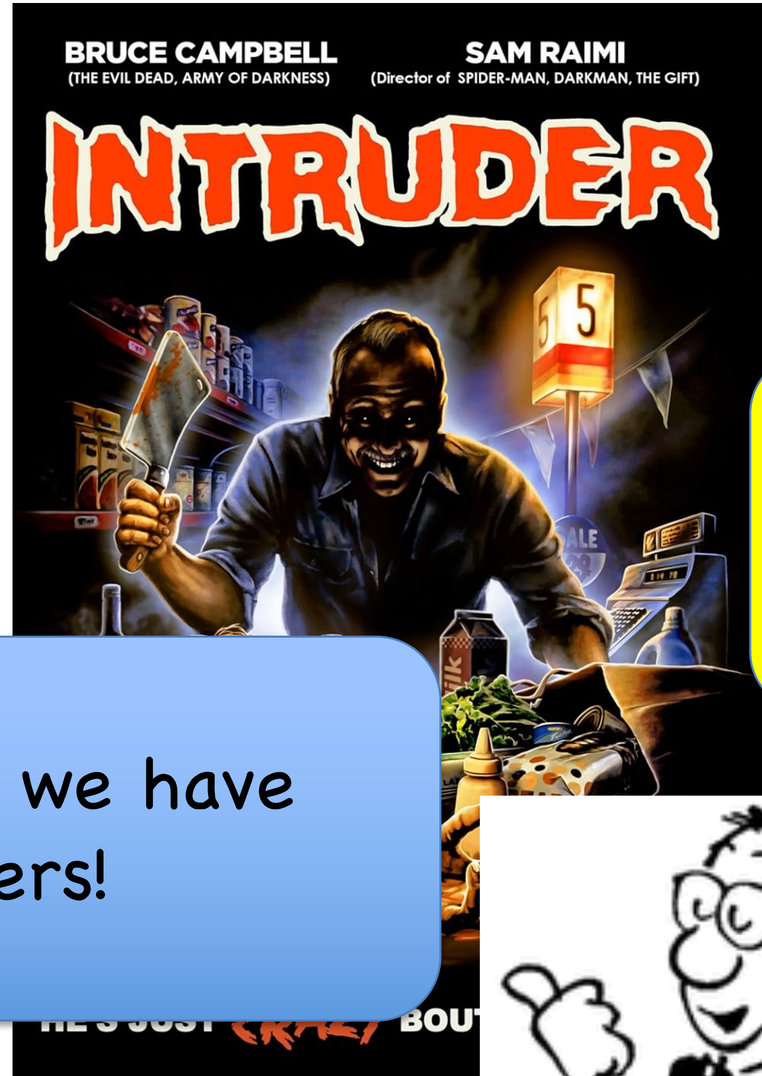
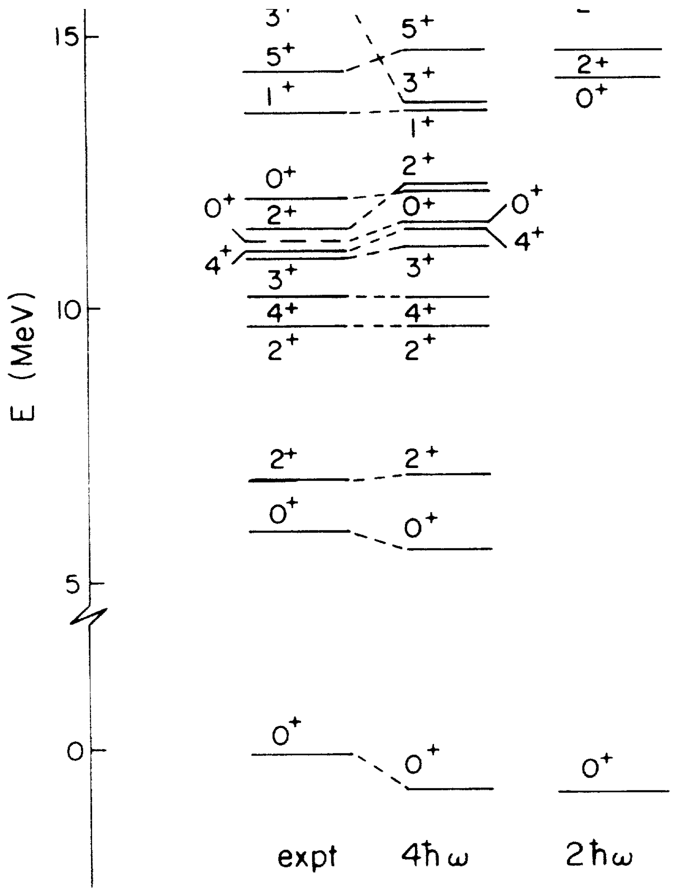
So basically we have intruders!




Yikes! Intruders are scary!

So basically we have intruders!

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




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

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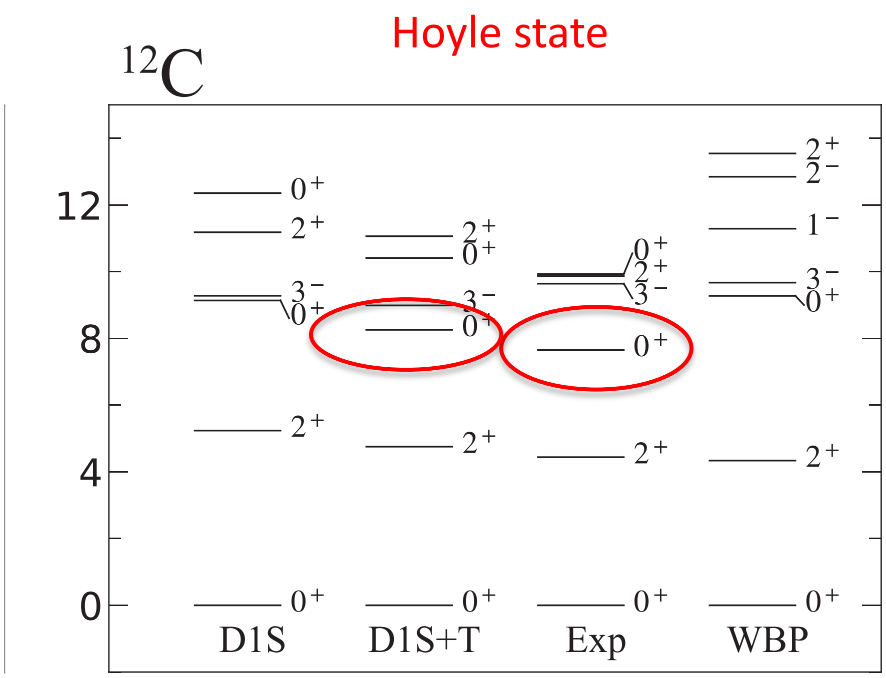
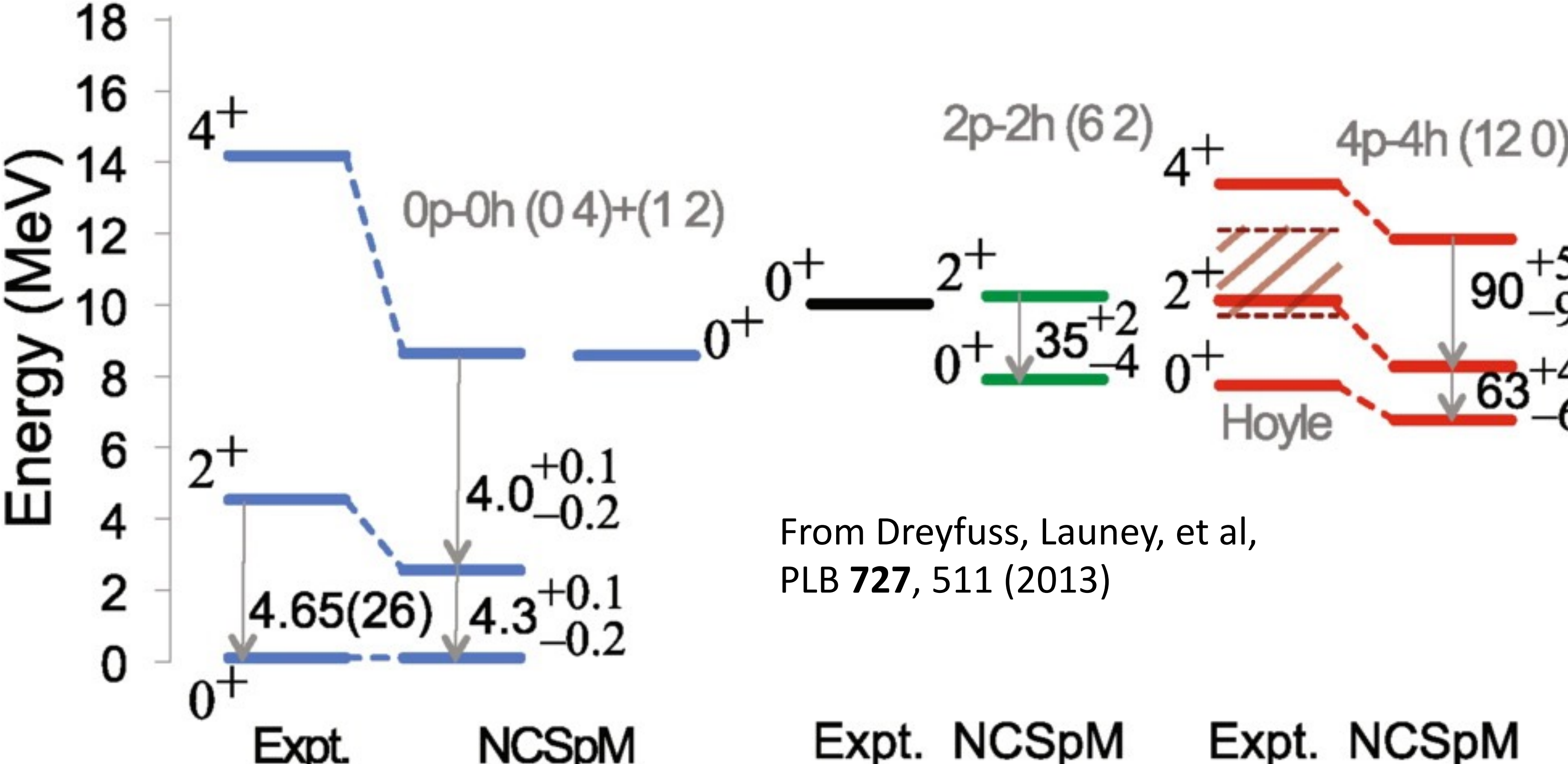
# One can phenomenologically reproduce spectra for example, by adjusting single particle energies




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)

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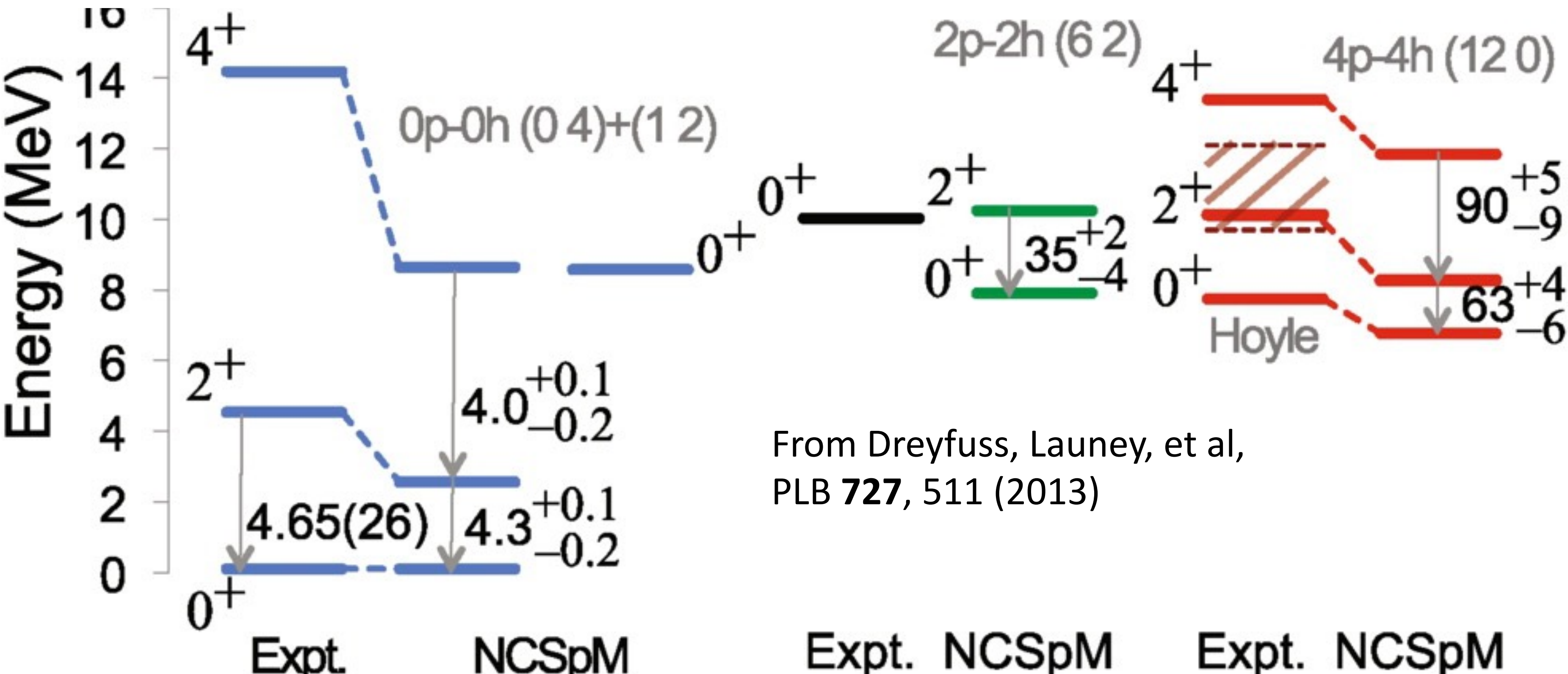
$$H_\gamma = \sum_{i=1}^{A}\left(\frac{\mathbf{p}_i^2}{2m} + \frac{m\Omega^2\mathbf{r}_i^2}{2}\right) + \frac{\chi}{2}\frac{(e^{-\gamma Q\cdot Q} - 1)}{\gamma}$$

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

a

r




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

Related to cluster states,
islands of inversions
and halo nuclei
form a similar **challenge** to
standard shell-model pictures

