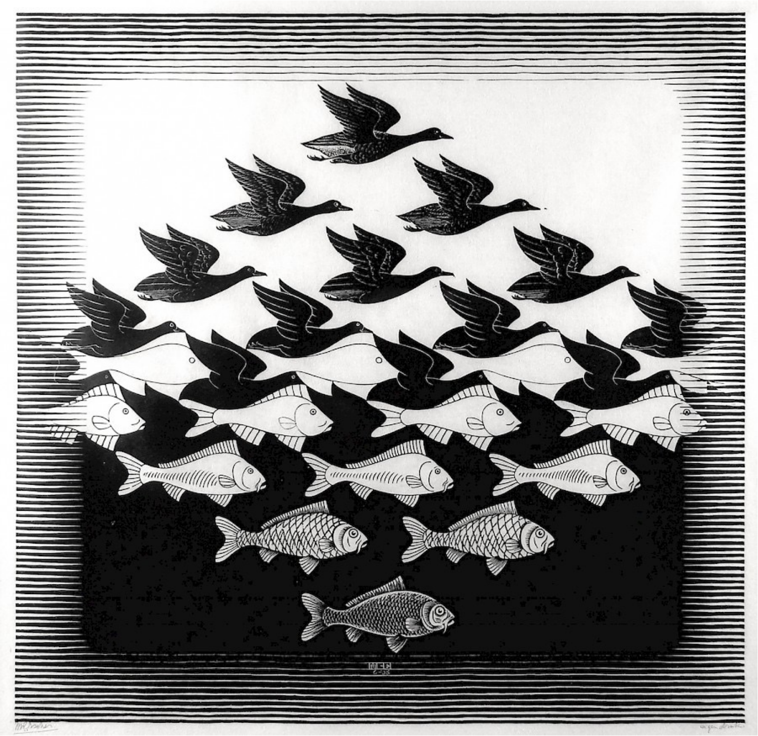
Deconstructing nuclear wave functions

San Diego State University



Calvin W. Johnson, San Diego State University

"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 "

XIV LASNPA, June 17, 2024

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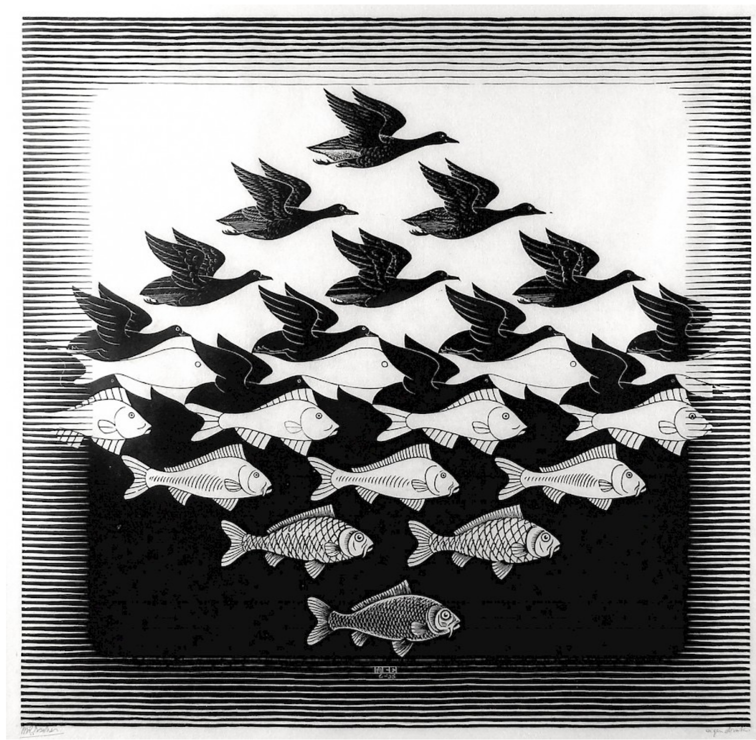

(75 YEARS!)

Calvin W. Johnson, San Diego State University

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XIV LASNPA, June 17, 2024

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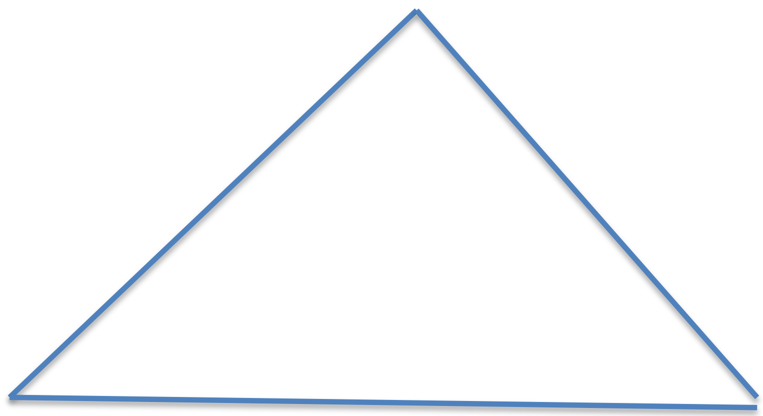
Themes of this talk
(and my research):



Large-scale computing

San Diego State University

Themes of this talk
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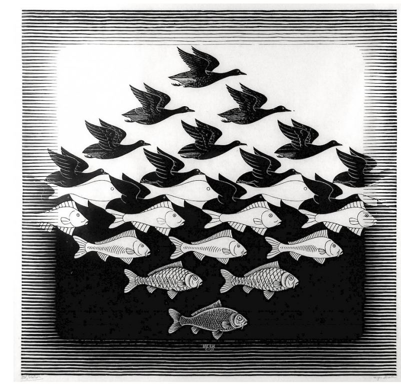
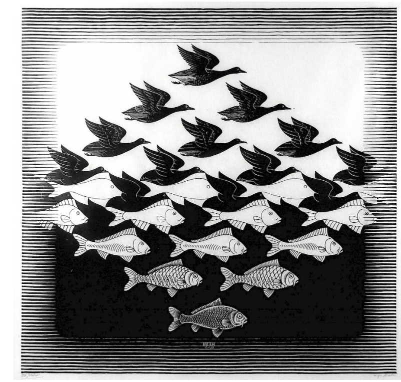


Symmetries

Large-scale computing

San Diego State University

Themes of this talk
(and my research):



Symmetries

Insight

Large-scale computing

- An outline of nuclear many-body calculations
  focus on: large scale shell-model calculations

- Using group theory to understand nuclear wave functions

- Apply to island of inversion nuclei ^{11}Li, ^{29}F

An all-too-common view:

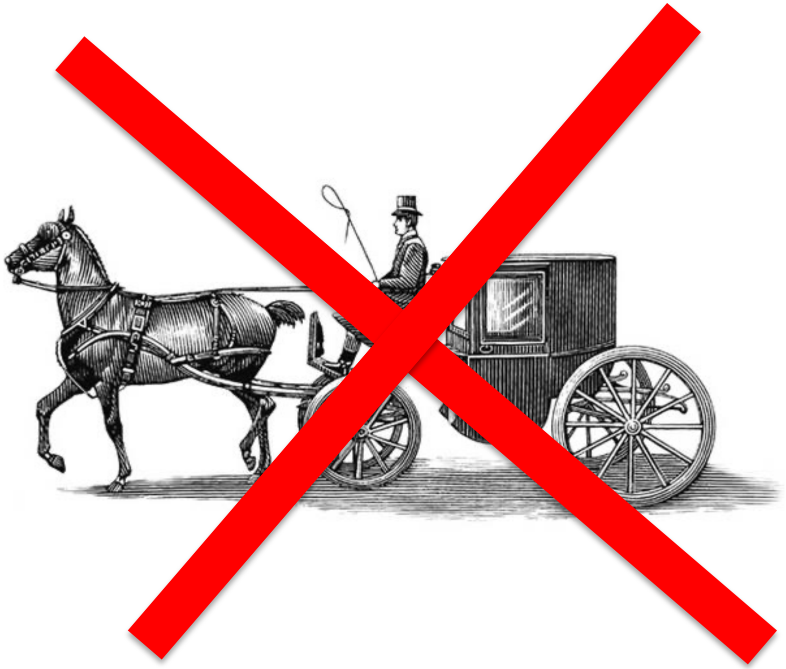
Dark matter, string theory, neutrino physics….

An all-too-common view:

Dark matter, string theory, neutrino physics....

Nuclear structure physics

An all-too-common view:



Dark matter, string theory, neutrino physics....

Nuclear structure physics

Modern nuclear structure physics is rigorous, vigorous, and *the launchpoint for many other investigations.*

To detect dark matter,
one needs **nuclear cross-sections**.
For neutrino physics, **nuclear cross-sections**.
For neutrinoless ββ decay, **need nuclear matrix element**
For parity/time-reversal violation (e.g. EDM),
need nuclear matrix elements….

The basic *science question* is to model detailed quantum structure of many-body systems, such the electronic structure of an atom, or structure of an atomic nucleus.

To answer this, we attempt to solve *Schrödinger's equation*:

$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j) \right) \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots) = E\Psi$$

or

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

The basic *science question* is to model detailed quantum structure of many-body systems, such the electronic structure of an atom, or structure of an atomic nucleus.

This differential equation is too difficult to solve directly

$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j) \right) \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots) = E\Psi$$

so we use the matrix formalism

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

The matrix formalism:
expand in some (many-body) basis

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

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

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

$|\Psi\rangle = c_1|1110001\rangle + c_2|1101010\rangle + c_3\,|0110101\rangle + \cdots$

- How the basis is represented

"occupation representation" $|\alpha\rangle = \hat{a}^+_{n_1}\hat{a}^+_{n_2}\hat{a}^+_{n_3}\ldots\hat{a}^+_{n_N}|0\rangle$

n_i	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0

Nuclear Hamiltonian: $\hat{H} = \sum_i -\frac{\hbar^2}{2M}\nabla_i^2 + \sum_{i<j} V(r_i, r_j)$

In the occupation representation:

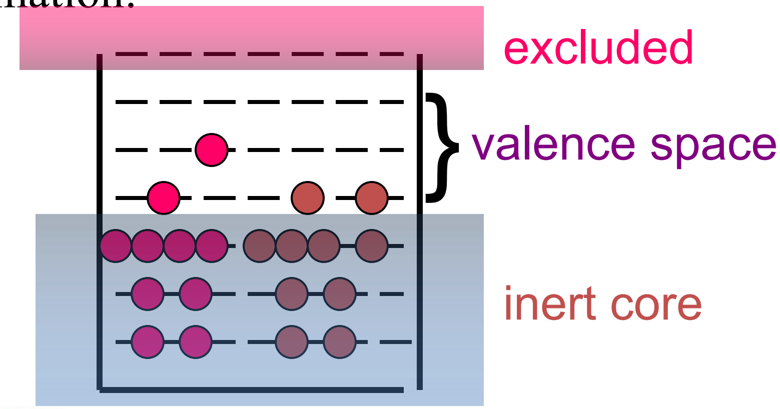
$$\hat{H} = \sum_i \varepsilon_i \hat{a}_i^+ \hat{a}_i + \frac{1}{4}\sum_{ijkl} V_{ijkl}\hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$

single-particle energies

two-body matrix elements

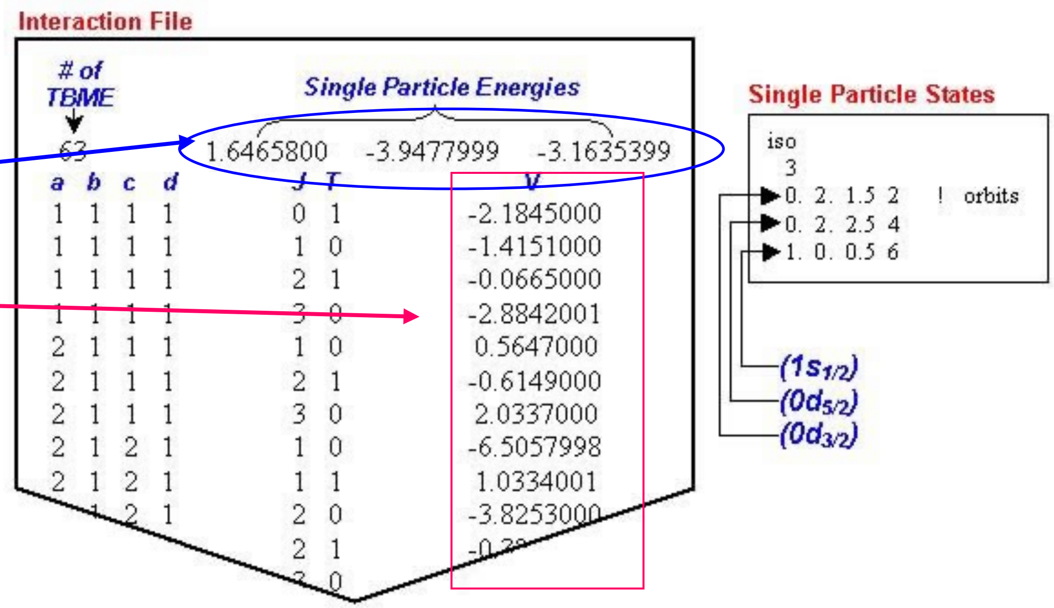
When running a fermion shell model code (e.g. MFD, BIGSTICK), one enters the following information:

(1) The single-particle valence space (such as *sd* or *pf*); assumes inert core



(2) The many-body model space (number of protons and neutrons, truncations, etc.)

(3) The interaction:
single-particle energies
and
two-body matrix elements
$V_{JT}(ab,cd)$



$$|\Psi\rangle = c_1|1110001\rangle + c_2|1101010\rangle + c_3\,|0110101\rangle + \cdots$$

Maria Mayer

Convenient for computers…

…and computers are needed, for we need millions or billions of such simple states.….

Largest (?) known M-scheme calculation
^{12}Be, N_{max}=12, **35 billion basis states**
(A. McCoy, arXiv:2402.12606)

Anna McCoy

in the matrix formalism

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

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

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

The shell-model wave functions can contain thousands, or millions, or billions of components

Normally it's very hard to understand what is going on

Group theory can illuminate how similar or different wave functions are (even for people who don't know group theory)

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Largest (?) kn

^{12}Be, N_{max}=1

(A. McCoy, a

“*The purpose of computing*
is
insight, not numbers”
--Richard Hamming

in

$\hat{\mathbf{H}}$

$c_\alpha|\alpha\rangle$

$$H_{\alpha\beta} = \langle\alpha|\hat{\mathbf{H}}|\beta\rangle$$

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

Largest (?) kn

^{12}Be, N_{max}=1

(A. McCoy, a

That's a lot of numbers!
How can we understand them?

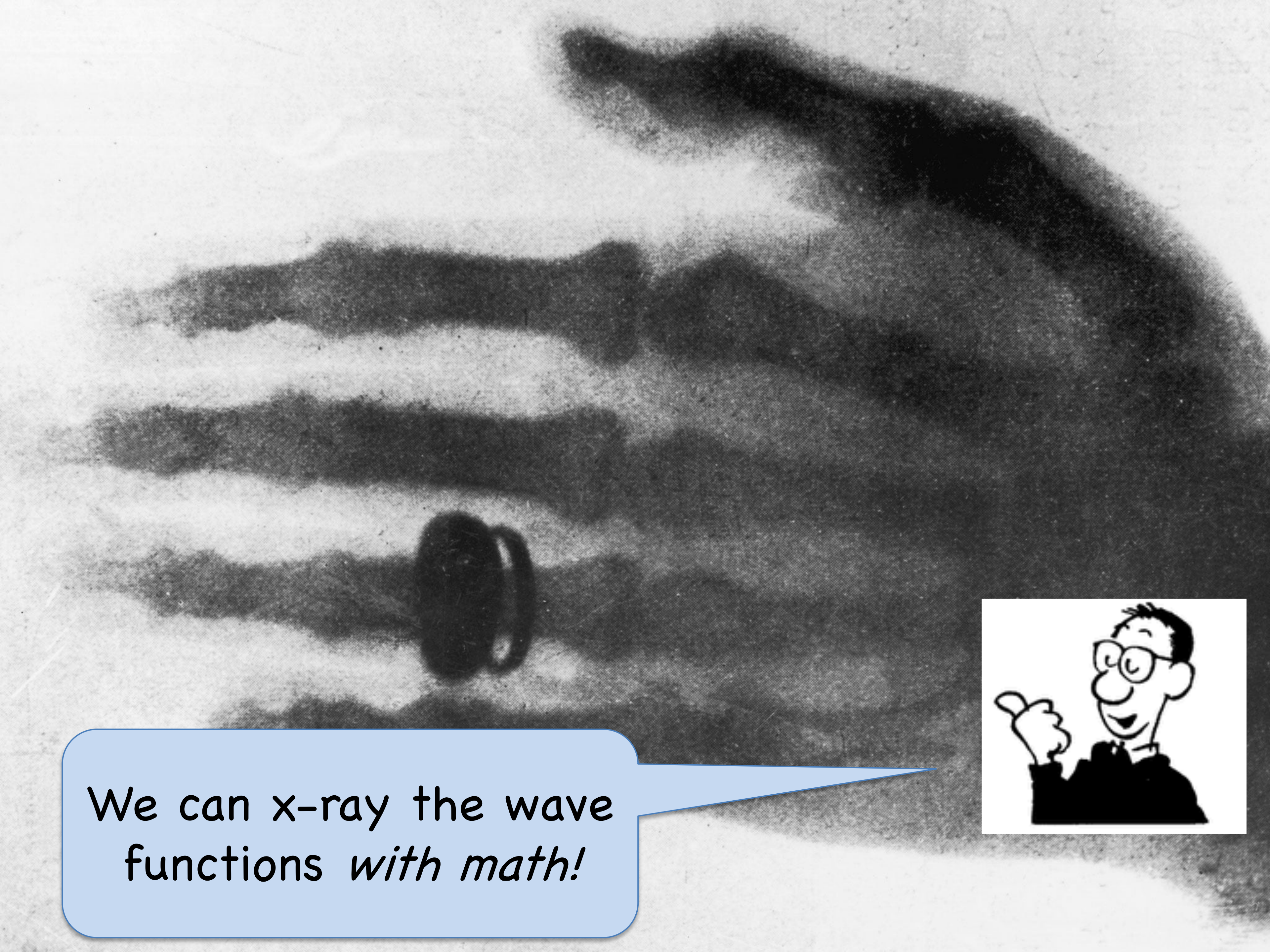
in

$\mathbf{H}$

$c_\alpha |\alpha\rangle$

$$H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} | \beta \rangle$$

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


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

Specifically, we use eigenvalues of Casimir operators to label subspaces (“irreps”)

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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 $j(j+1)$

Casimir

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

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

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

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

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 $| \Psi >$, we define
the *fraction of the wavefunction in an irrep*