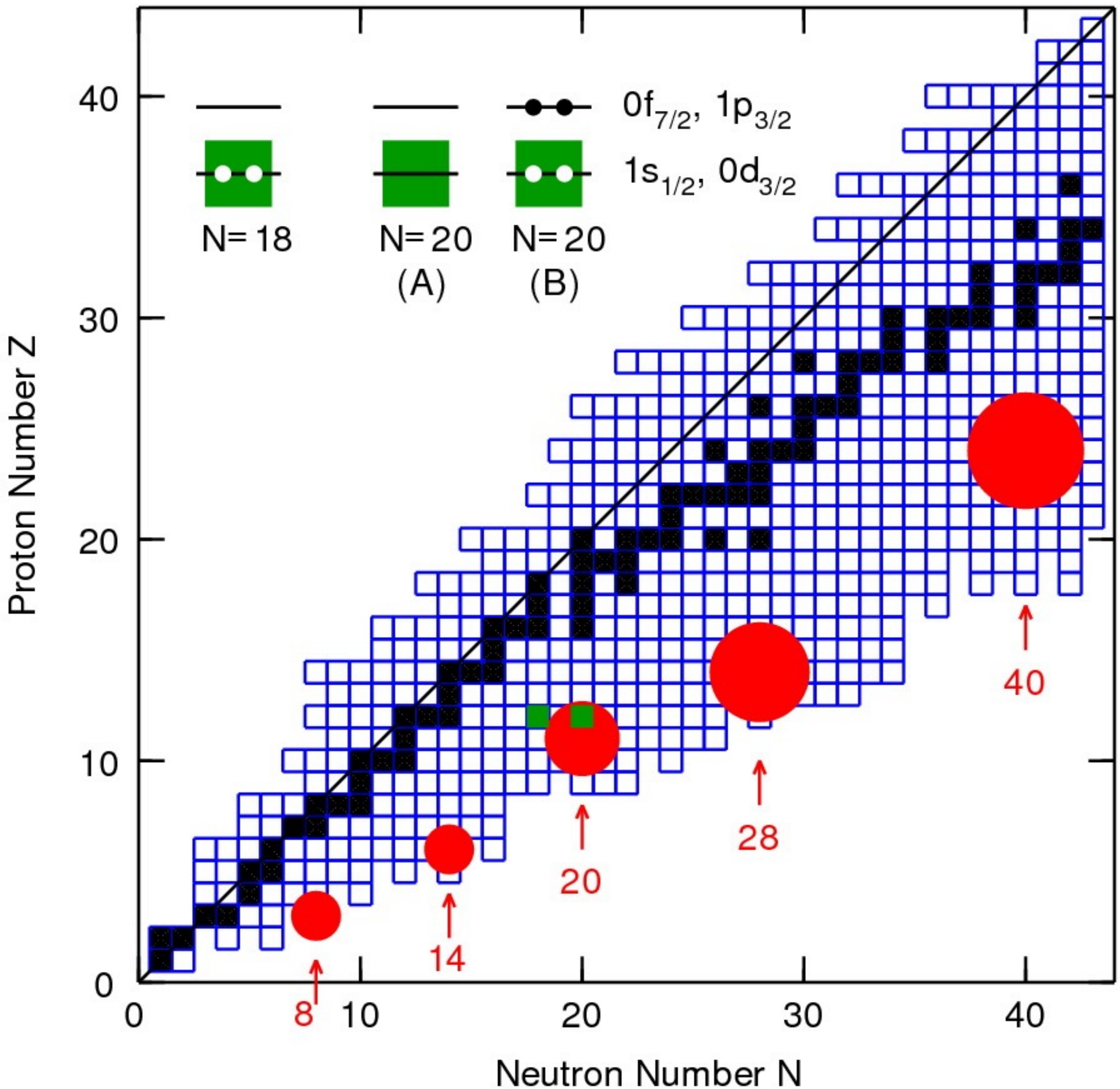



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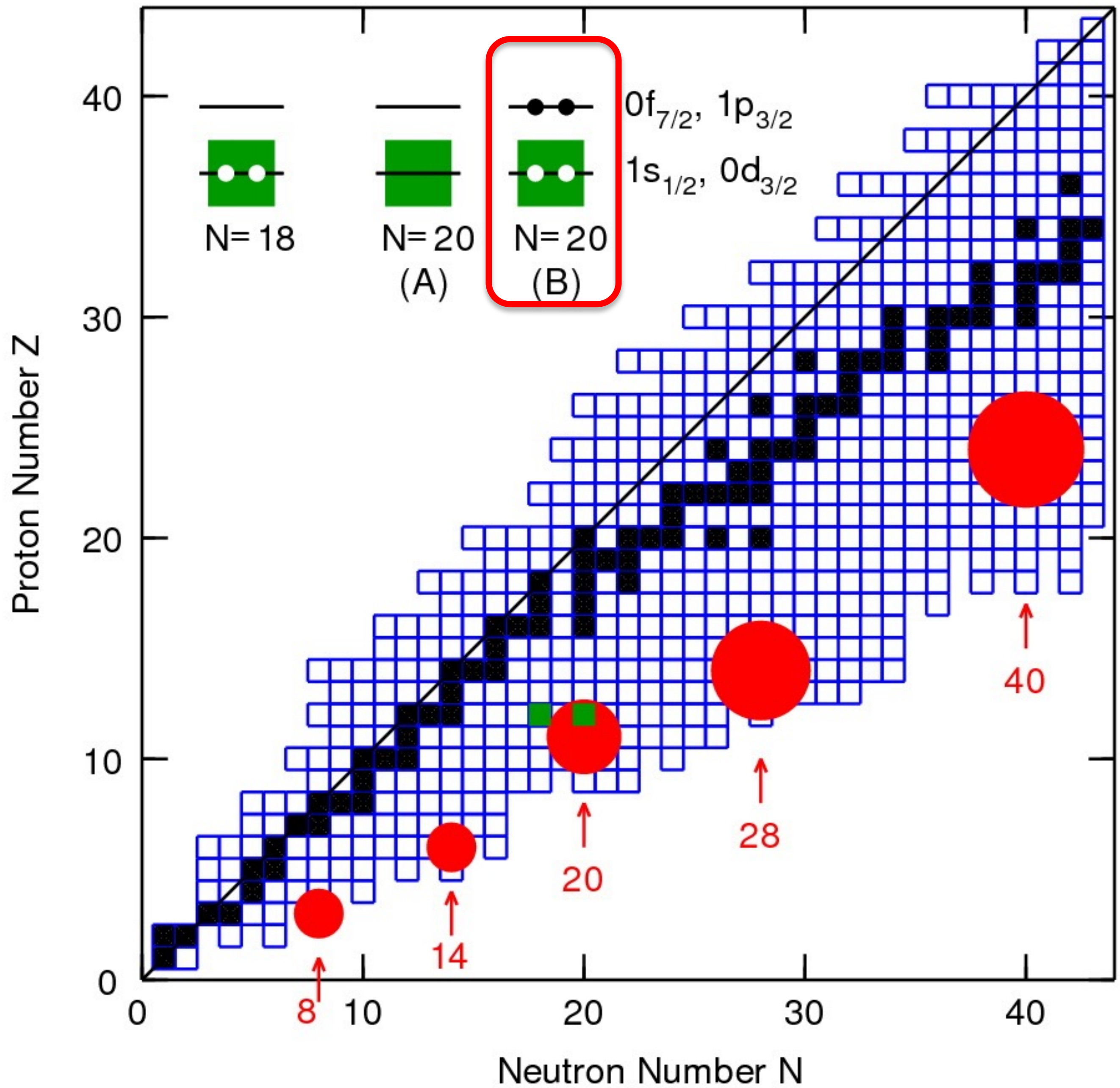
Figure:
Alex Brown




San Diego State University

Figure:
Alex Brown

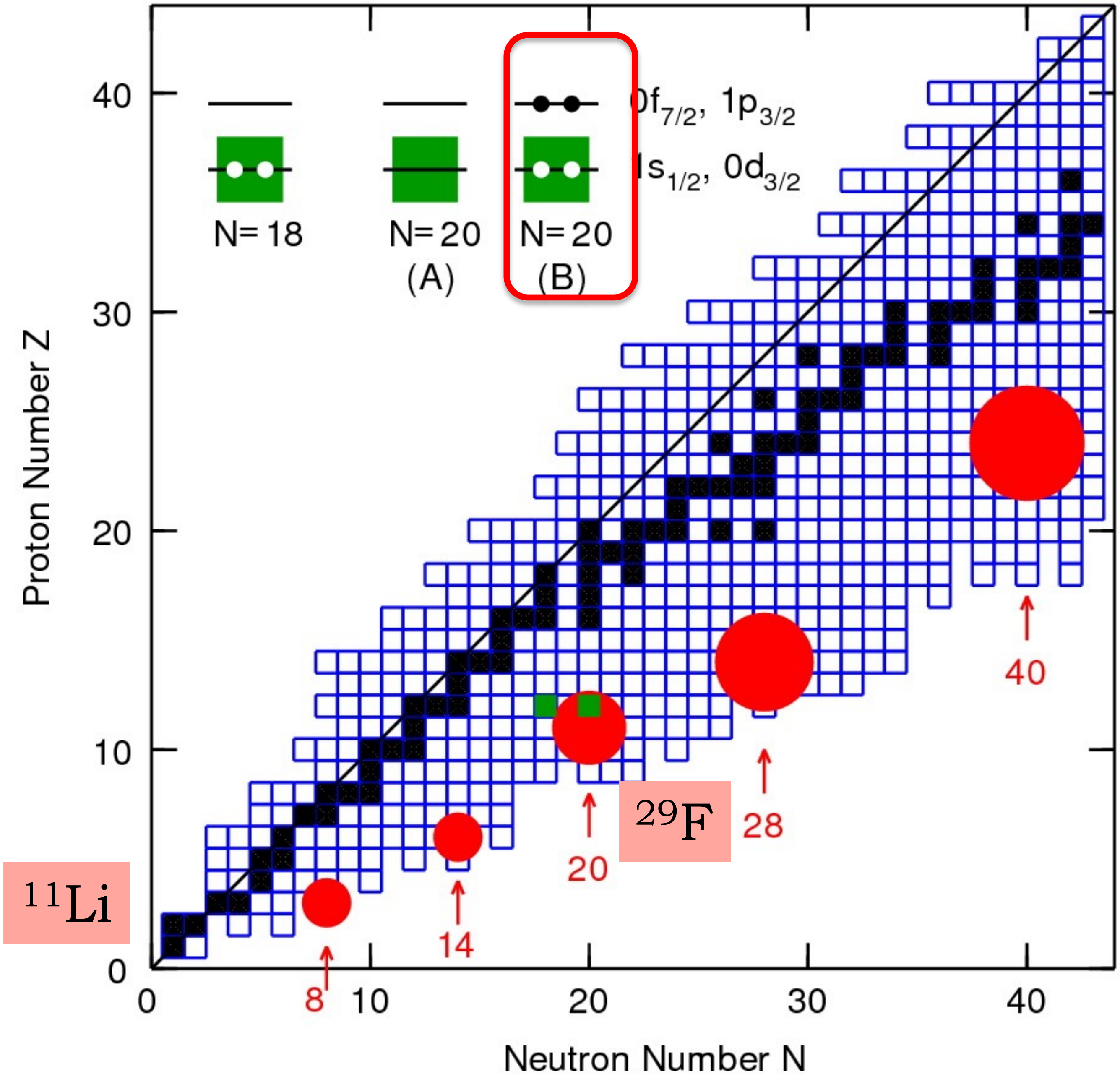




Figure:
Alex Brown

# 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; large deformation
- Small enough to be tackled numerically
- Testbed for techniques

# Case study: $^{11}$Li

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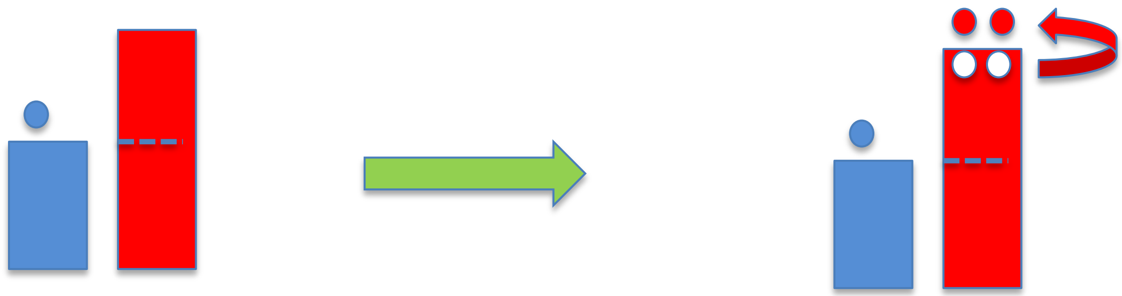


One proton outside a filled shell
+ filled neutron shell

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

"island of inversion"

# CASE STUDY: $^{11}$LI

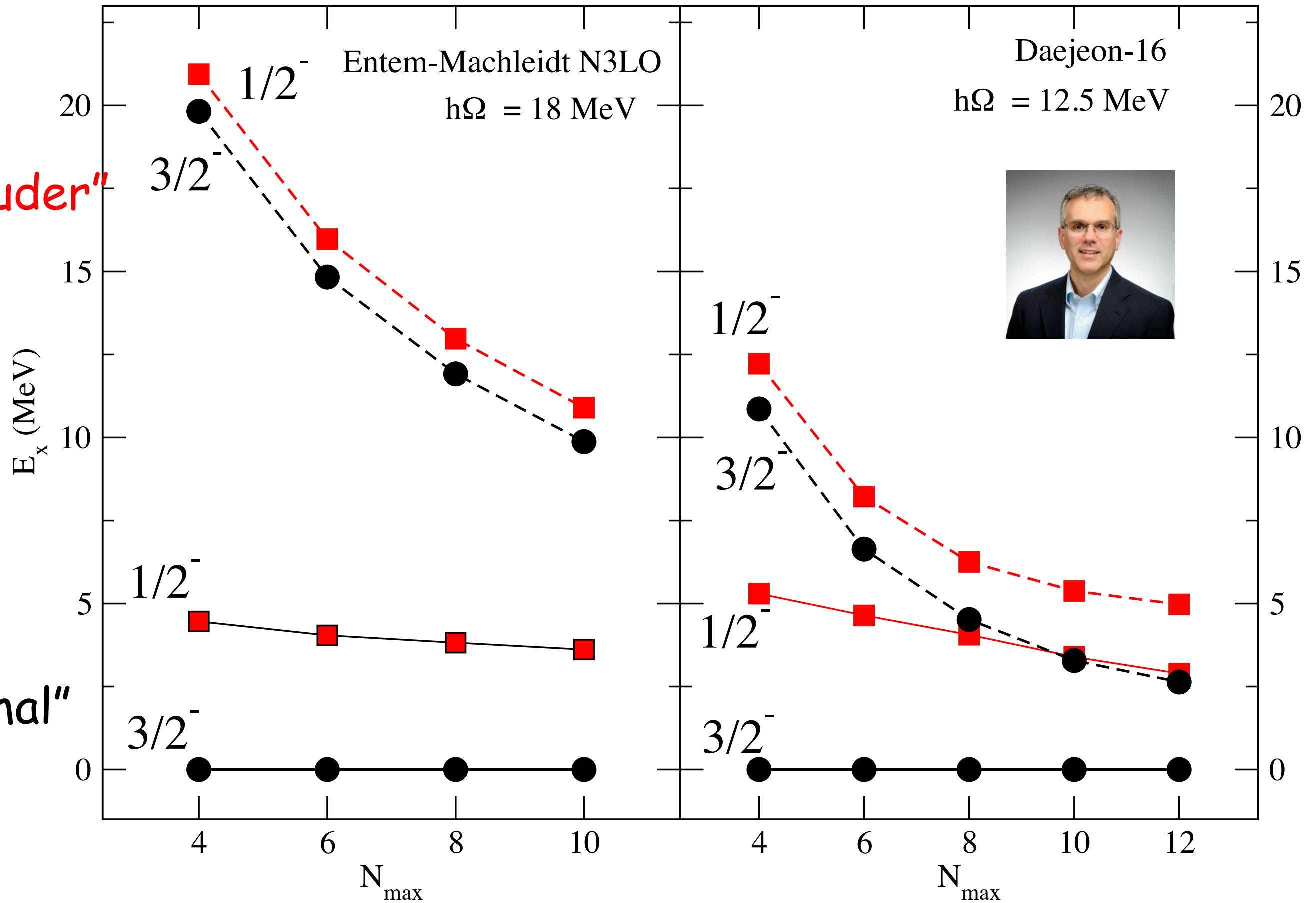
$^{11}$Li makes for an excellent case study

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

# CASE STUDY: $^{11}$LI

"intruder"

"normal"