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

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

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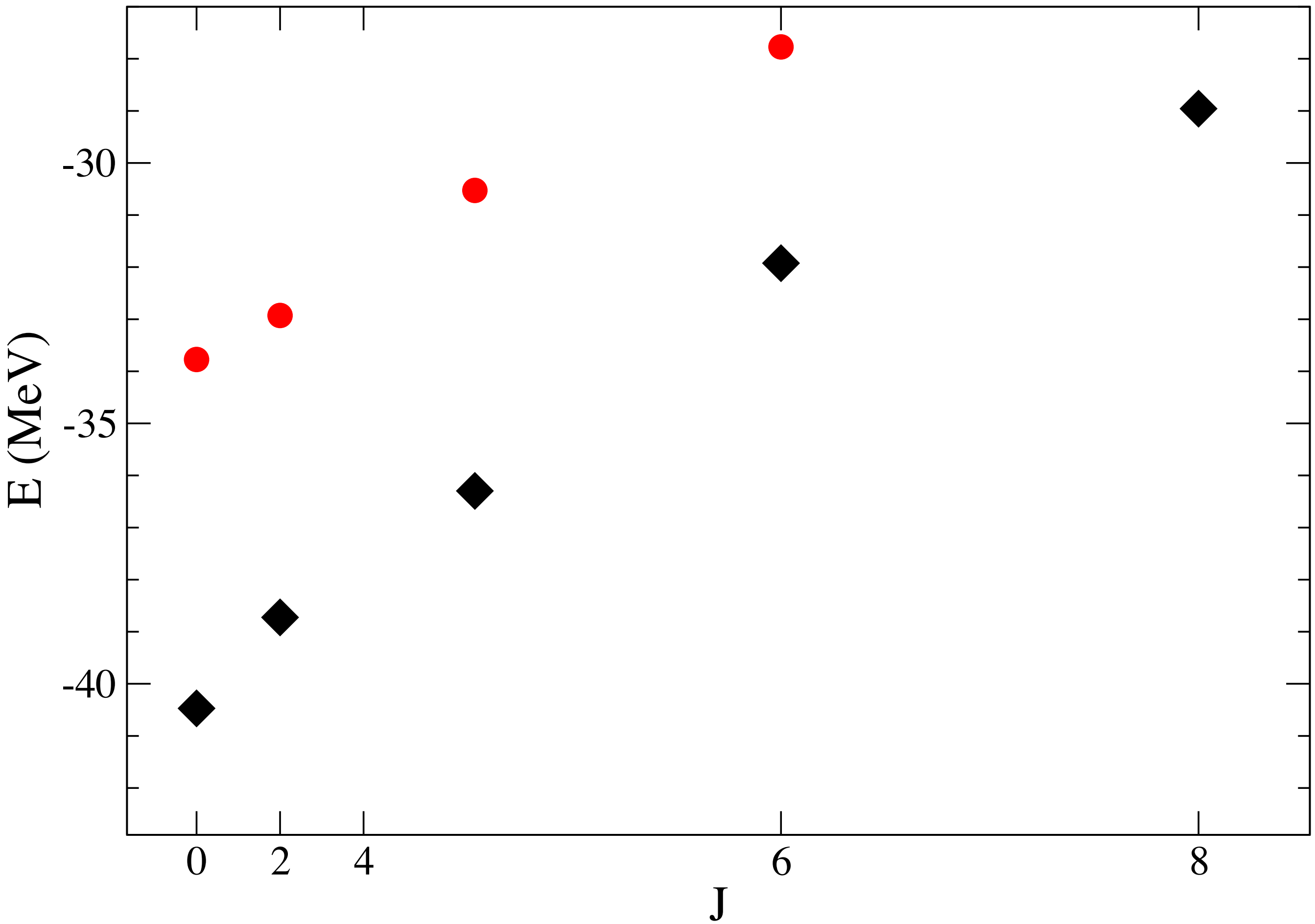


^{20}Ne

USDB interaction

^{20}Ne using phenomenological USDB force

1p-0f

-------- ^{40}Ca

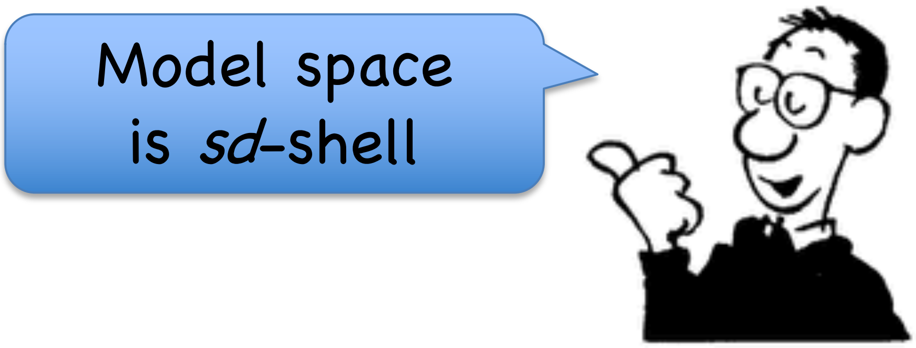
0d-1s

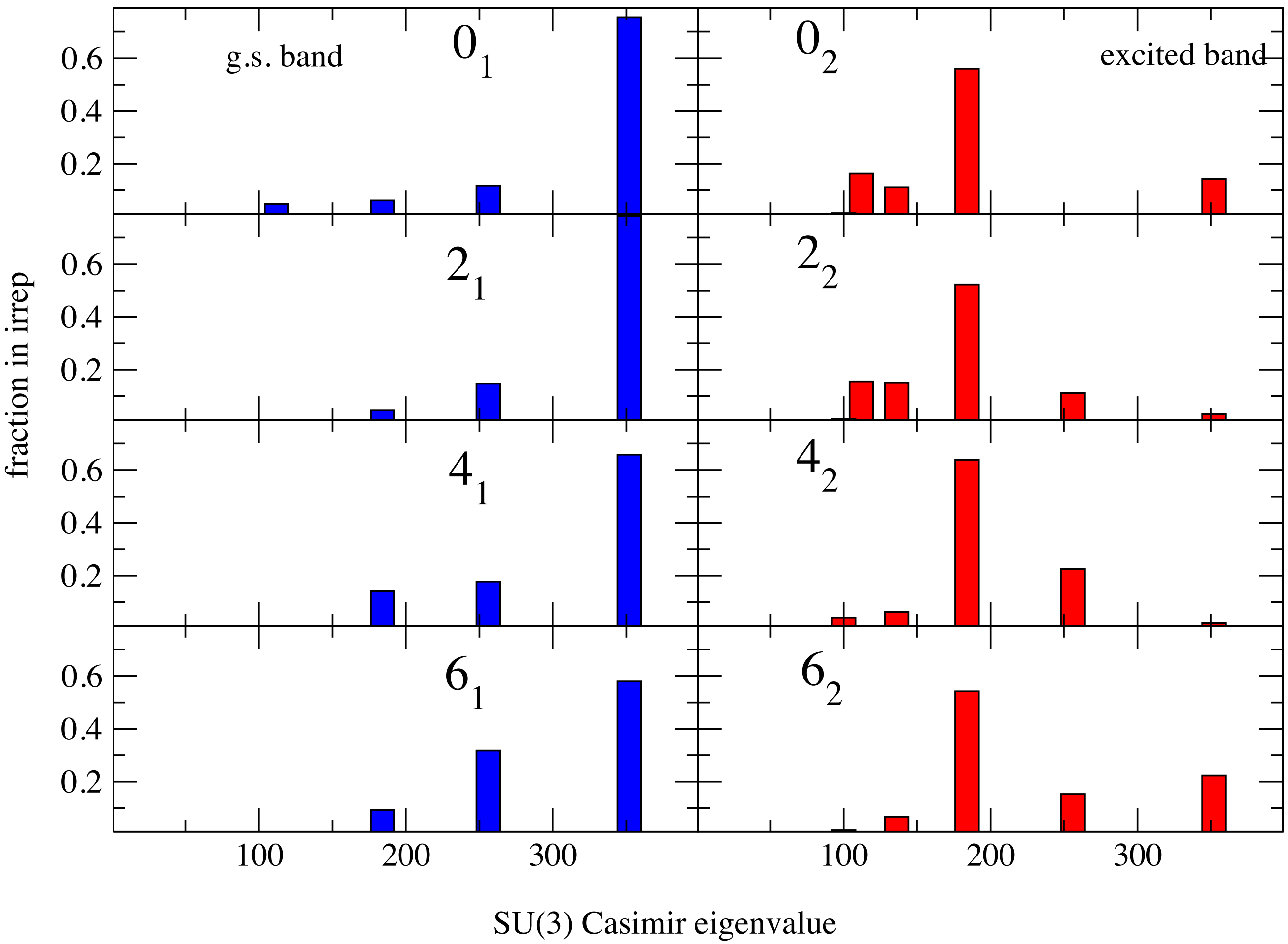
------- ^{16}O

0p

------ ^{4}He

0s



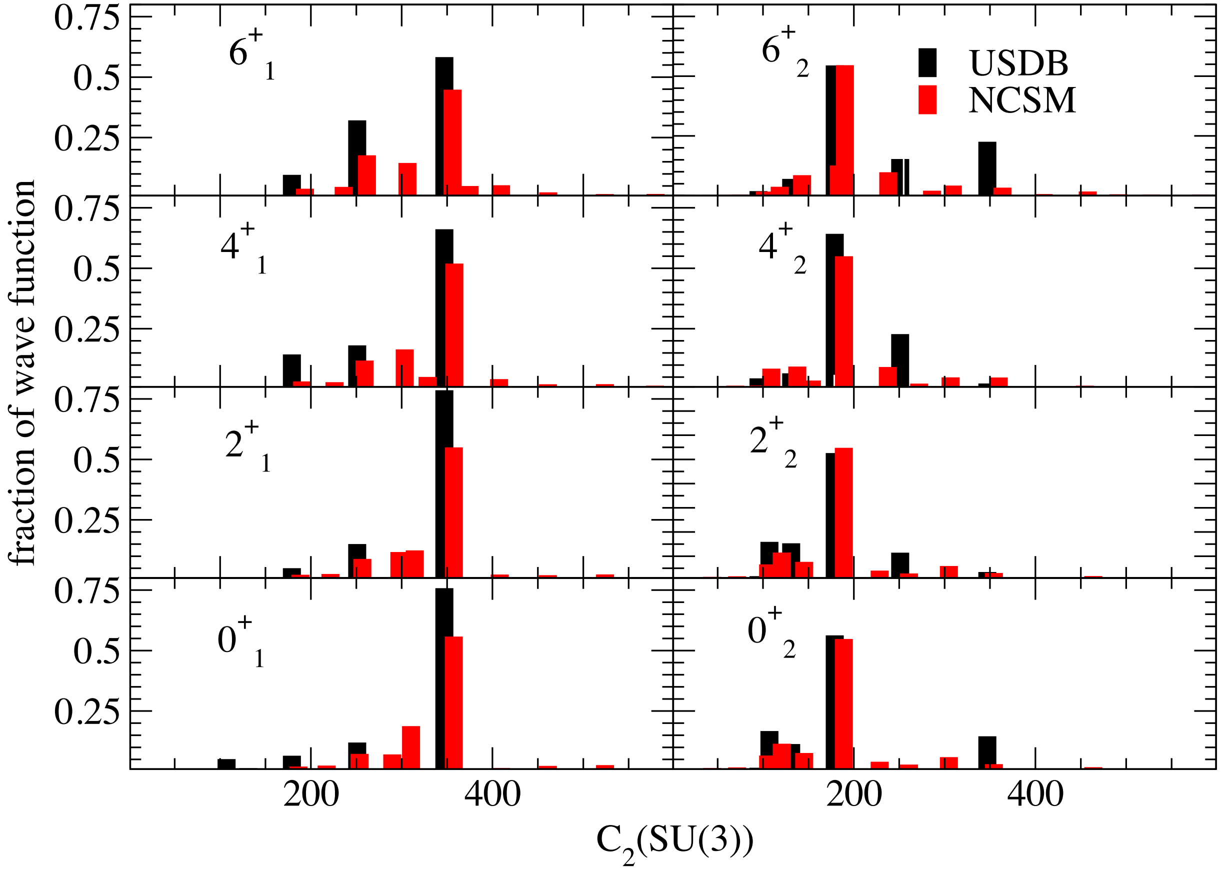


^{20}Ne

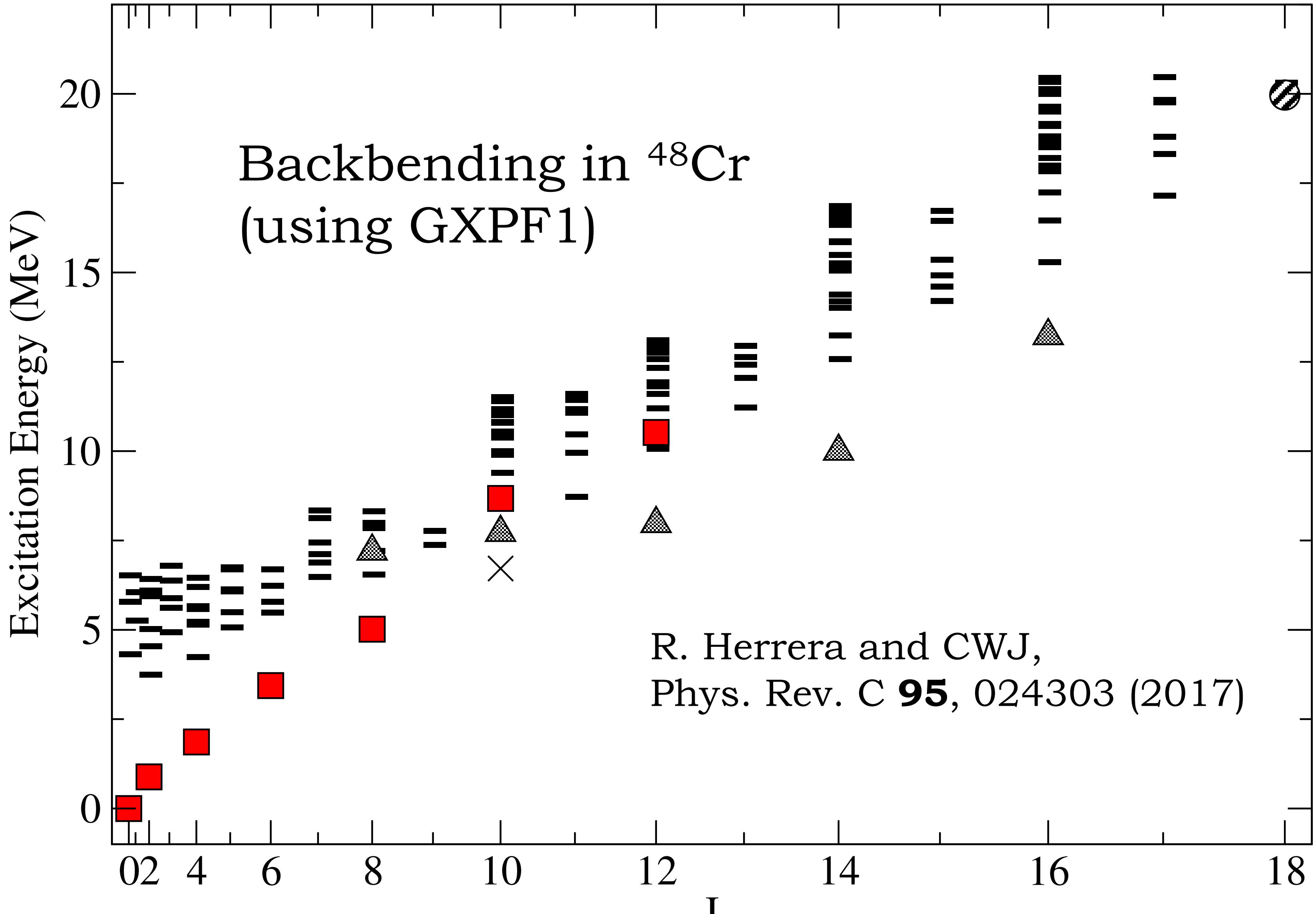
USDB interaction

dimension = 640

^{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!


Backbending in ⁴⁸Cr
(using GXPF1)
R. Herrera and CWJ,
Phys. Rev. C **95**, 024303 (2017)
Excitation Energy (MeV)
I
0
5
10
15
20
0
2
4
6
8
10
12
14
16
18

Backbending in ^{48}Cr
(using GXPF1)

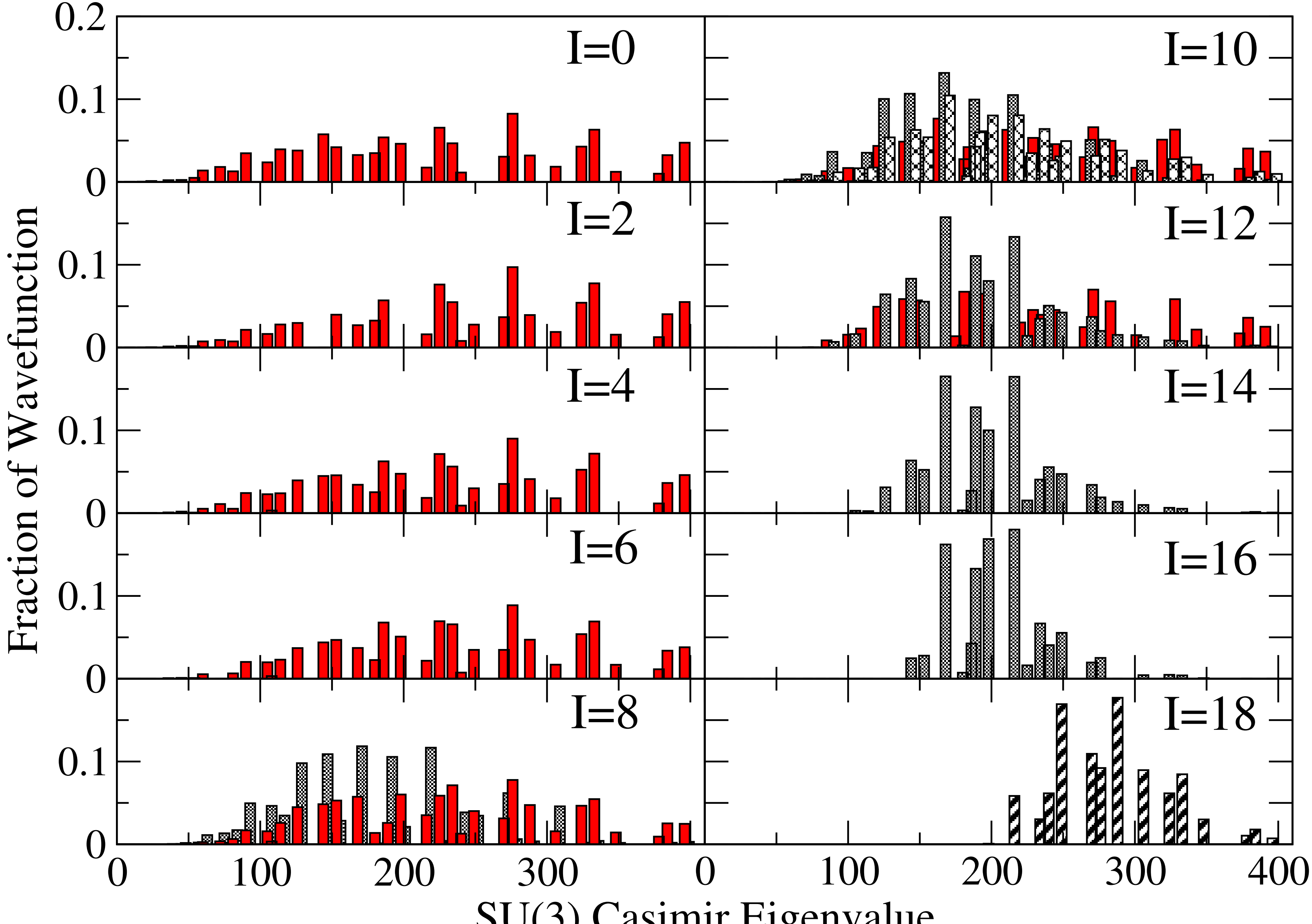
0f –1p
-------- ^{40}Ca
0d-1s
------ ^{16}O
0p
------ ^{4}He
0s

Model space
is *pf*-shell

Backbending in ^{48}Cr
(using GXPF1)