# CASE STUDY: $^{11}$LI

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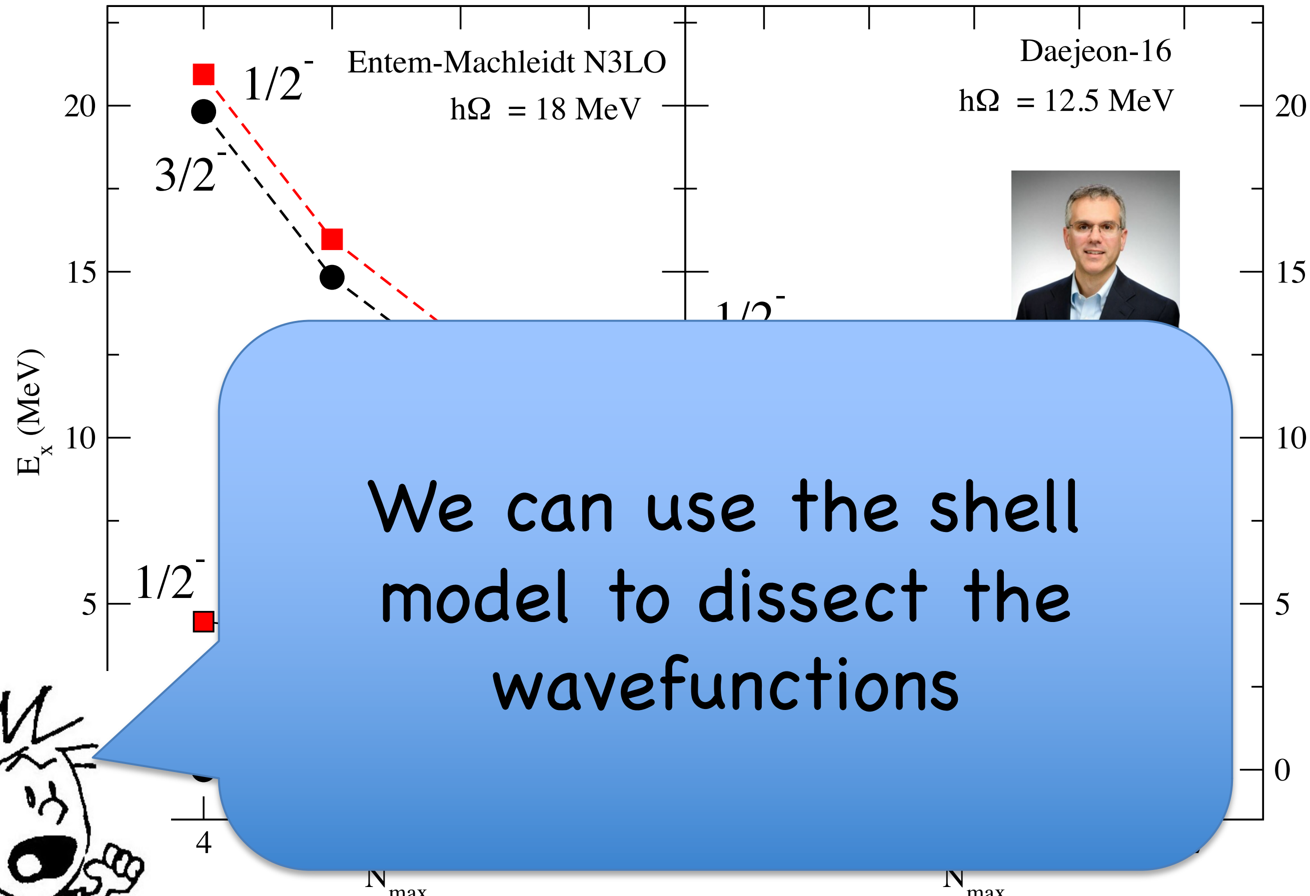
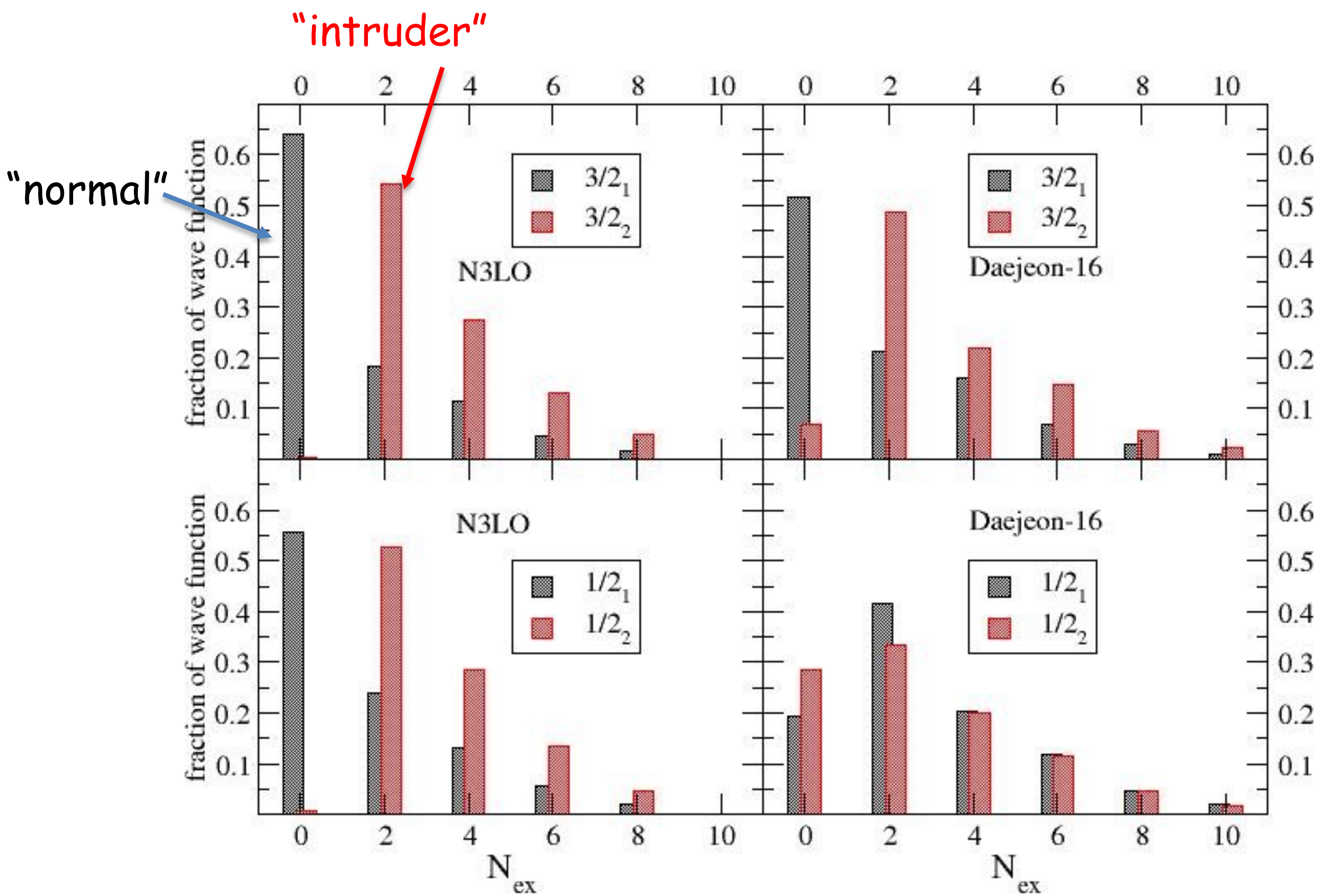
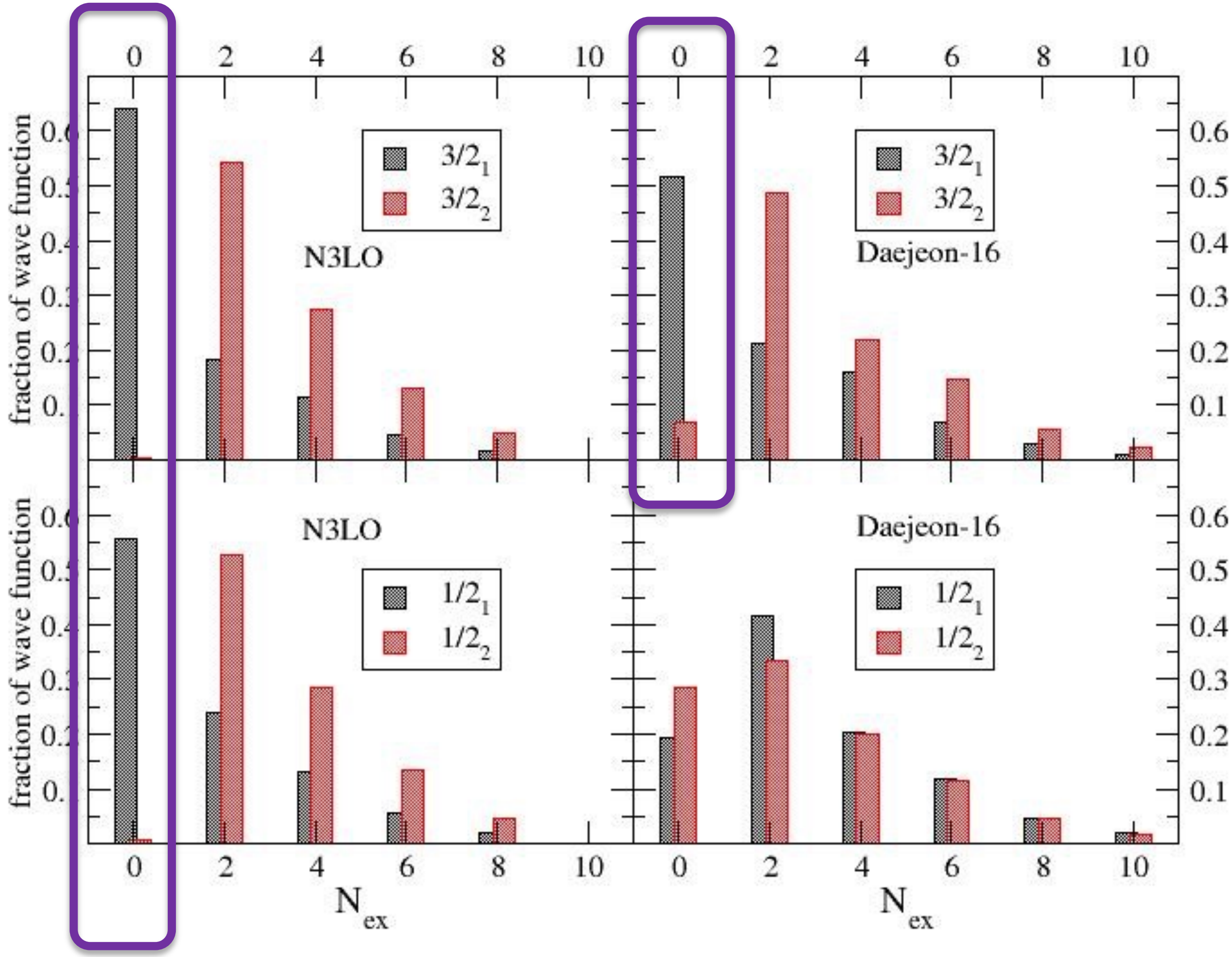



We can use the shell model to dissect the wavefunctions

# CASE STUDY: $^{11}$LI

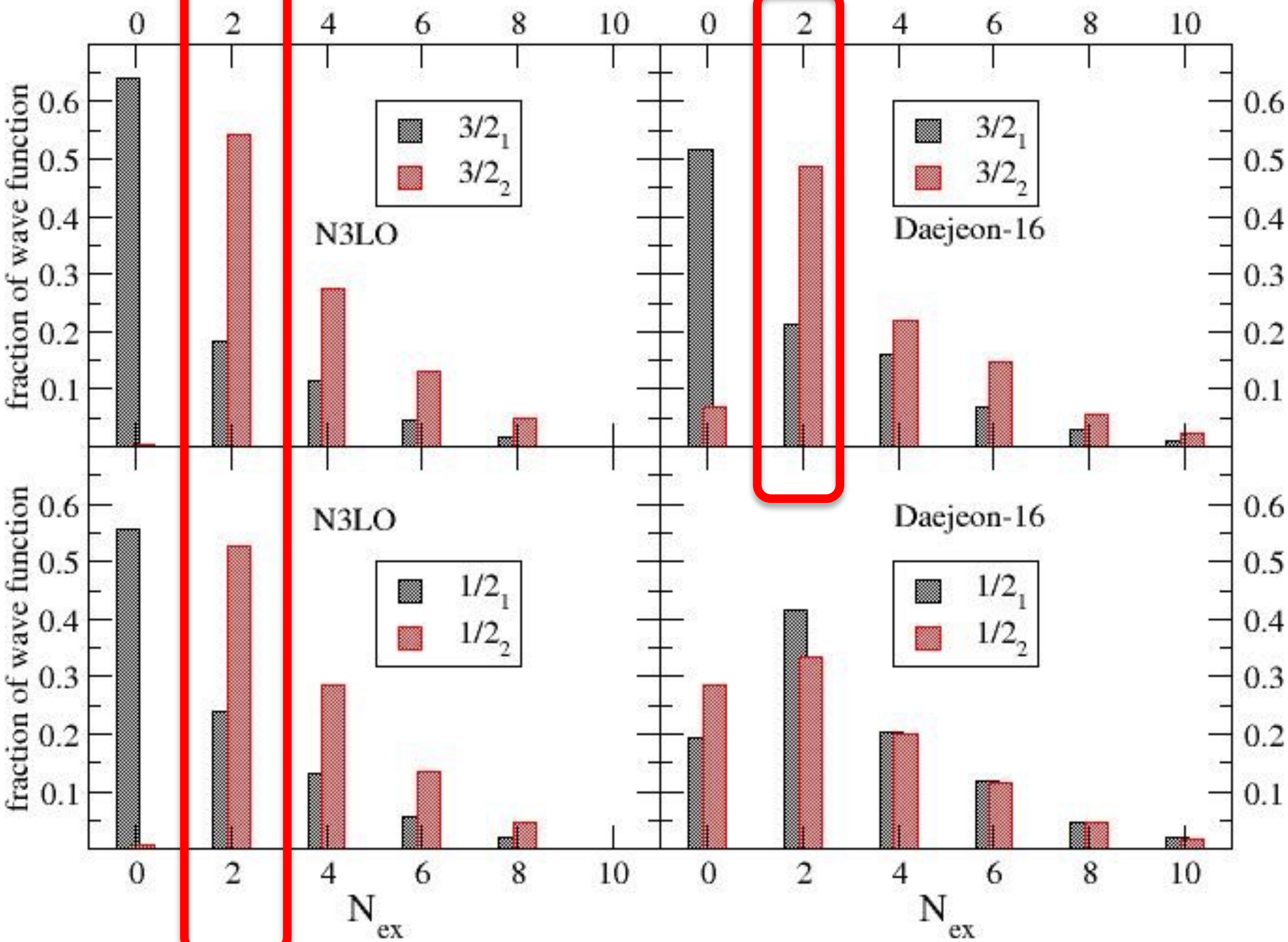


# CASE STUDY: $^{11}$LI



# CASE STUDY: $^{11}$Li

“intruder”



# CASE STUDY: $^{11}$LI

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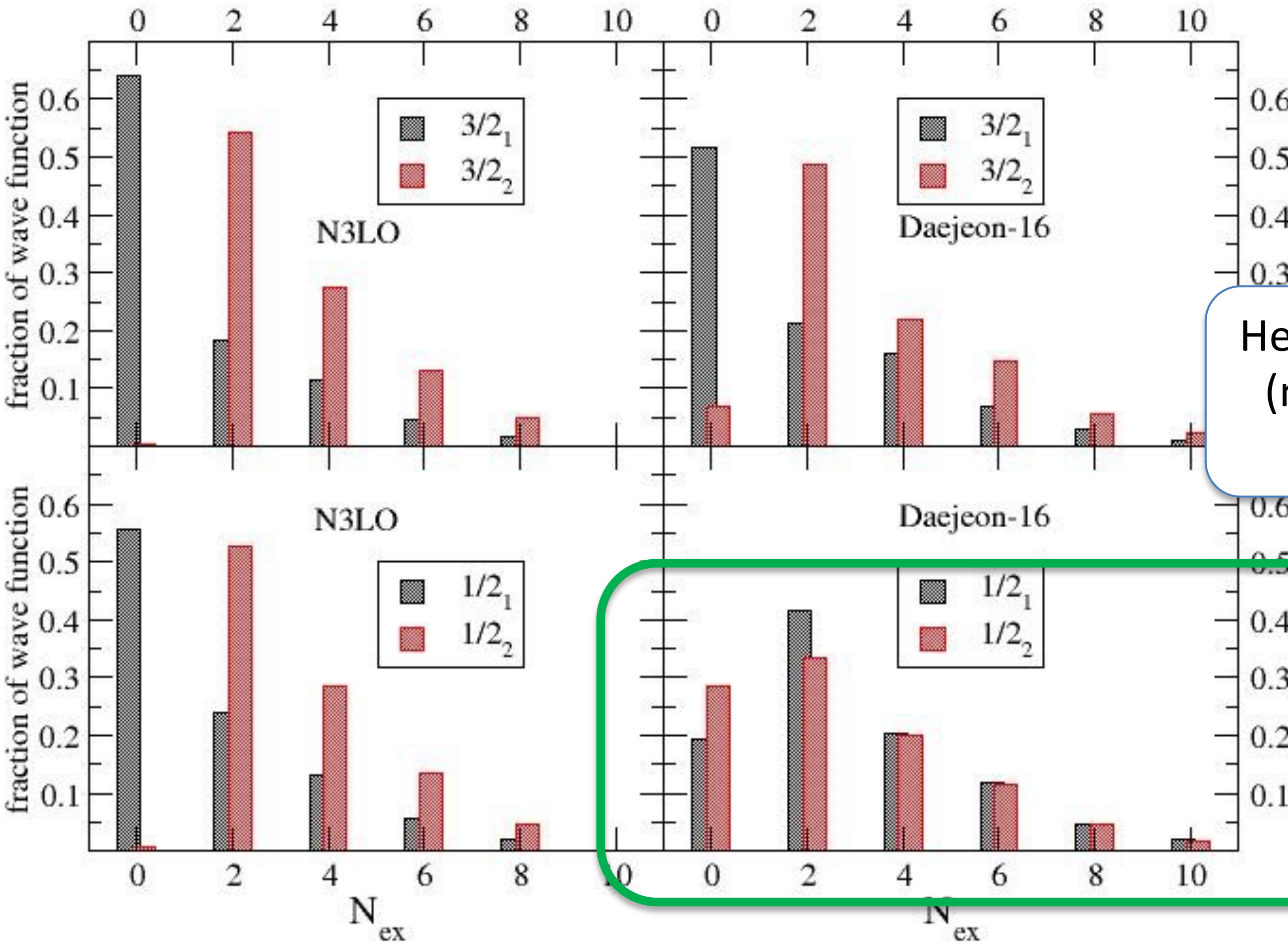


Here we see mixing (more in my talk, next!)

# CASE STUDY: $^{11}$LI

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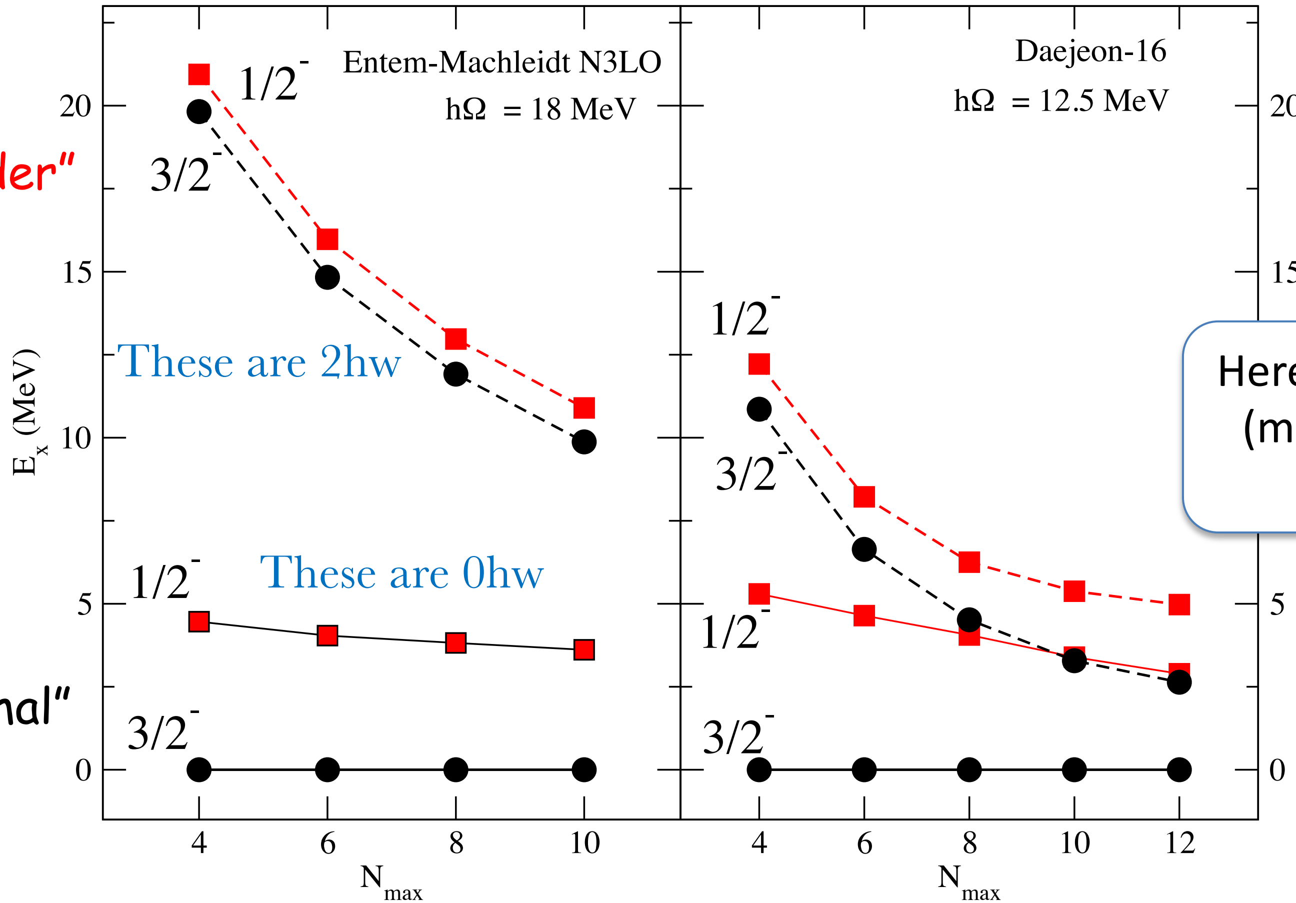
"intruder"

"normal"

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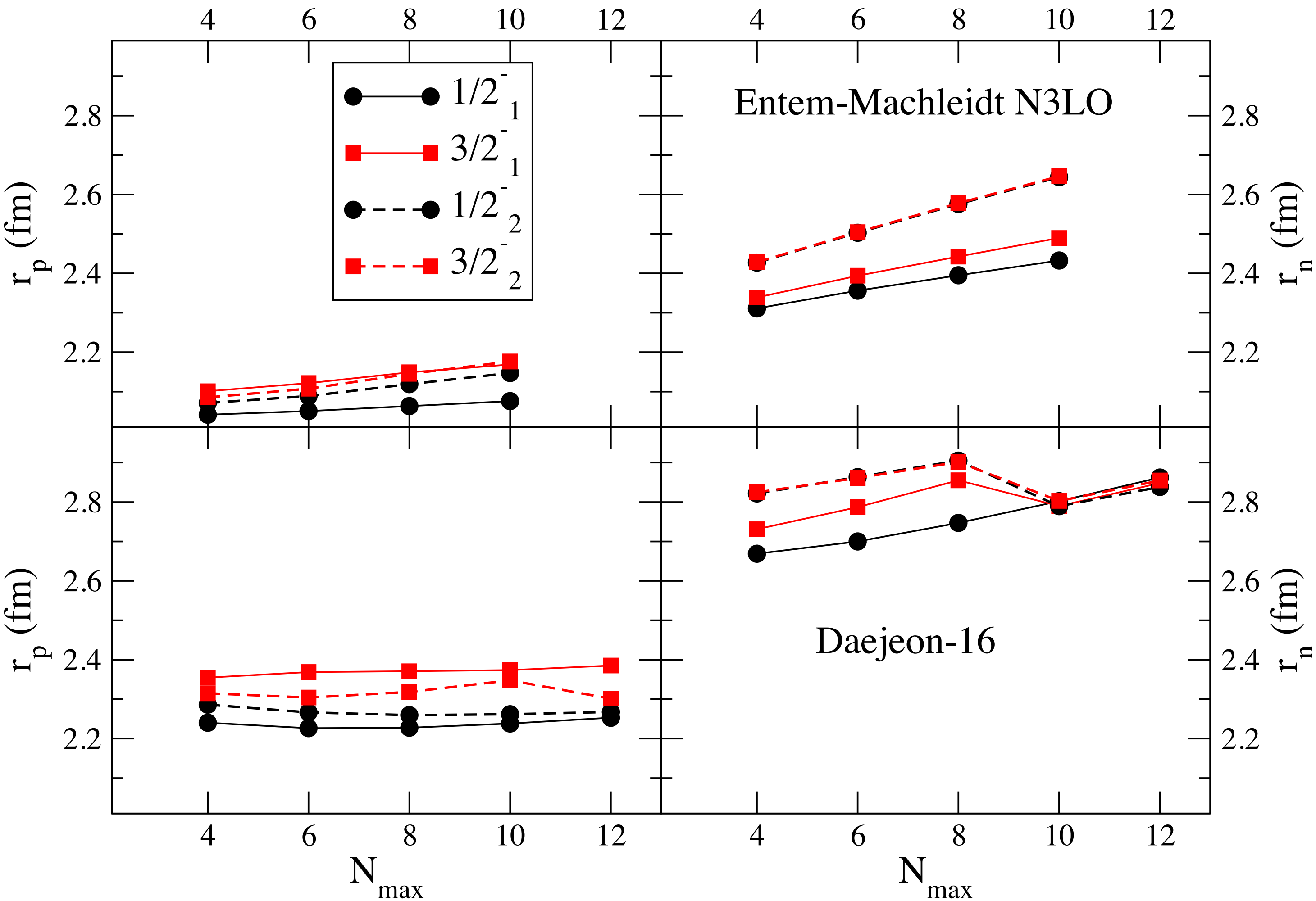
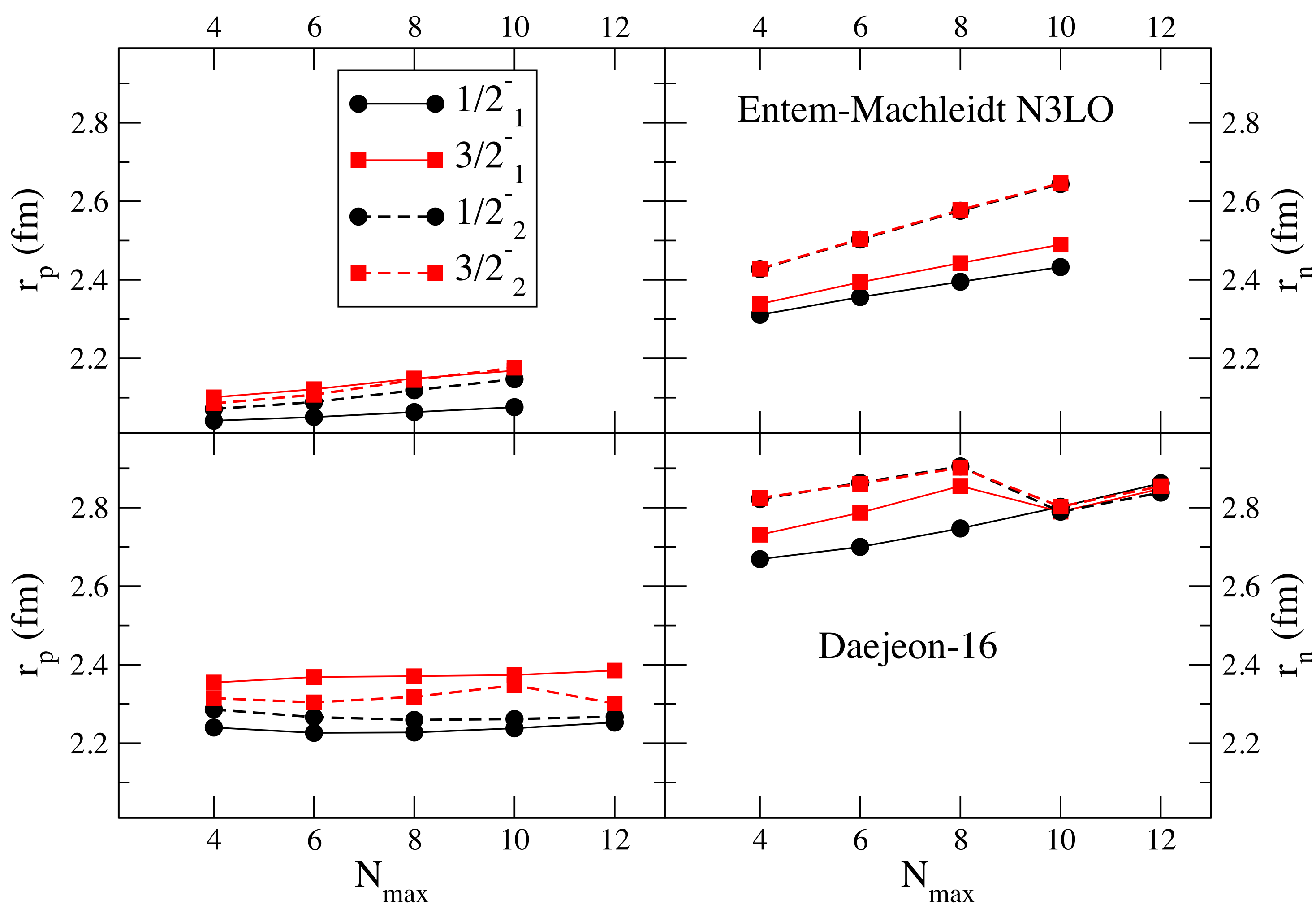
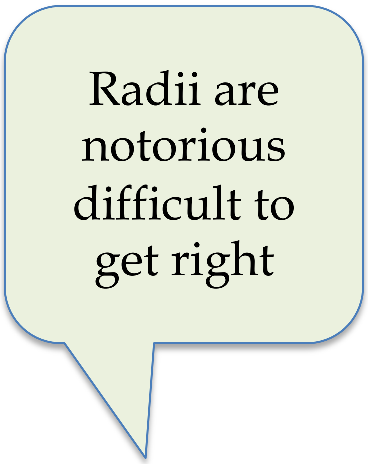
# CASE STUDY: $^{11}$LI