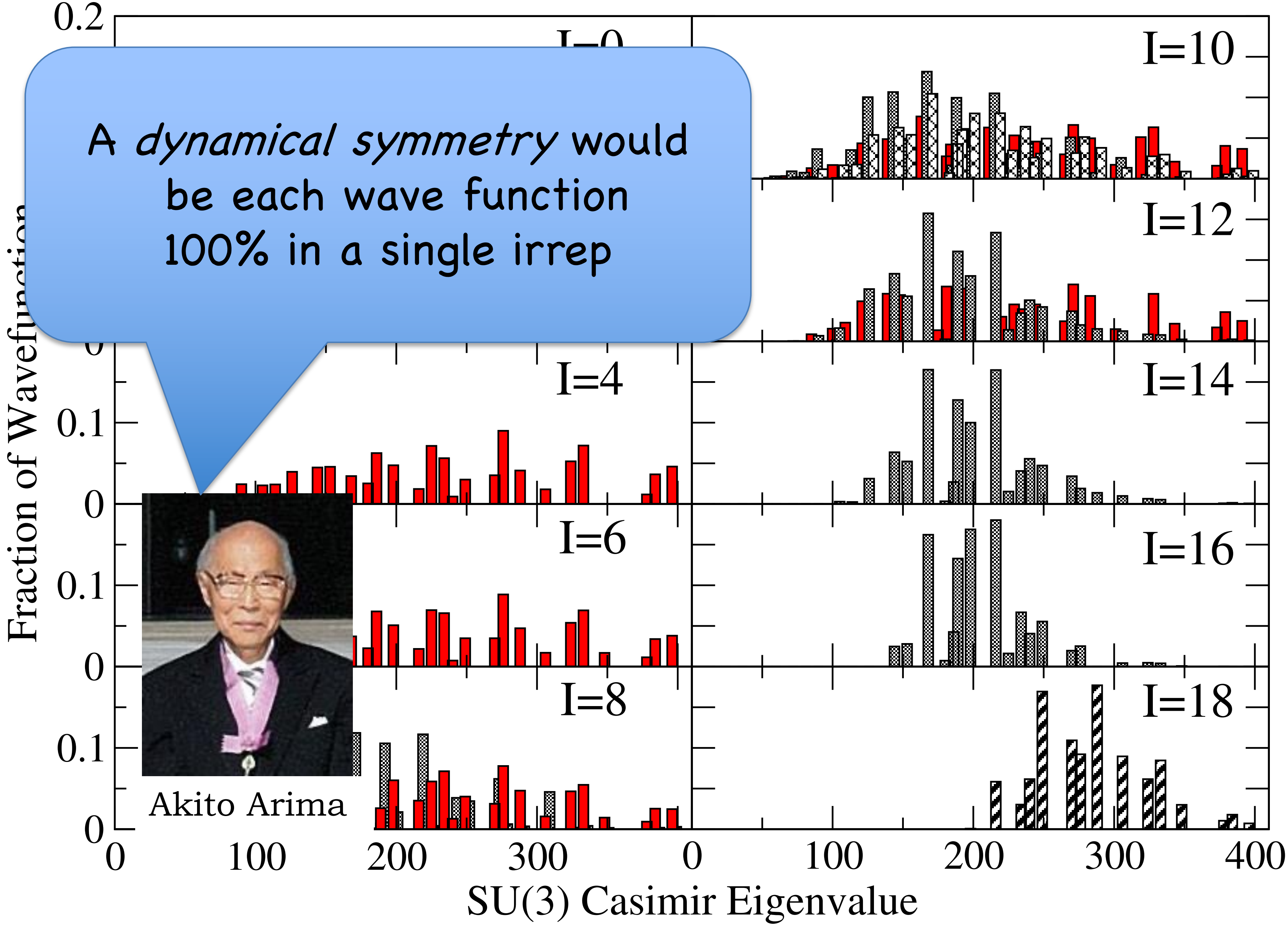
Wave functions computed in interacting shell model* using GXPF1 interaction; then SU(3) 2-body Casimir read in and decomposition done with Lanczos

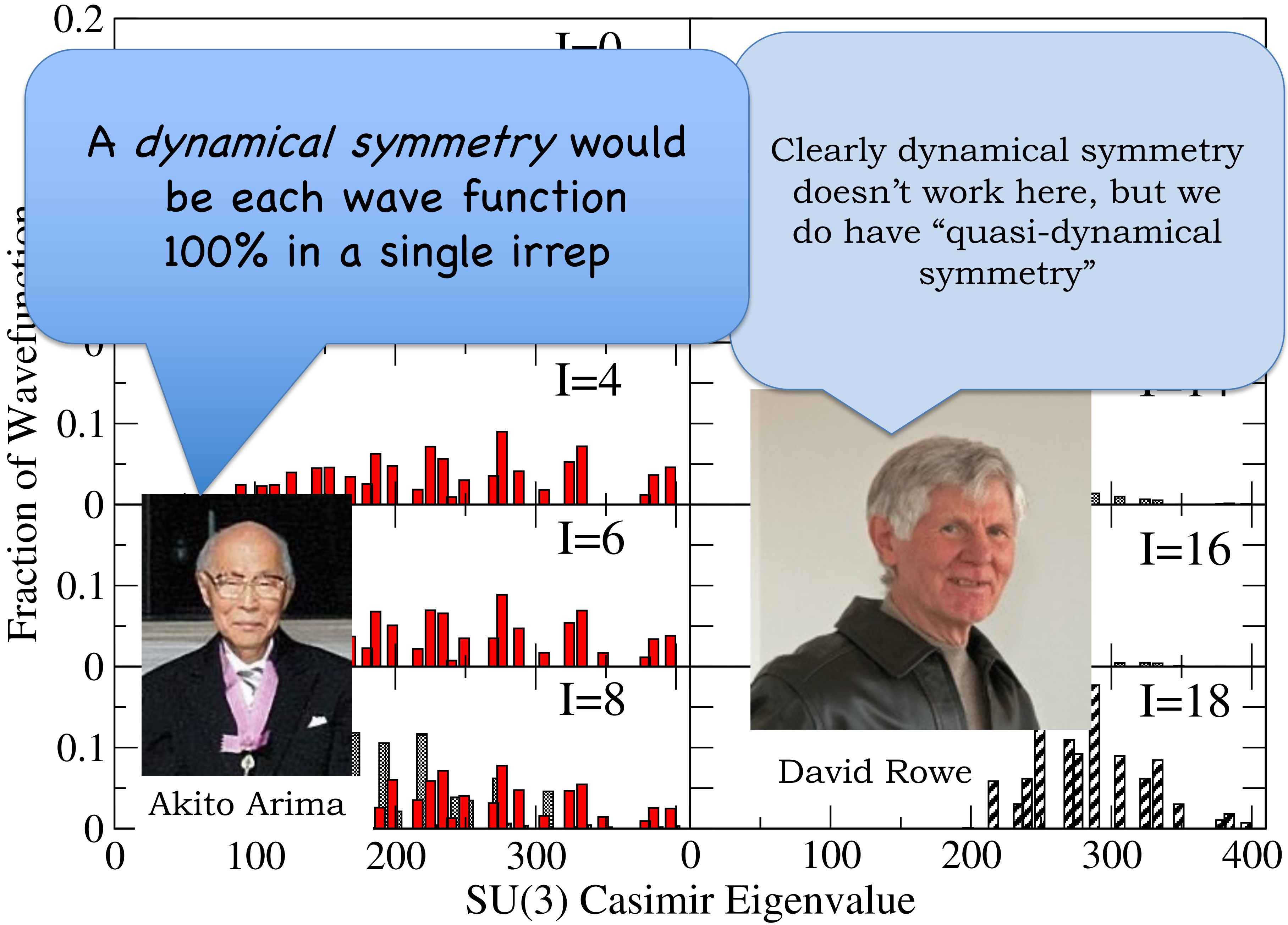
R. Herrera and CWJ,
Phys. Rev. C **95**, 024303 (2017)



I=0
I=2
I=4
I=6
I=8
I=10
I=12
I=14
I=16
I=18
0.2
0.1
0
0
100
200
300
400
Fraction of Wavefunction
SU(3) Casimir Eigenvalue

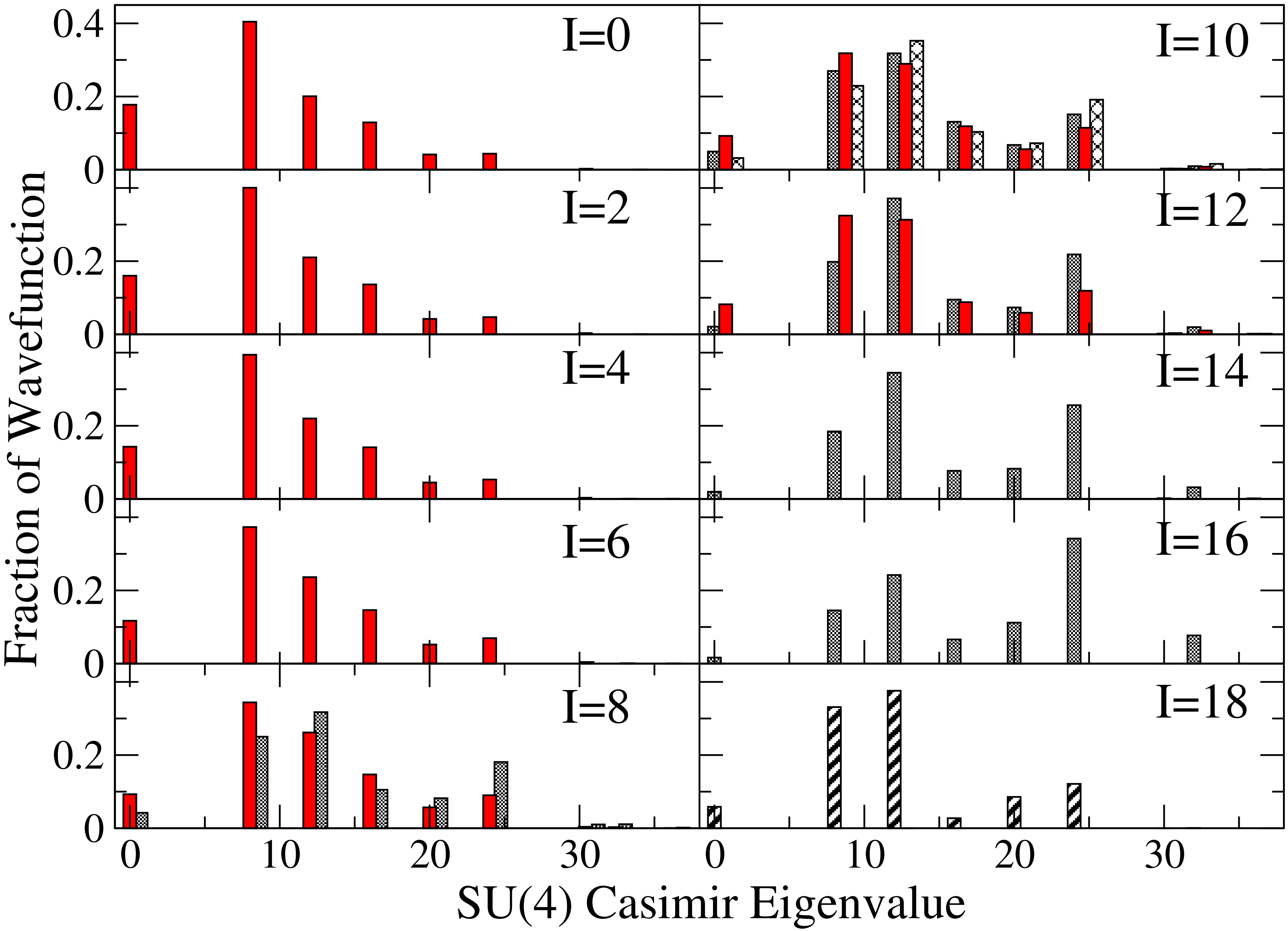
A *dynamical symmetry* would be each wave function 100% in a single irrep




A *dynamical symmetry* would be each wave function 100% in a single irrep
Clearly dynamical symmetry doesn't work here, but we do have "quasi-dynamical symmetry"
Akito Arima
David Rowe
I=4
I=6
I=8
I=16
I=18
0.2
0.1
0
Fraction of Wavefunction
0
100
200
300
400
SU(3) Casimir Eigenvalue

What about
other groups?

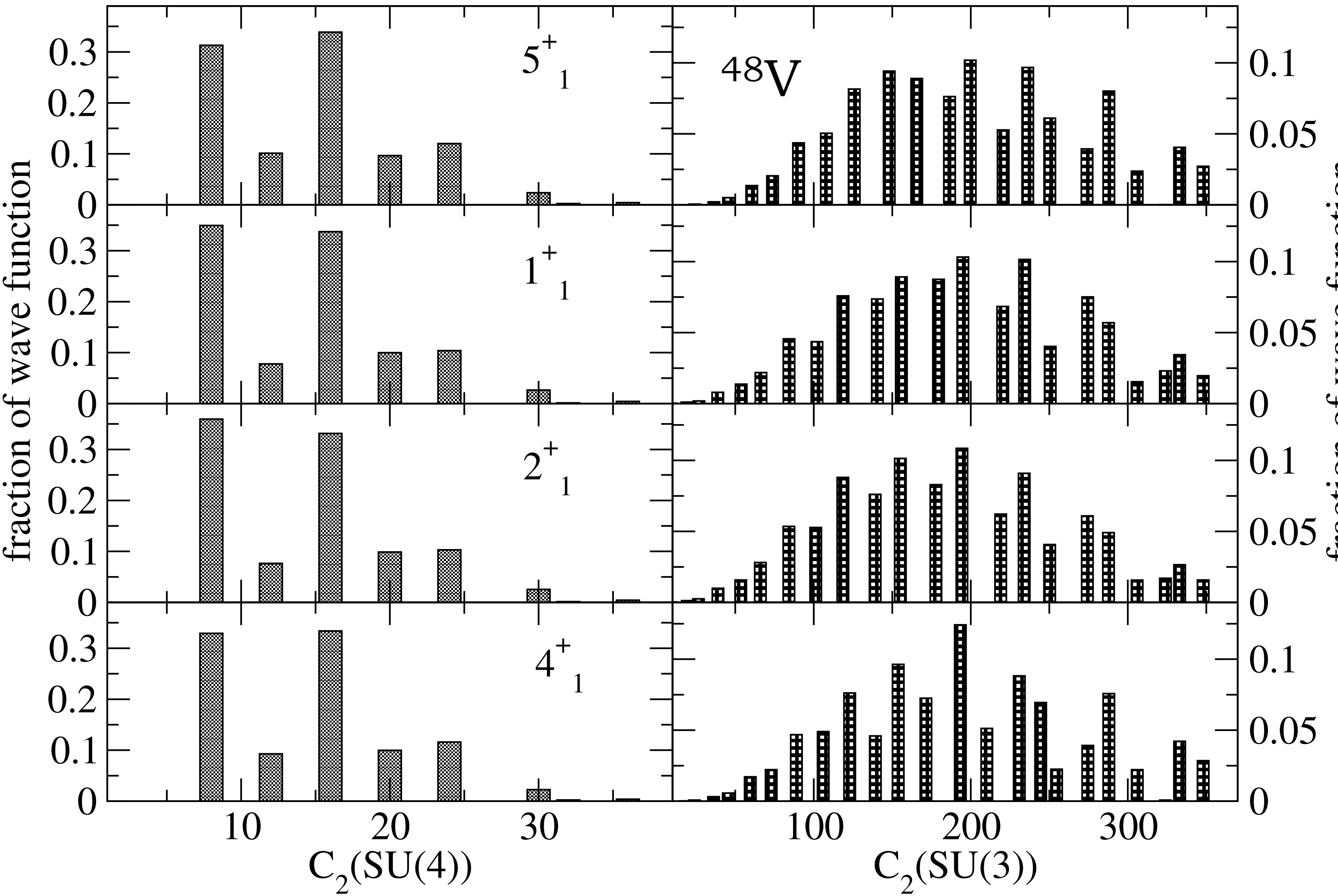
Eugene Wigner

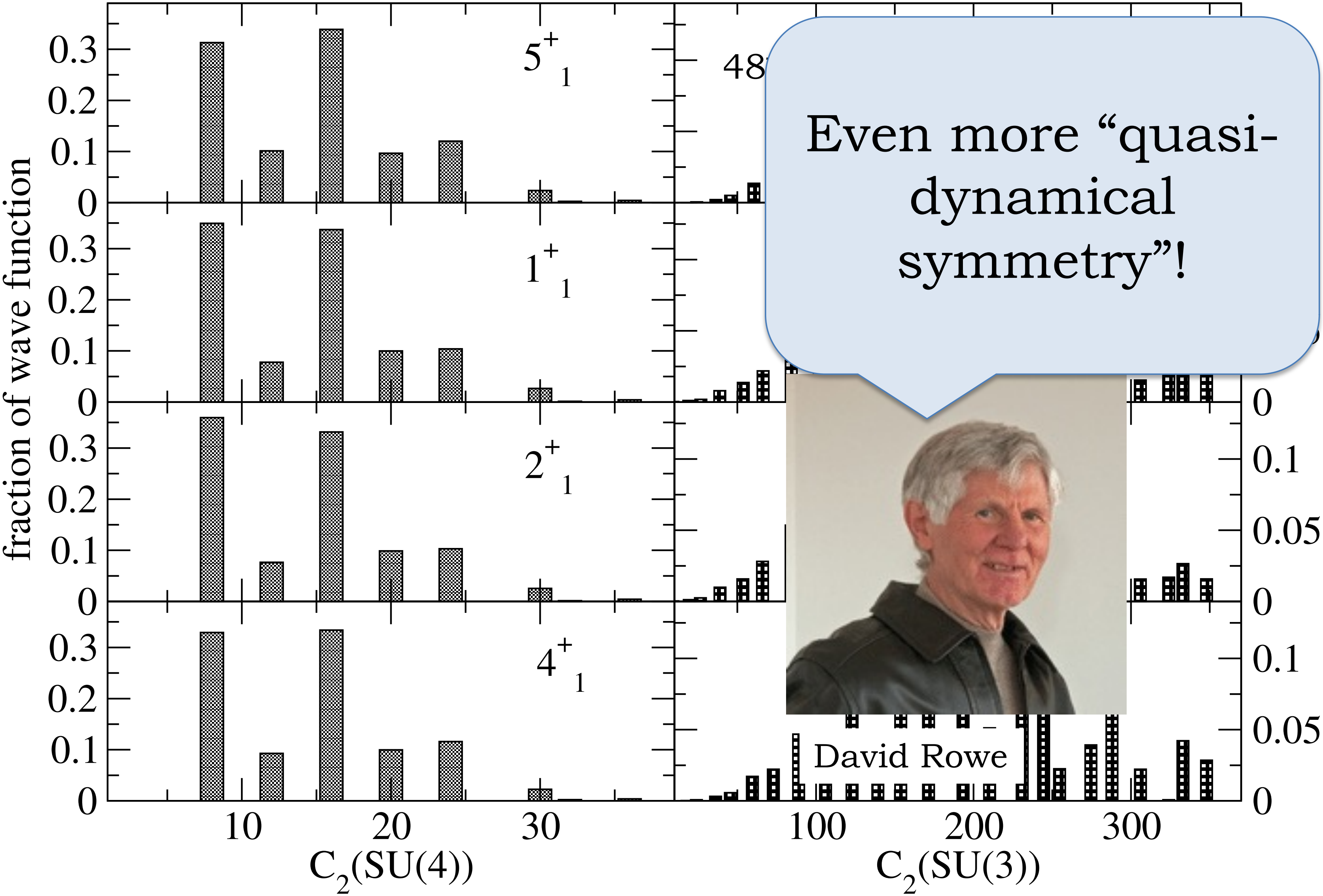


I=0
I=2
I=4
I=6
I=8
I=10
I=12
I=14
I=16
I=18
0.4
0.2
0
0
10
20
30
Fraction of Wavefunction
SU(4) Casimir Eigenvalue

What about non-rotational nuclei?

Eugene Wigner


fraction of wave function
fraction of wave function
^{48}V
5^+_1
1^+_1
2^+_1
4^+_1
0
0.1
0.2
0.3
0
0.05
0.1
10
20
30
100
200
300
$C_2(SU(4))$
$C_2(SU(3))$

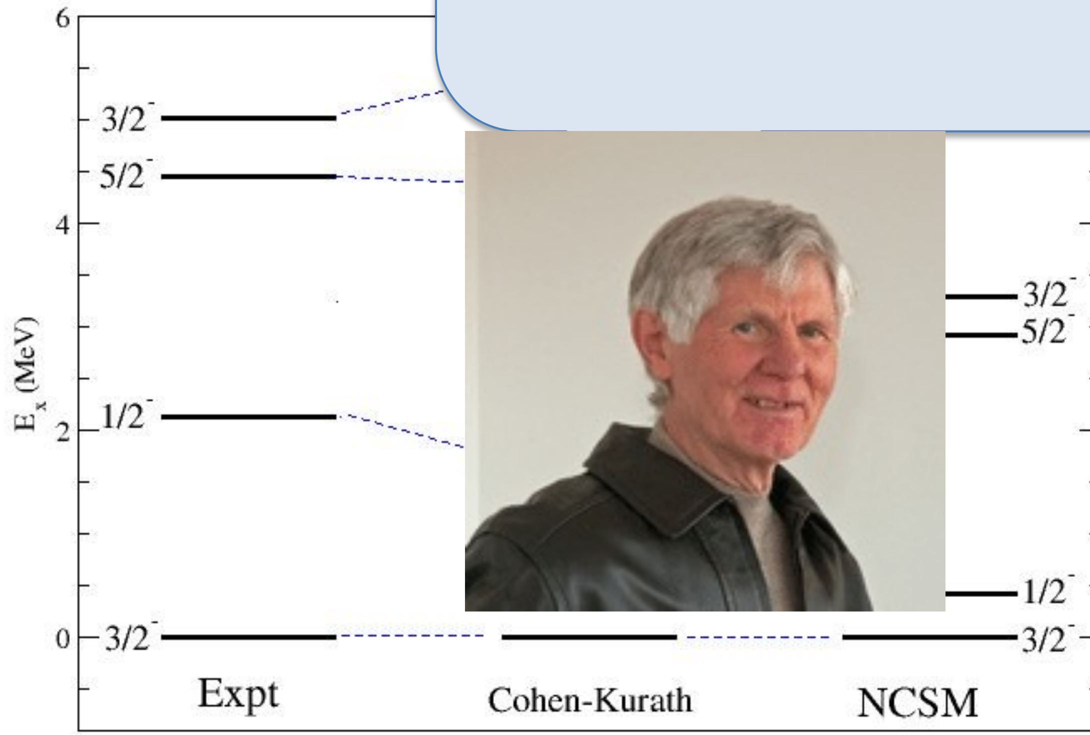

Even more "quasi-dynamical symmetry"!
David Rowe
fraction of wave function
0.3
0.2
0.1
0
5^+_1
1^+_1
2^+_1
4^+_1
48
10
20
30
100
200
300
0.1
0.05
$C_2(SU(4))$
$C_2(SU(3))$