# CASE STUDY: $^{11}$LI

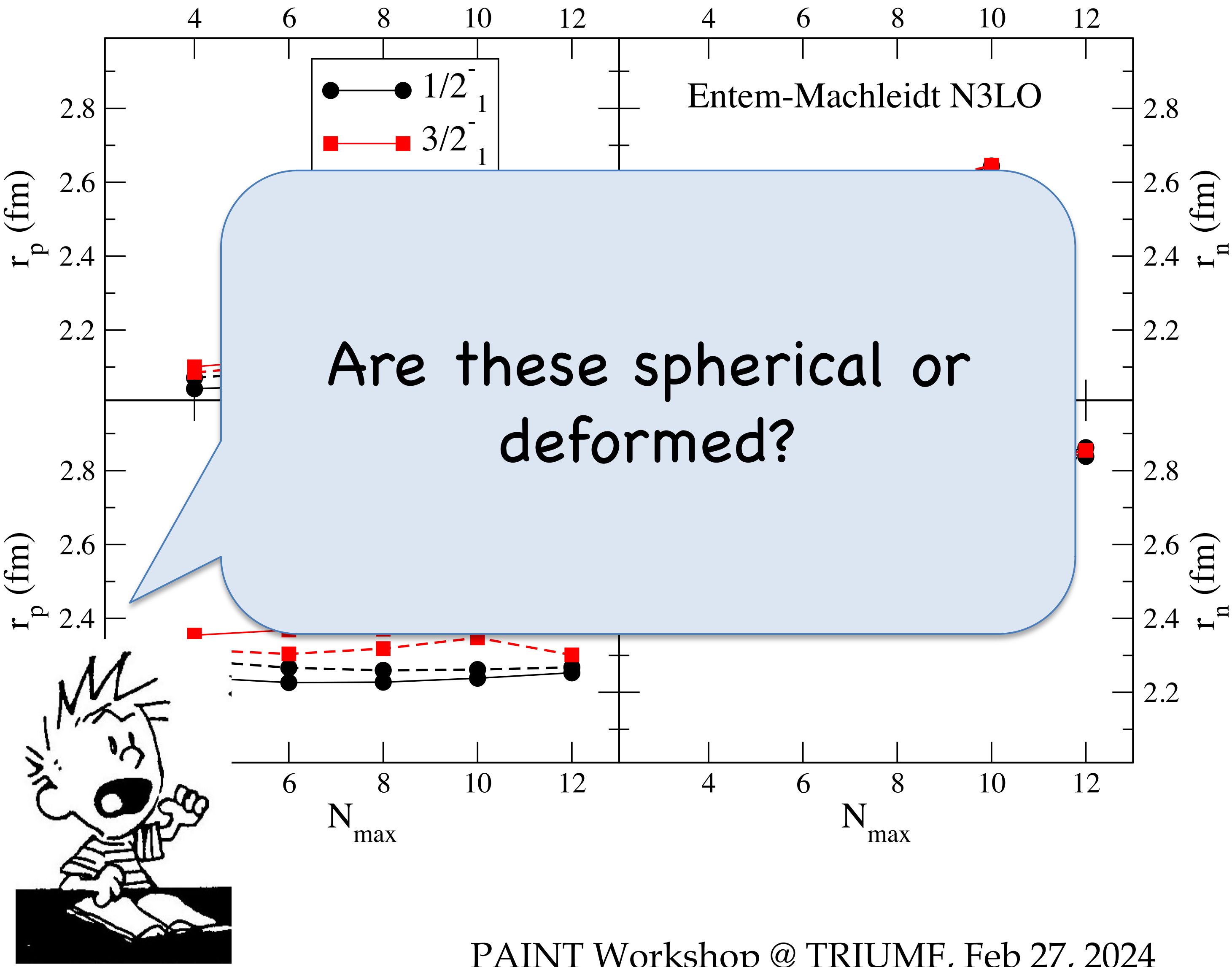



Mark Caprio

# CASE STUDY: $^{11}$LI

SAN DIEGO STATE UNIVERSITY

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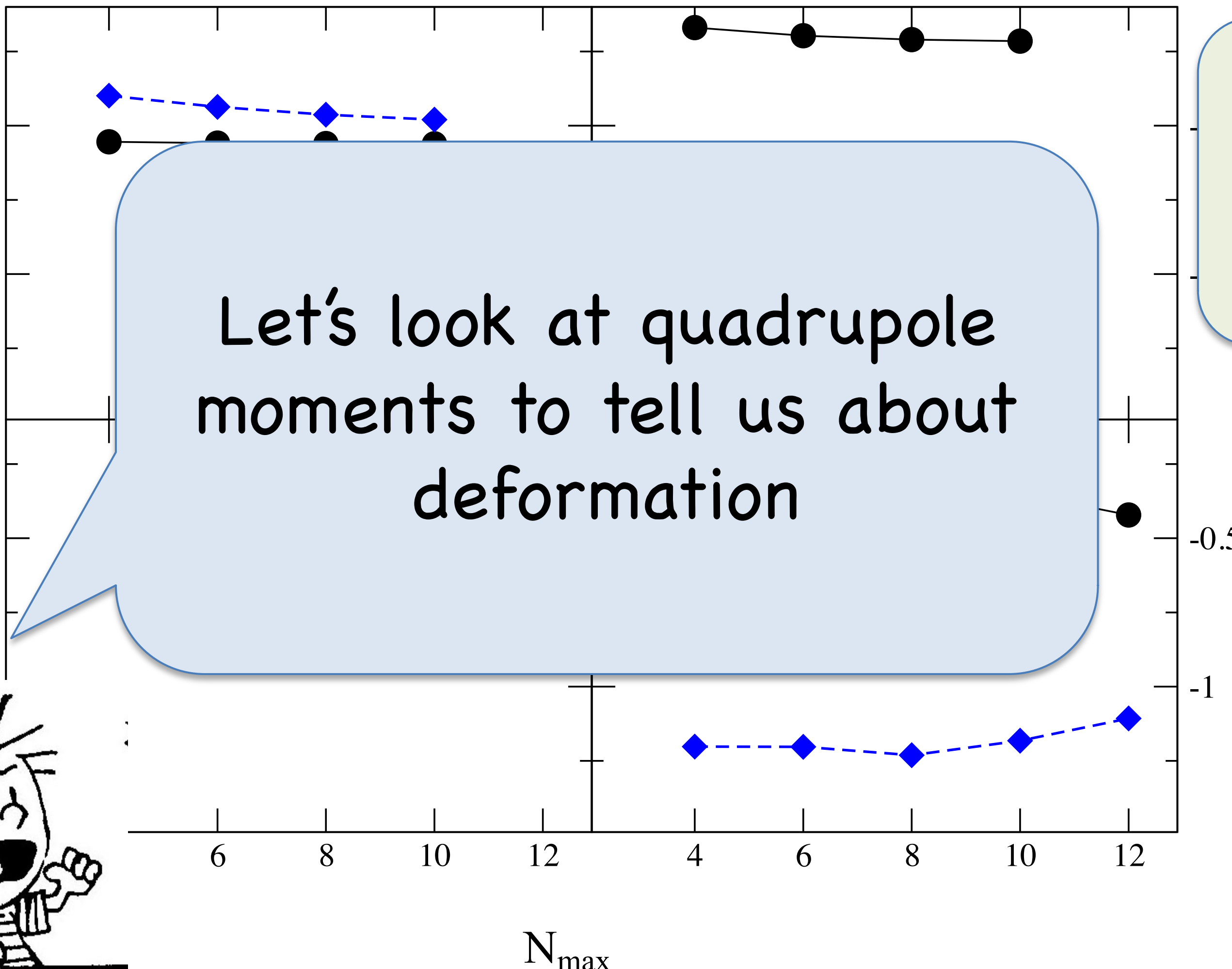


Let's look at quadrupole moments to tell us about deformation

Divide by radius$^2$ for more robust results

Mark Caprio

San Diego State University

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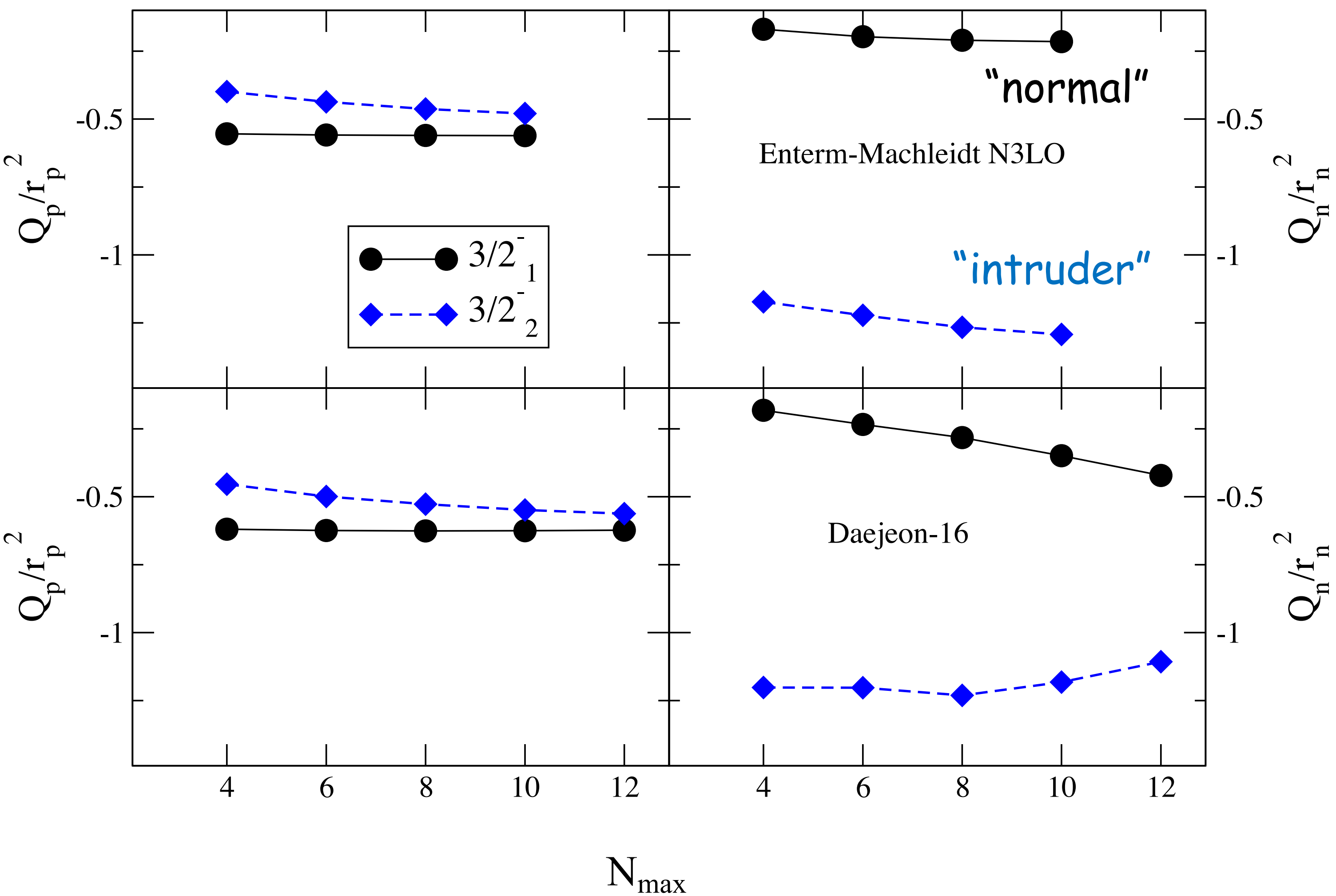

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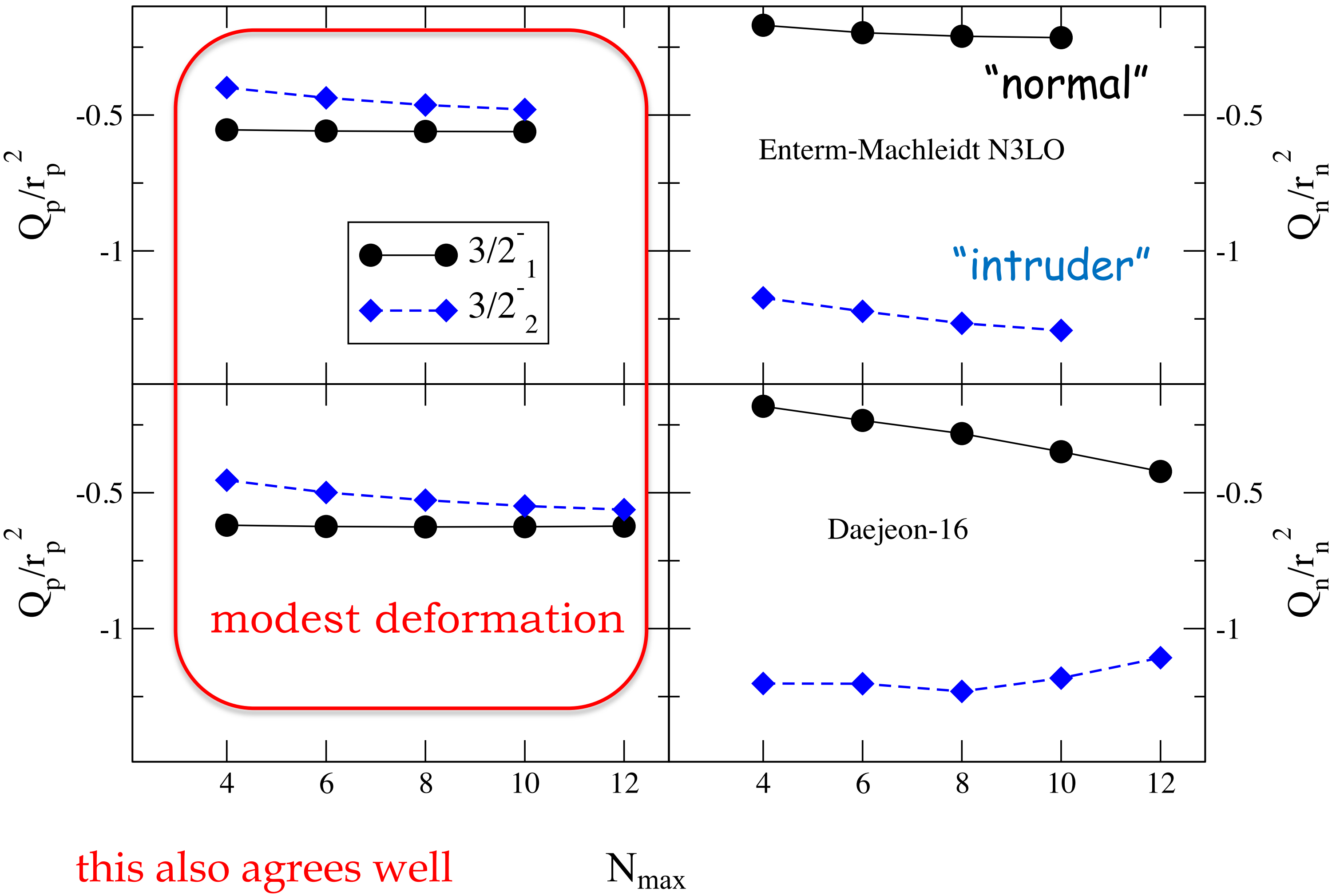
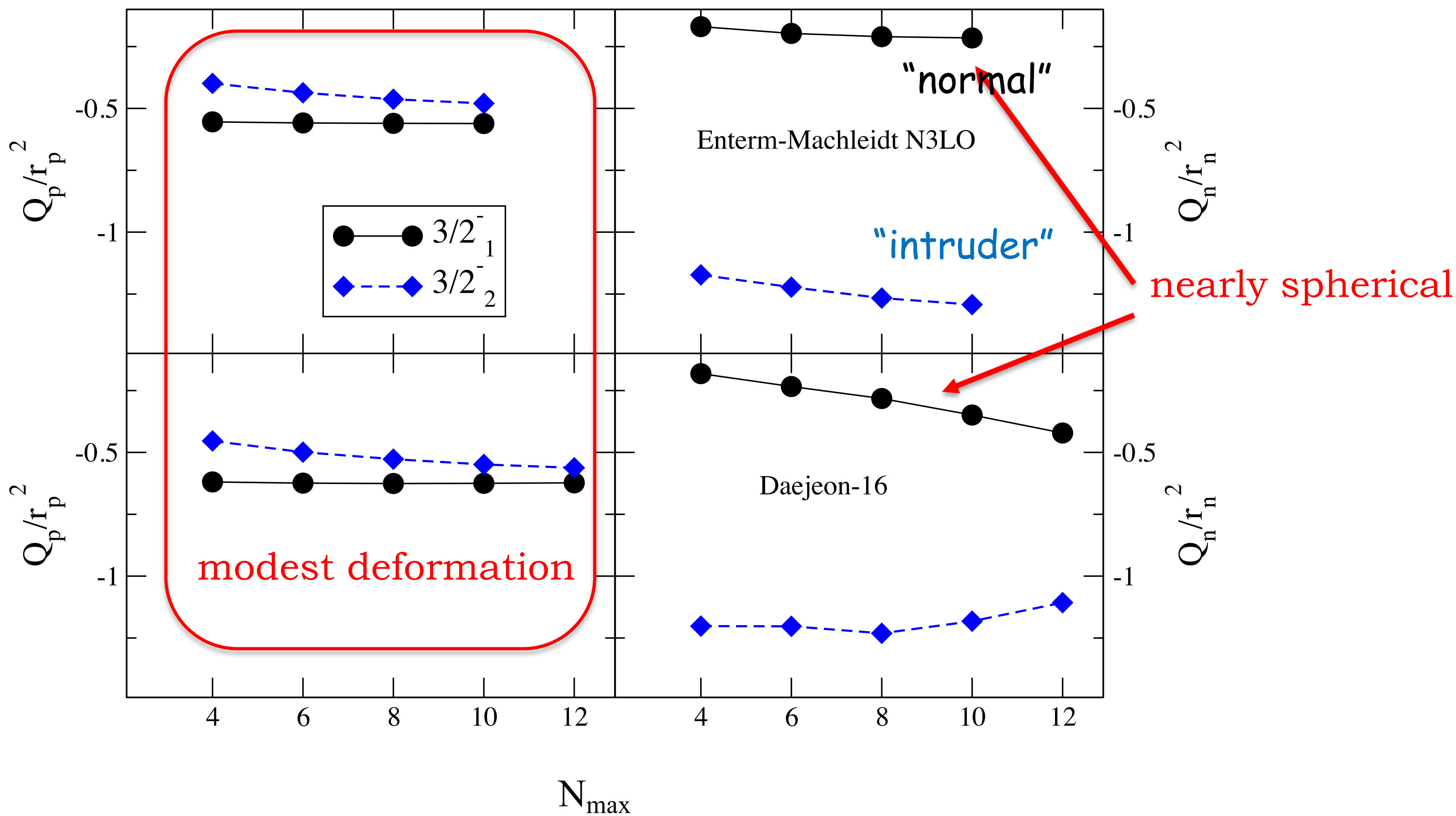