^{11}B

Phenomenological Cohen-Kurath *m*-scheme dim

NCSM: N3LO chiral 2-body force SRG evolved t
m-scheme dimension: 20 million

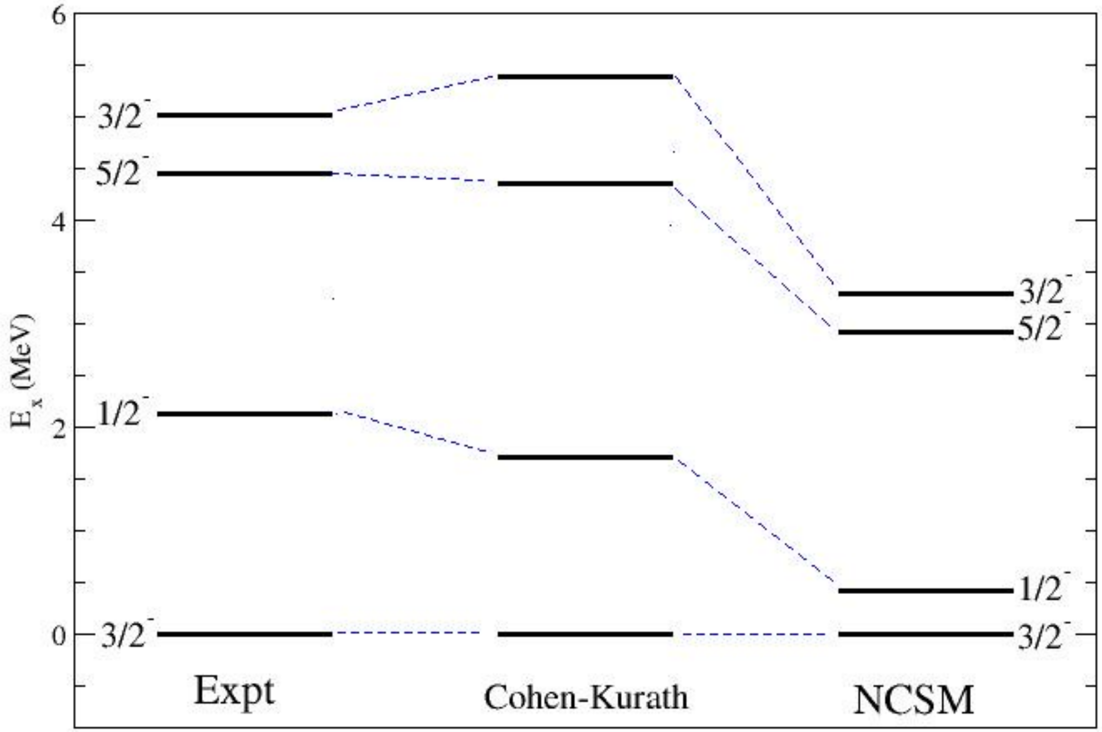
What about
in the
NCSM?

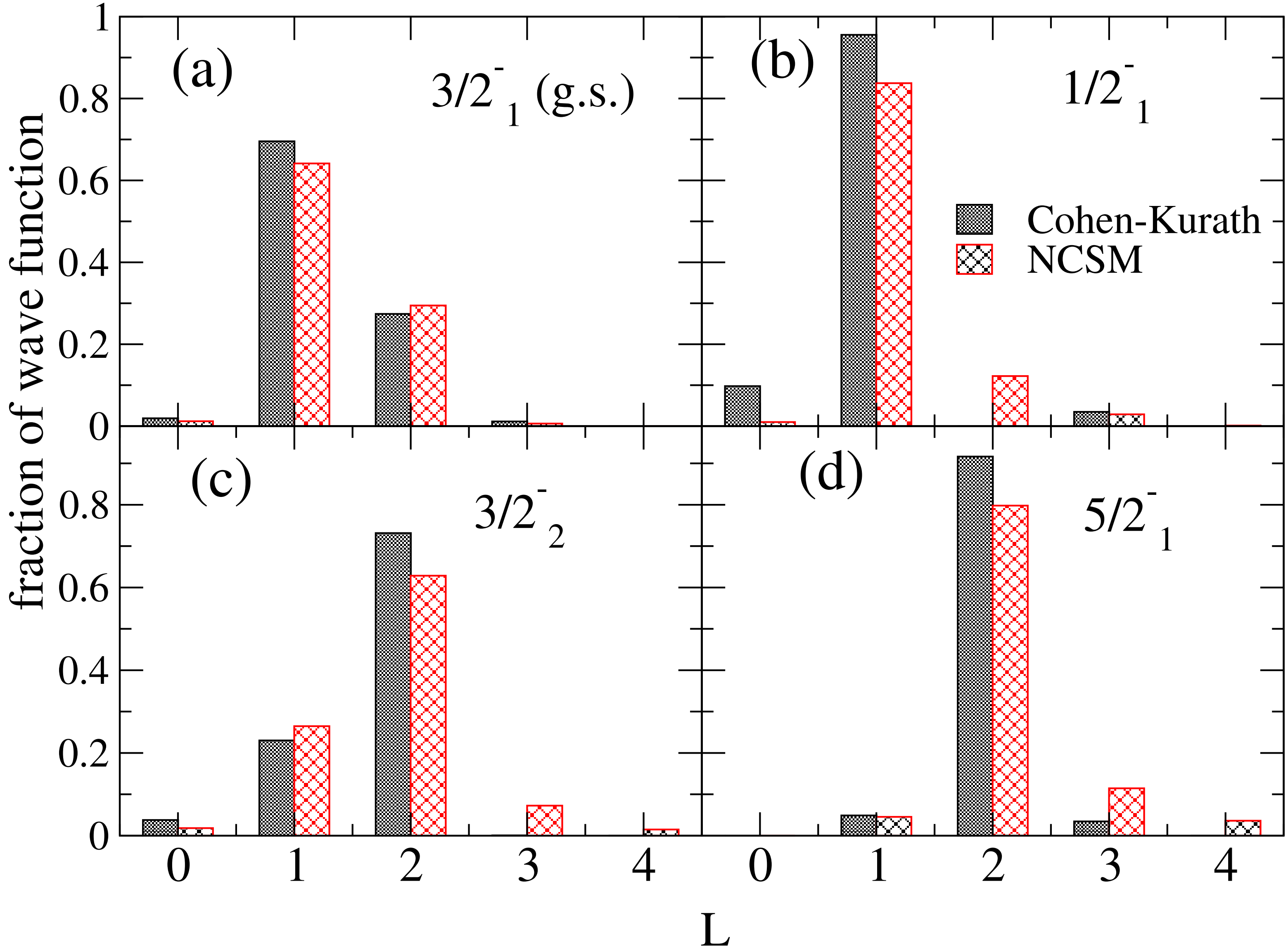


^{11}B

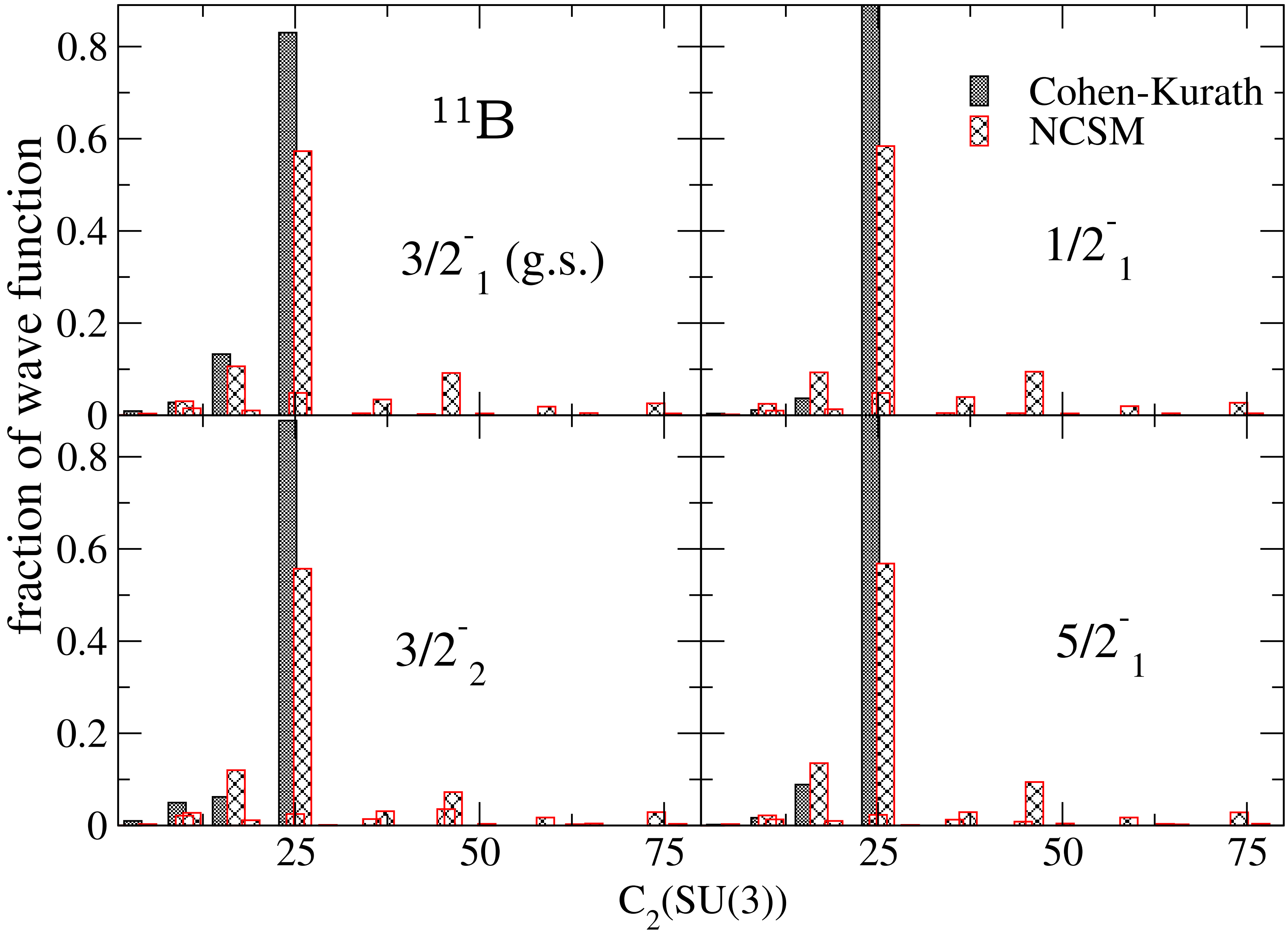
Phenomenological Cohen-Kurath *m*-scheme dimension: 62