this also agrees well with experiment

# CASE STUDY: $^{11}$LI



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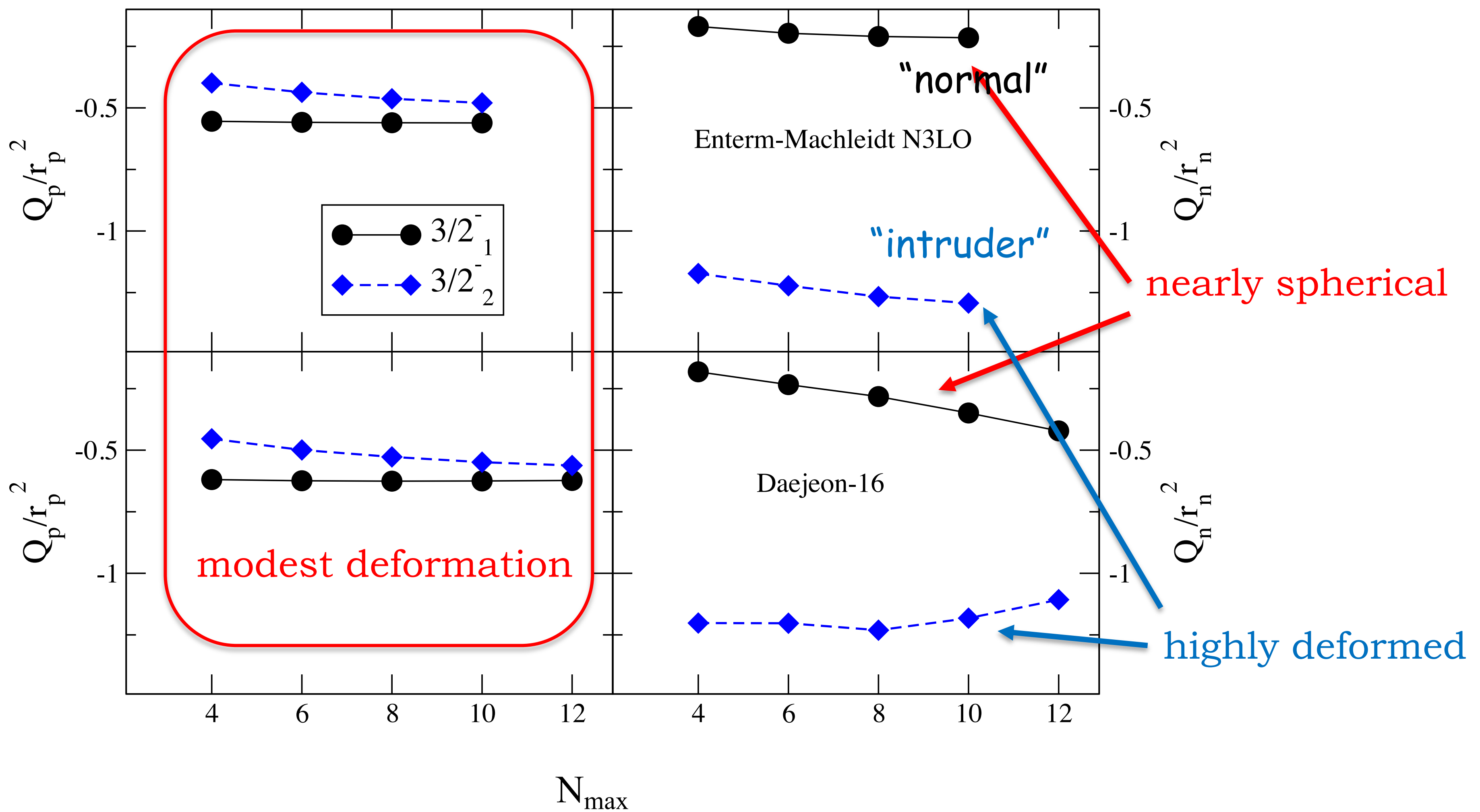

# CASE STUDY: $^{11}$LI

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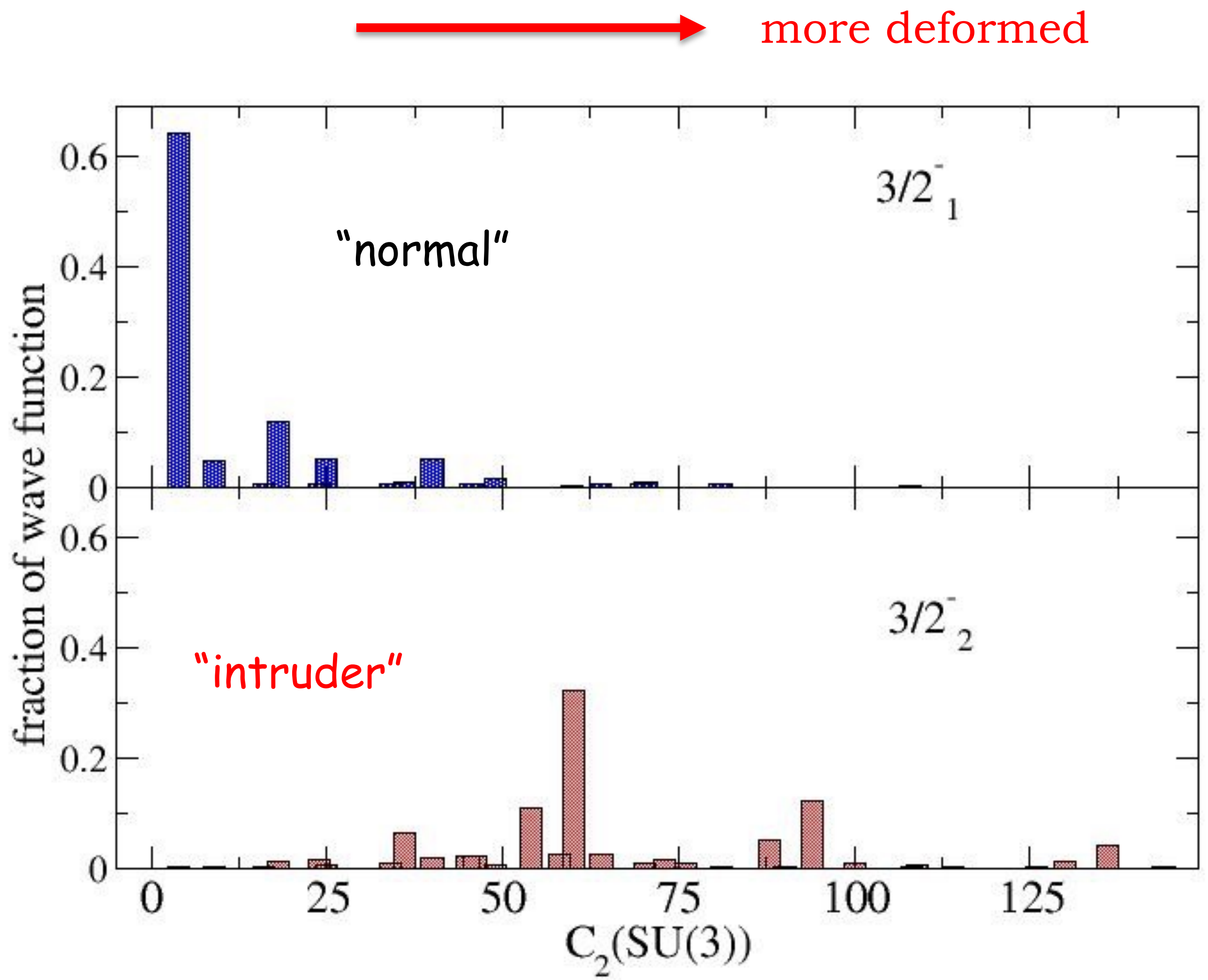
We can use the shell model to dissect the wavefunctions

# CASE STUDY: $^{11}$LI




Group-theoretical Decomposition

Elliot SU(3)

# CASE STUDY: $^{11}$LI

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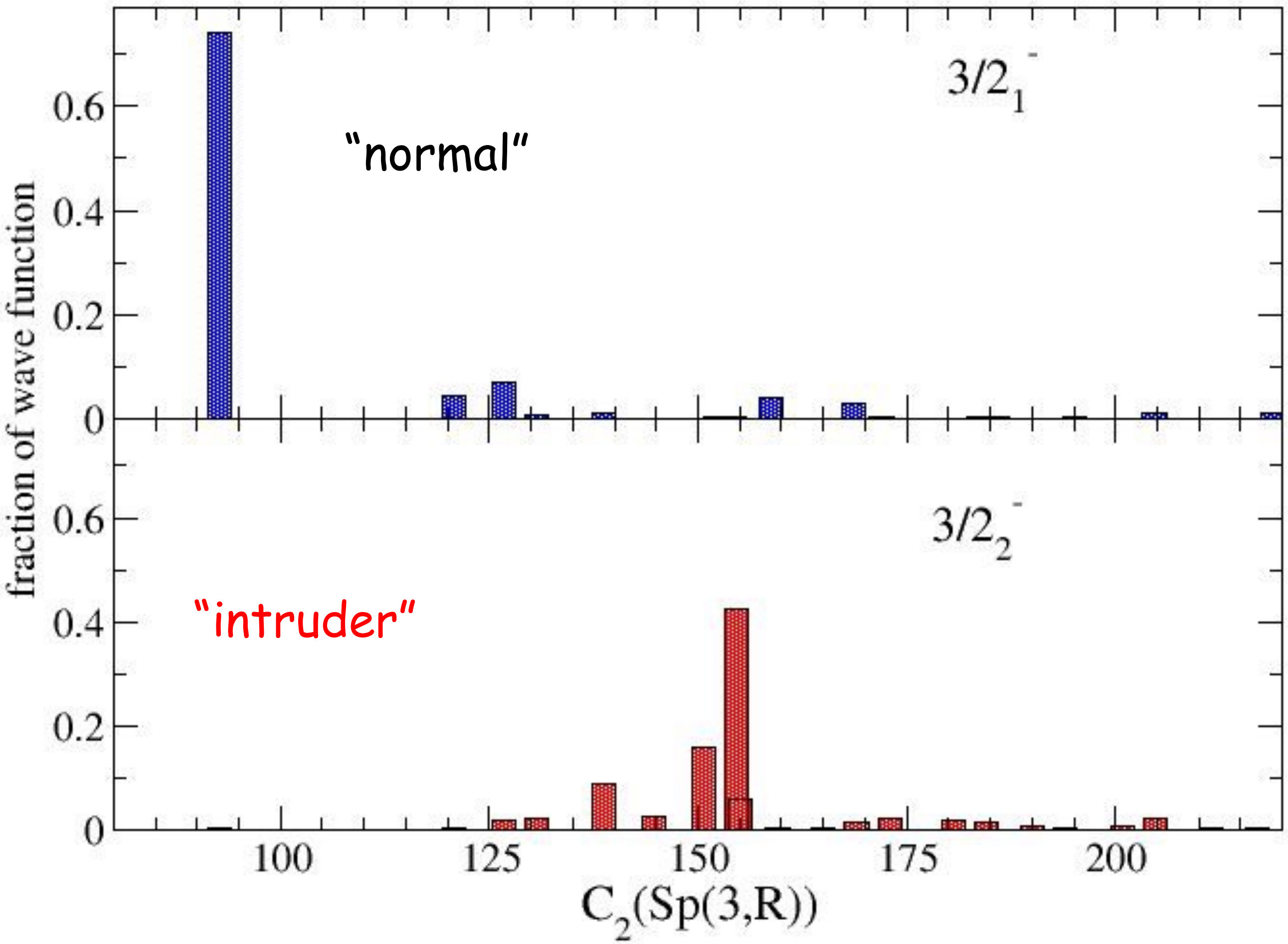
more deformed




Group-theoretical Decomposition

Symplectic Sp(3,R)

# CASE STUDY: $^{11}$LI

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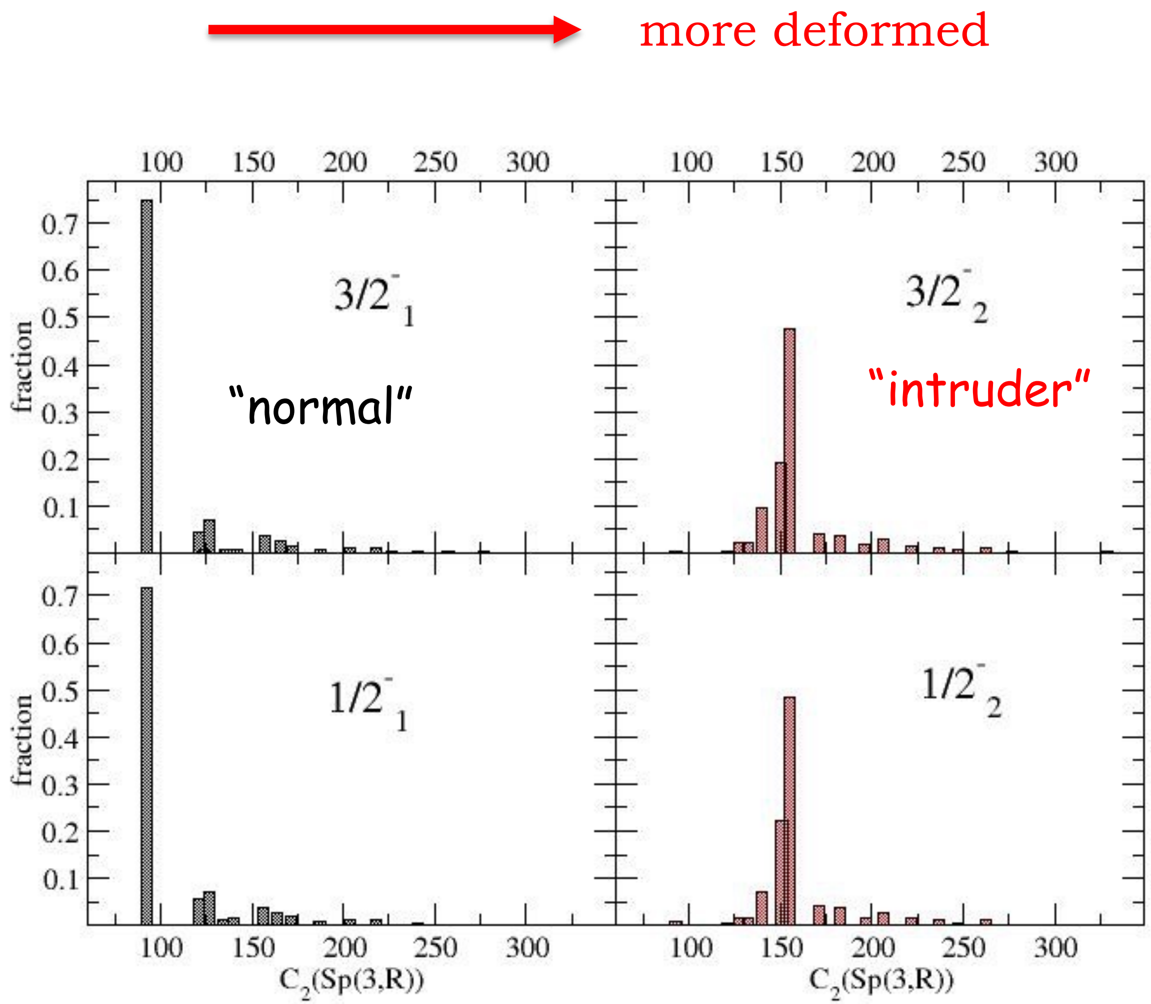
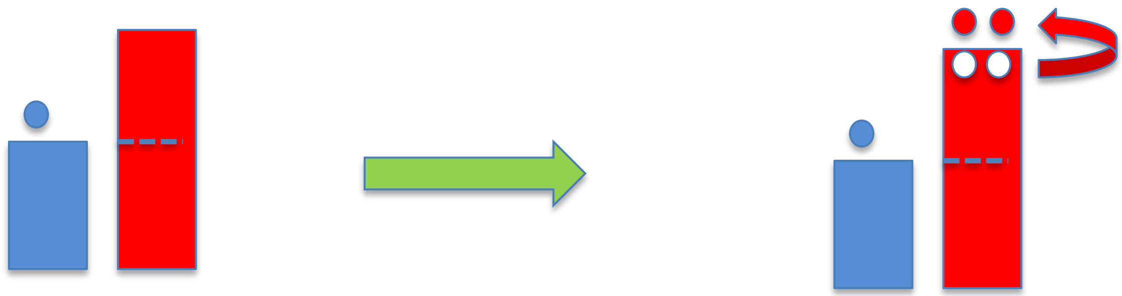



Group-theoretical Decomposition

Symplectic Sp(3,R)

# Case study: $^{29}$F

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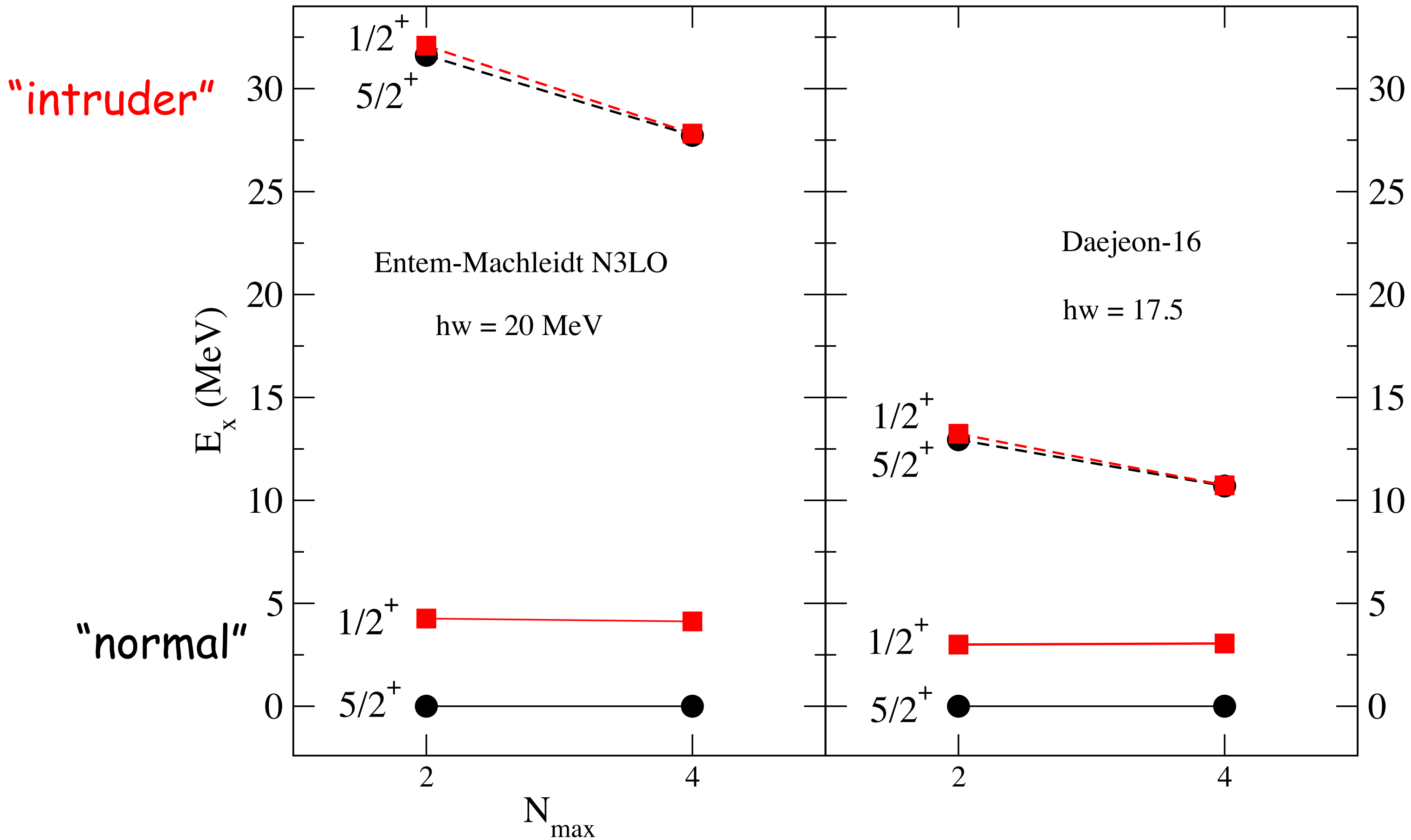
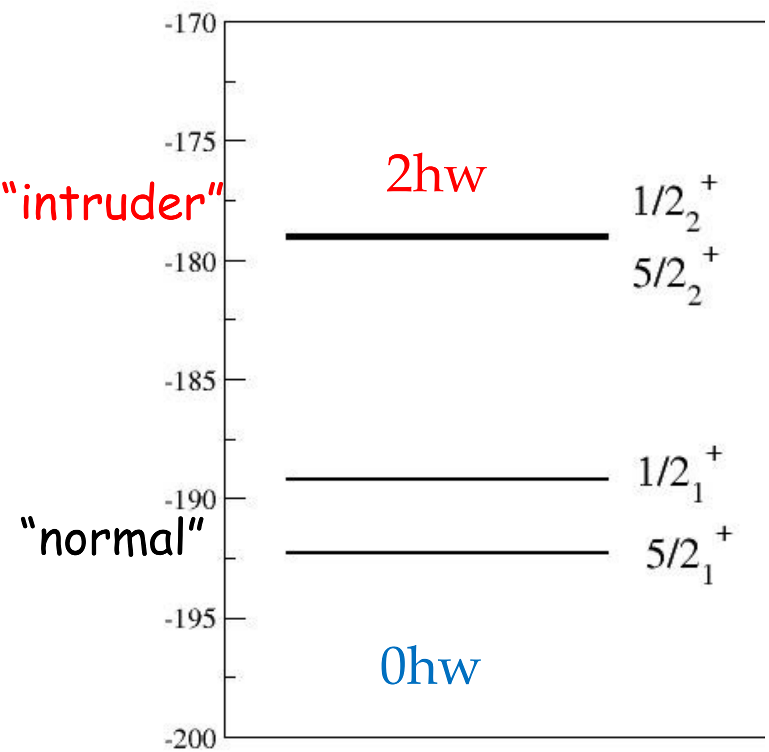
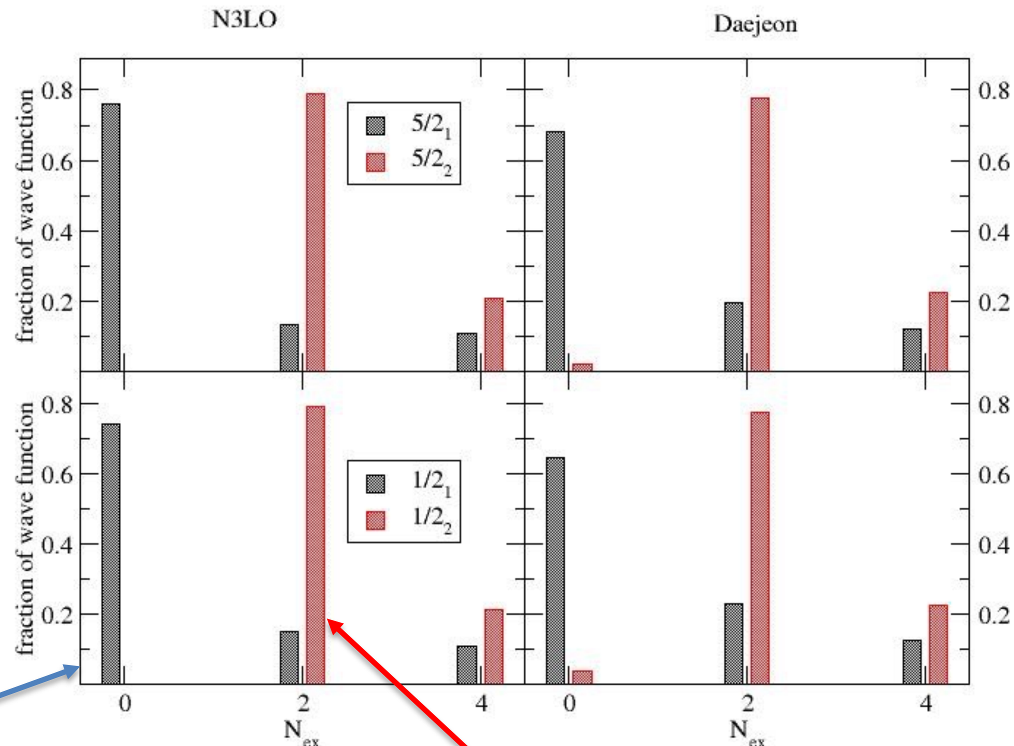
$^{29}F$ is an analog of $^{11}Li$



# Case study: $^{29}$F

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

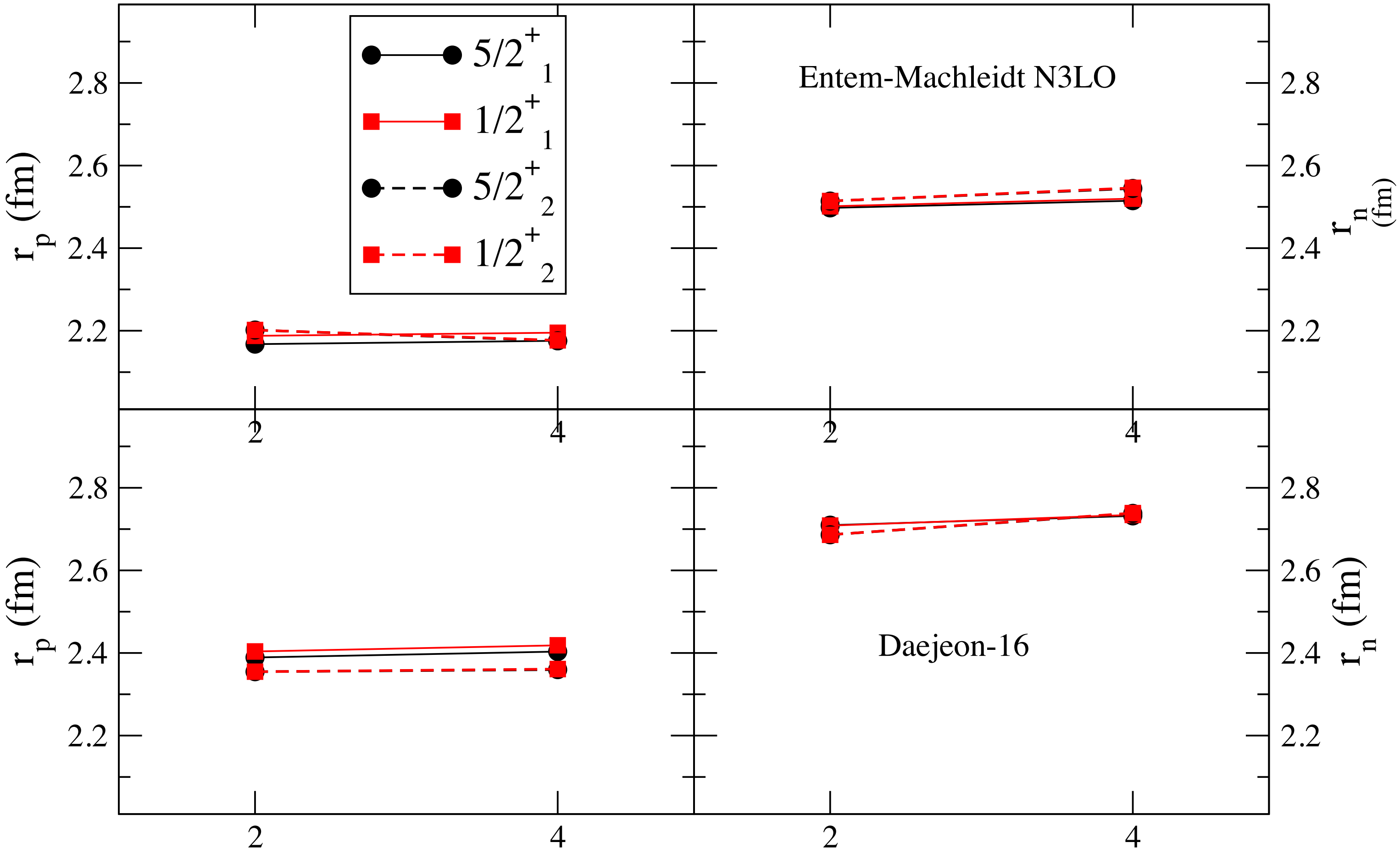



"normal"

"intruder"

# CASE STUDY: $^{29}$F



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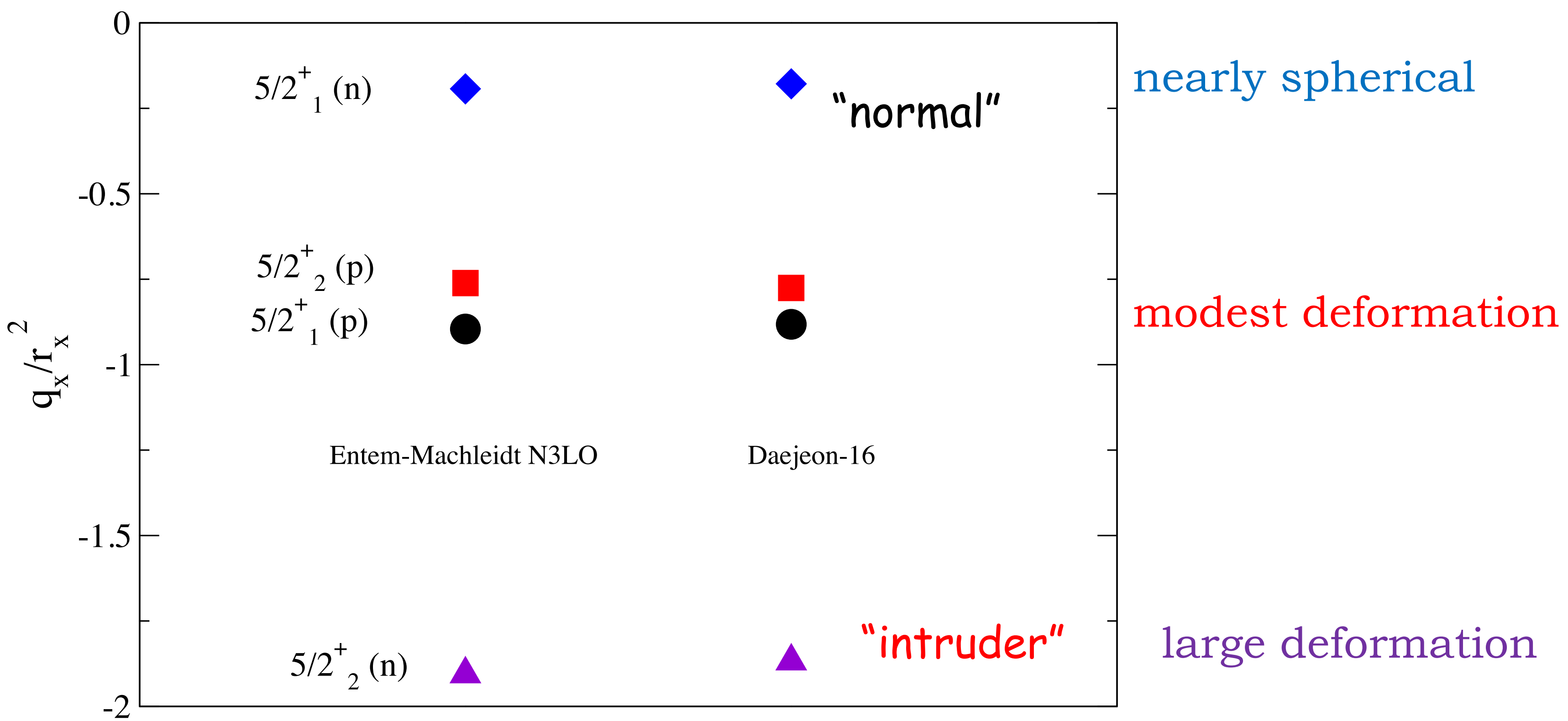

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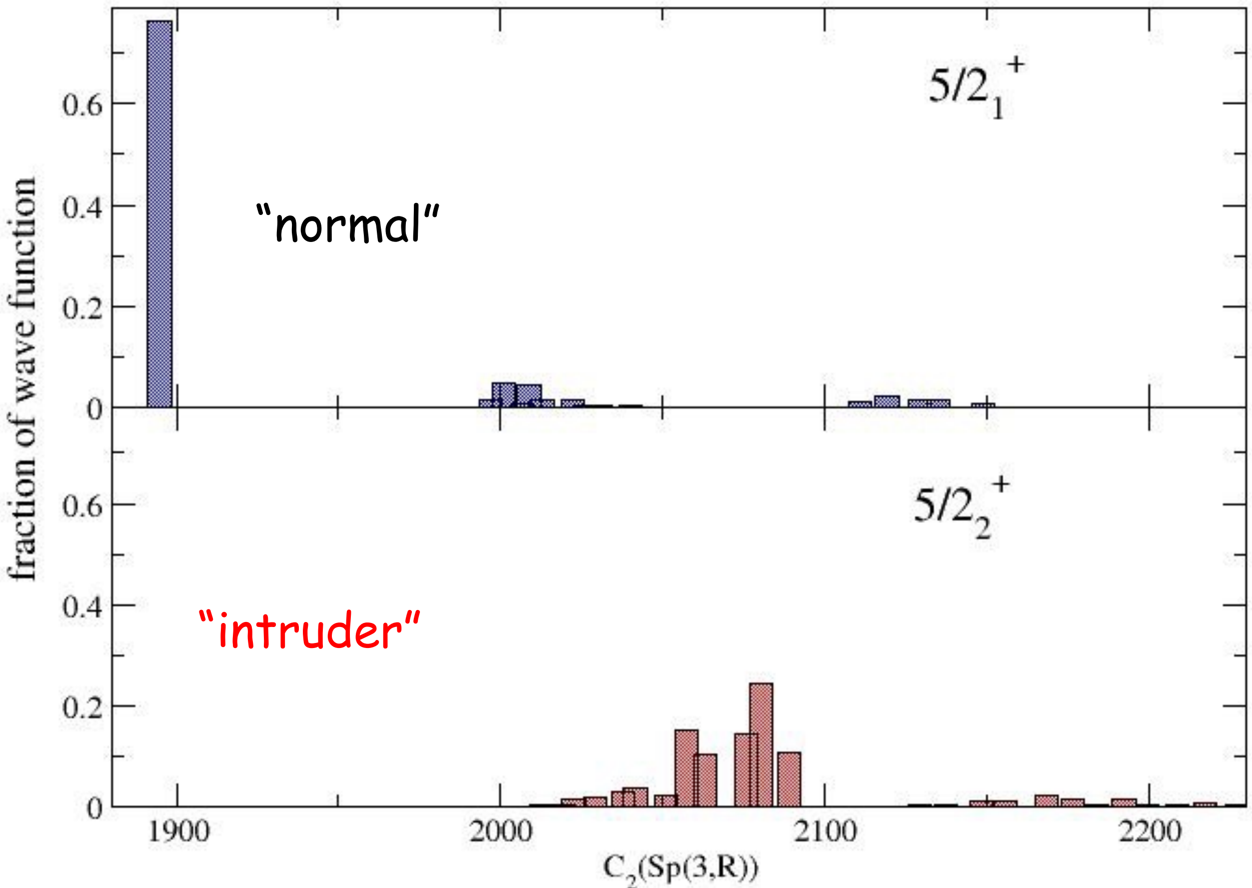


$N_{max}$ = 4 (natural orbitals)

Group-theoretical Decomposition

Symplectic Sp(3,R)

# CASE STUDY: $^{29}F$

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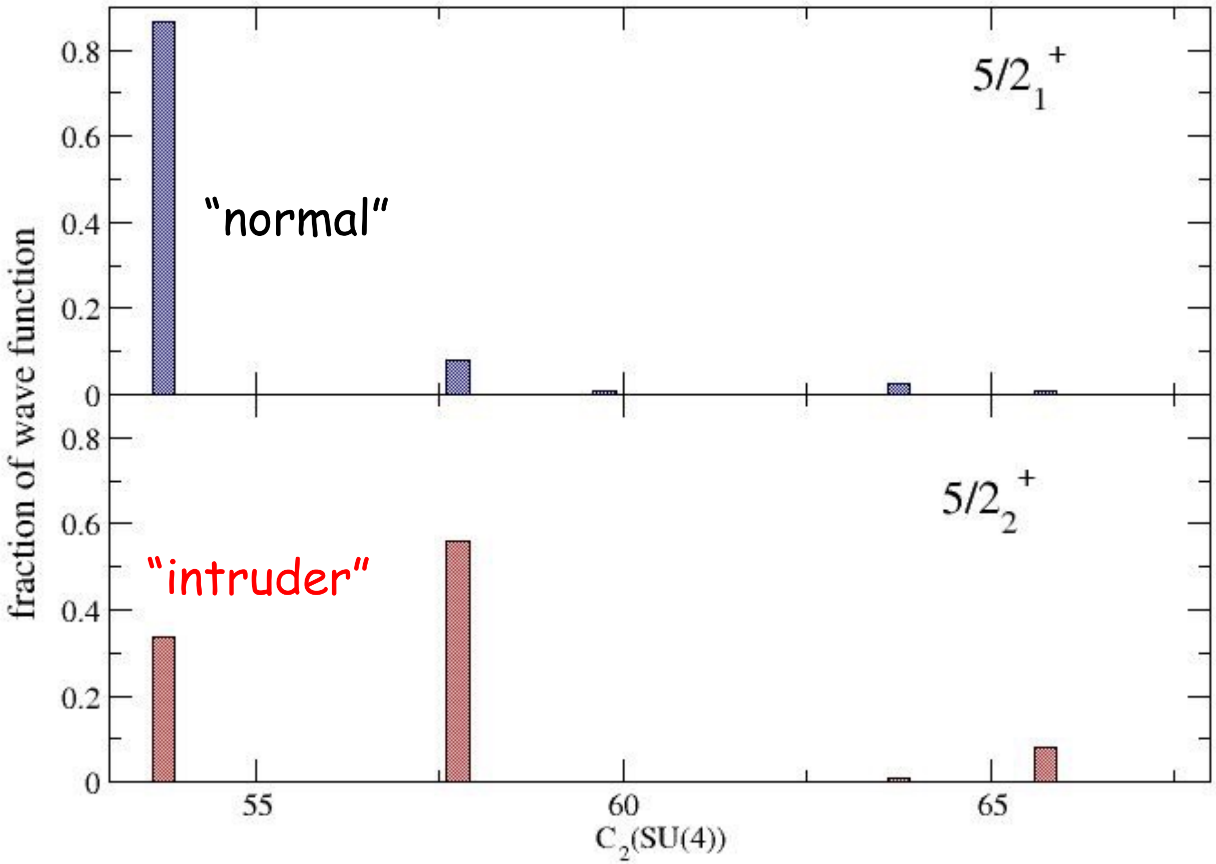


$N_{max}$ = 4, natural orbitals

Group-theoretical decomposition

SU(4)

# Case studies: $^{11}$Li, $^{29}$F

San Diego State University

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

San Diego State University

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

Note: these are technically closed-shells +1 nuclides.

For example, does **coupled-clusters** with a **spherical reference** eventually regain the deformation?
Or does one need a **deformed reference** state?

# Symplectic Sp(3,R) Symmetry

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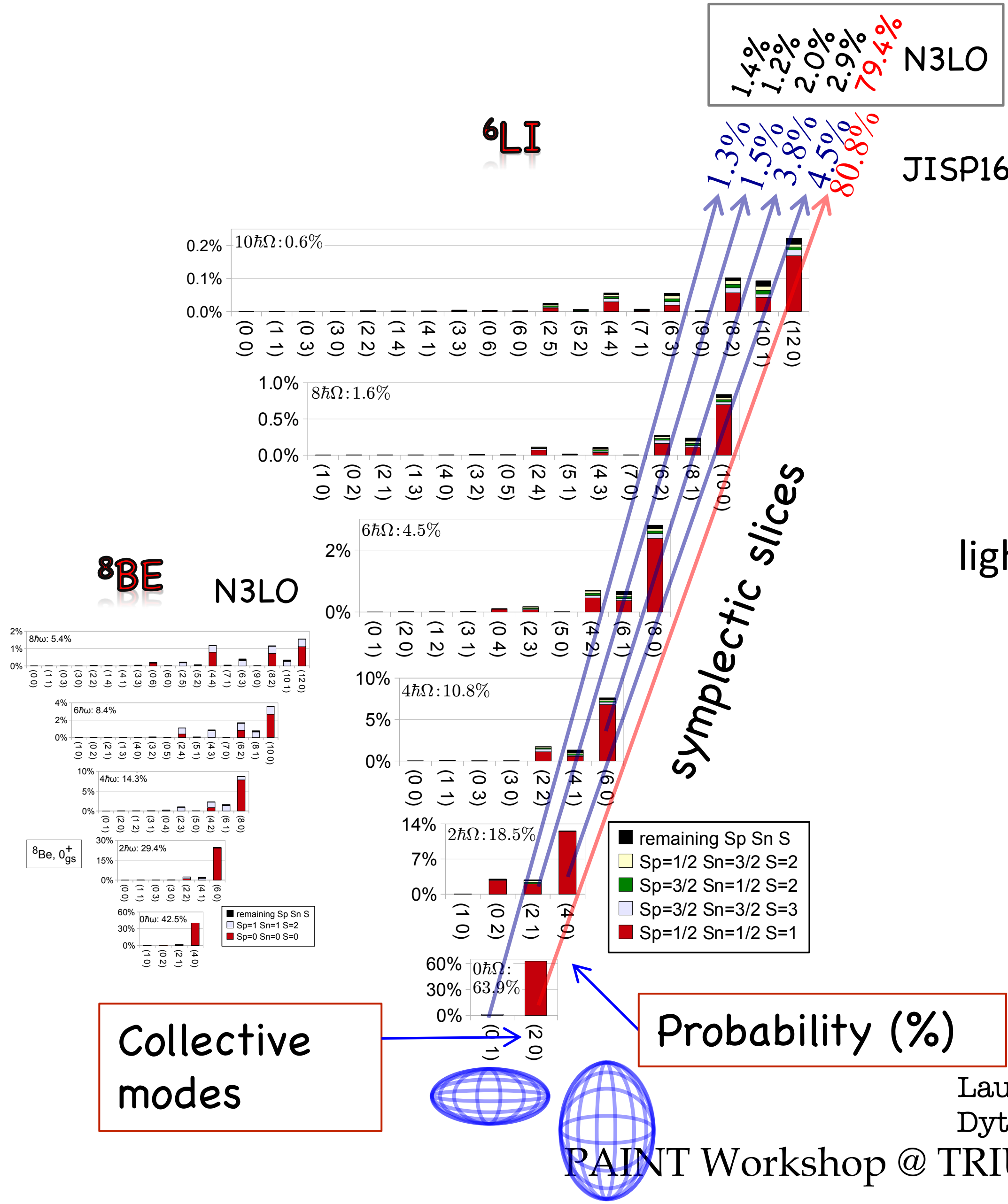



(From K. Launey, LSU)

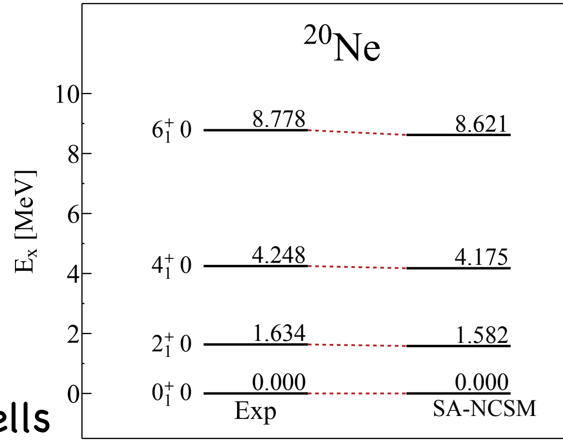
From first principles: light/intermediate-mass nuclei, low-lying states

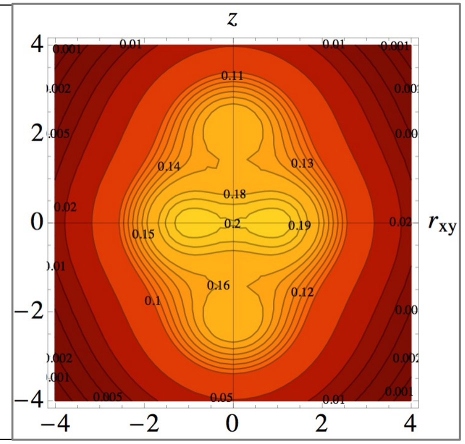
Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

# Collectivity features

San Diego State University

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: $2^+ \rightarrow 0^+$)

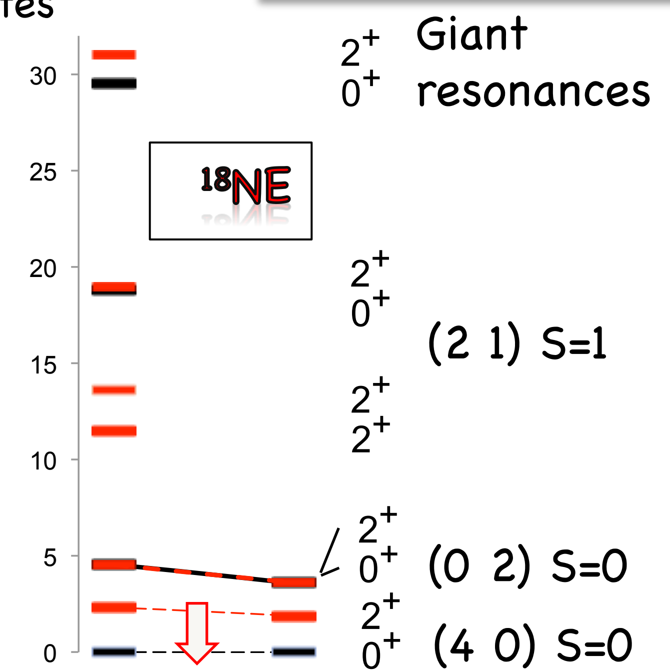
--------------------------

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)

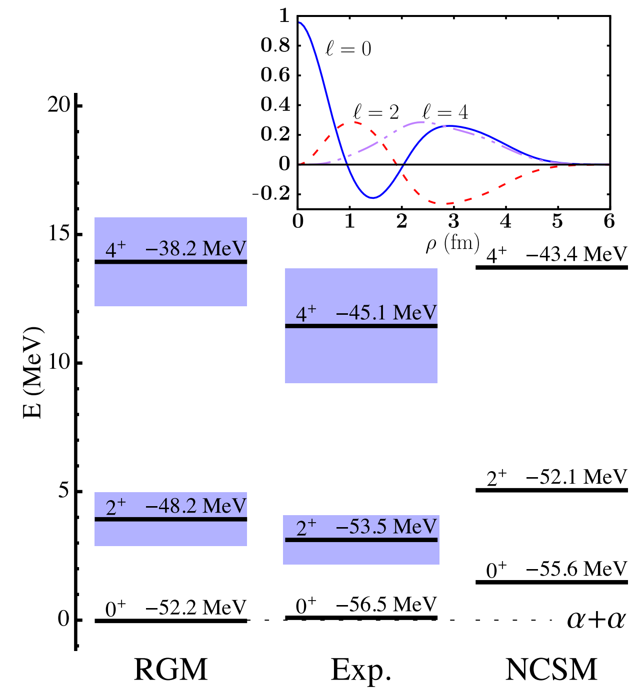


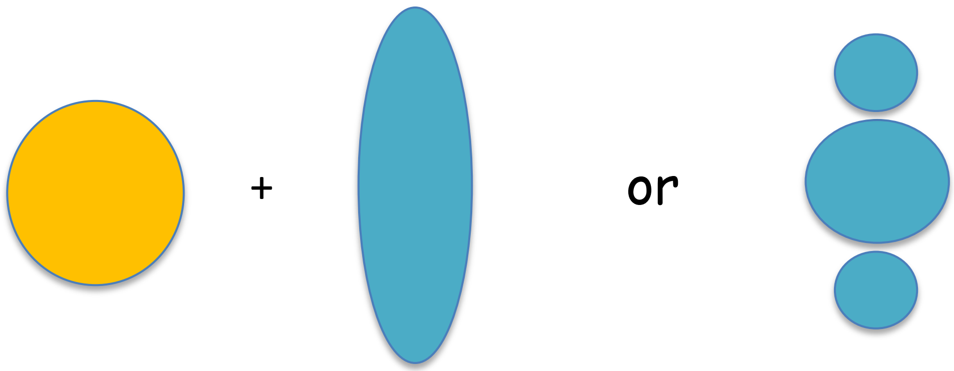

FIG. 1. Spectrum of RGM Hamiltonian with the SRG softened N3LO interaction ($\lambda = 1.5$ fm$^{-1}$) and $\hbar\Omega = 25$ MeV for a $2\alpha$ system. Zero on the energy scale is set by the $\alpha + \alpha$ breakup threshold of the corresponding model. Levels are marked by spin and parity and by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

# Summary

The no-core configuration-interaction **shell model** remains useful.

But 'intruder' states are very challenging! They are highly deformed and require large model spaces

# Summary




'deformation' or 'cluster' or
'particle-hole' or….

…but at times the correlation energy
in these states bring them low in the spectrum
(or even to the ground state)

# Summary

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The no-core configuration-interaction **shell model** remains useful.

But 'intruder' states are very challenging! They are highly deformed and require large model spaces

We can use the shell-model to 'x-ray' the problems....

...and maybe find a way forward!

# Summary

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In particular we suggest $^{11}$Li

...and $^{29}$F...

...as model cases to stress-test our many-body methods (CC, IMSRG, Sp(3,R), GCM, etc.)

Let the computing begin!