NCSM: N3LO chiral 2-body force SRG evolved to $\lambda = 2.0\ fm^{-1}$, $N_{max} = 6$, $\hbar\omega$=22 MeV
m-scheme dimension: 20 million





(a)
3/2⁻₁ (g.s.)
(b)
1/2⁻₁
(c)
3/2⁻₂
(d)
5/2⁻₁
Cohen-Kurath
NCSM
fraction of wave function
L
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4



fraction of wave function
0.8
0.6
0.4
0.2
0
^{11}B
$3/2^-_1$ (g.s.)
$1/2^-_1$
$3/2^-_2$
$5/2^-_1$
Cohen-Kurath
NCSM
25
50
75
$C_2(SU(3))$

Islands of inversions
and halo nuclei
form a **challenge** to standard
shell-model pictures

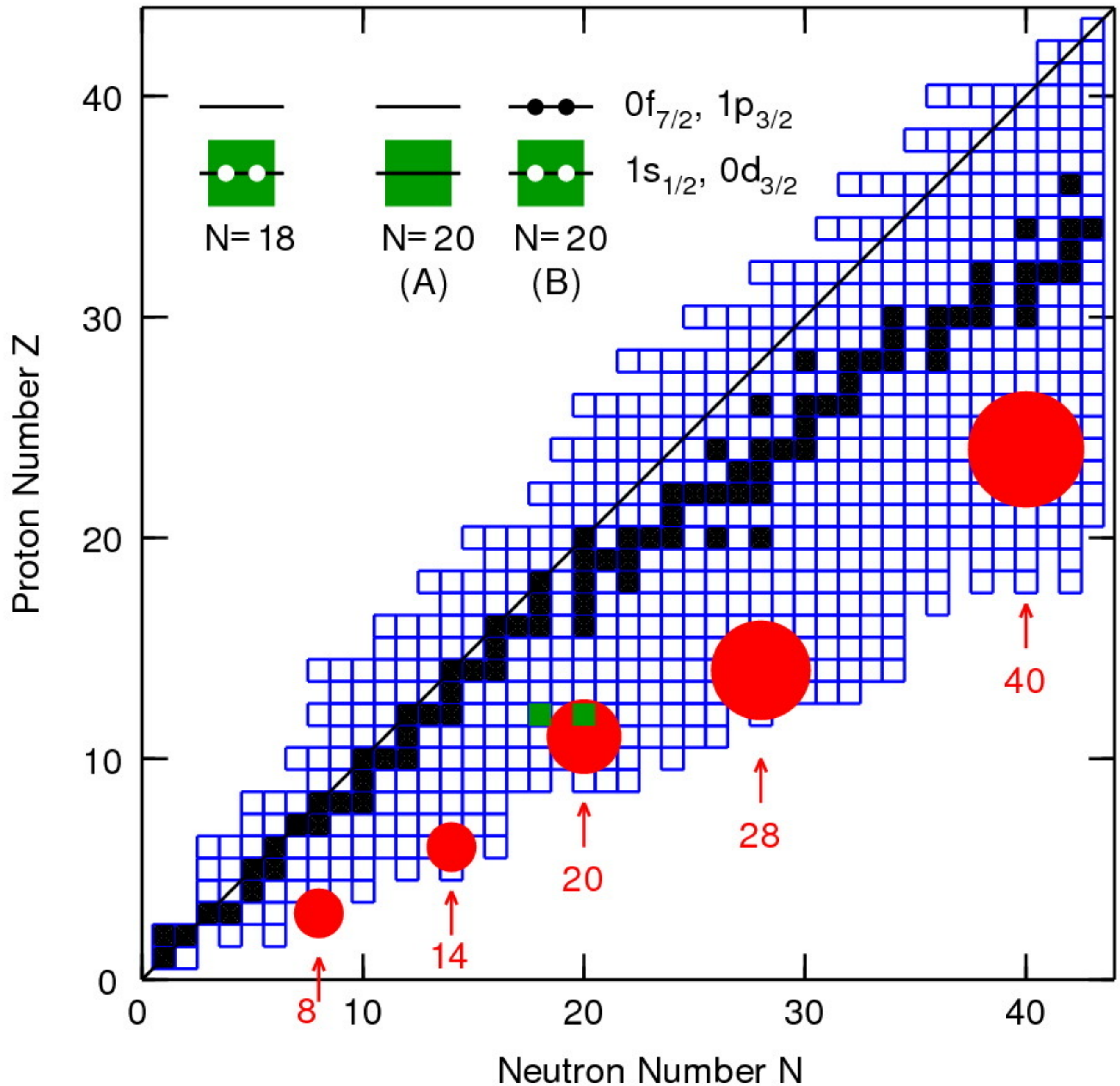


Figure: Alex Brown

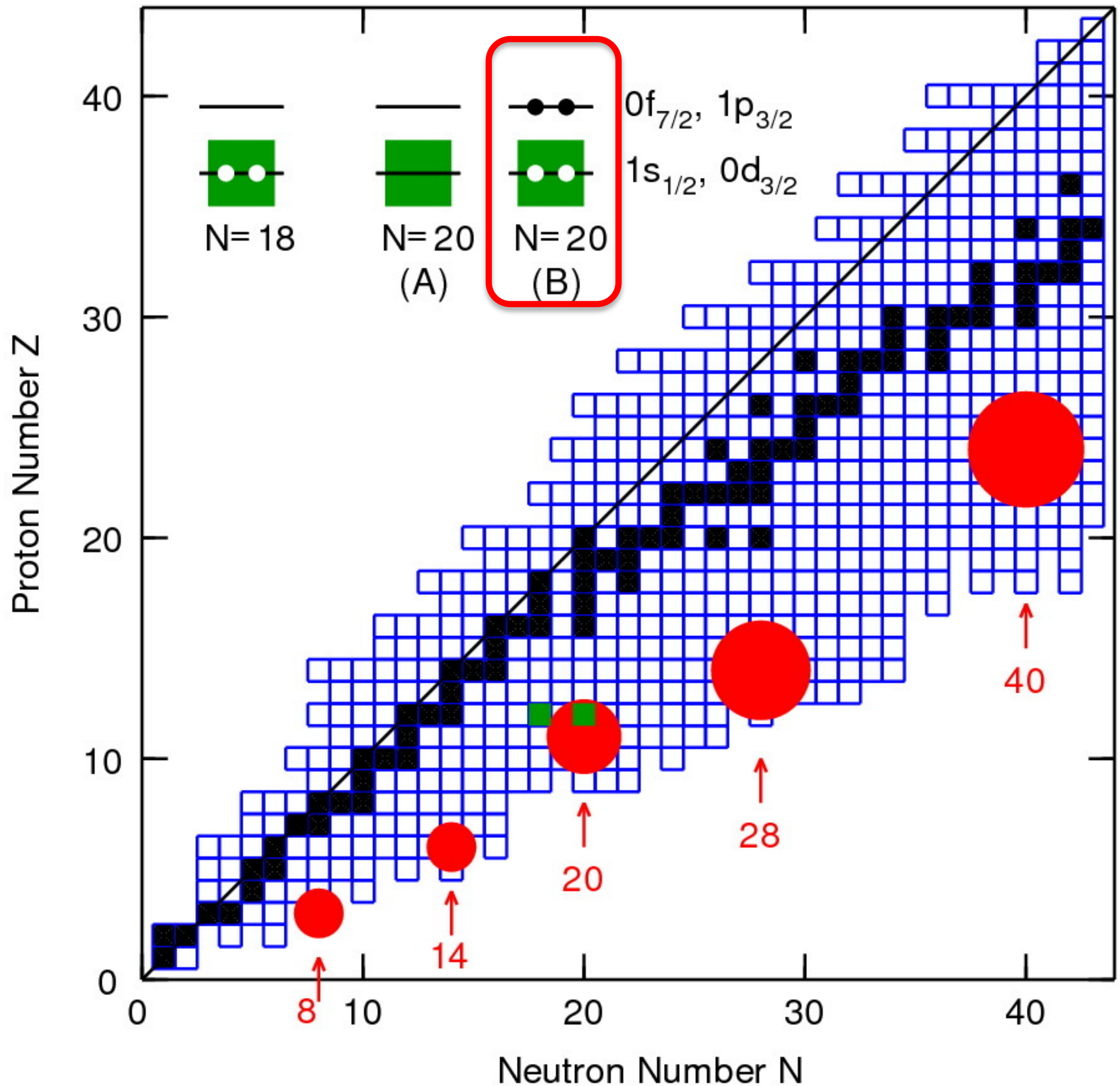


Figure: Alex Brown

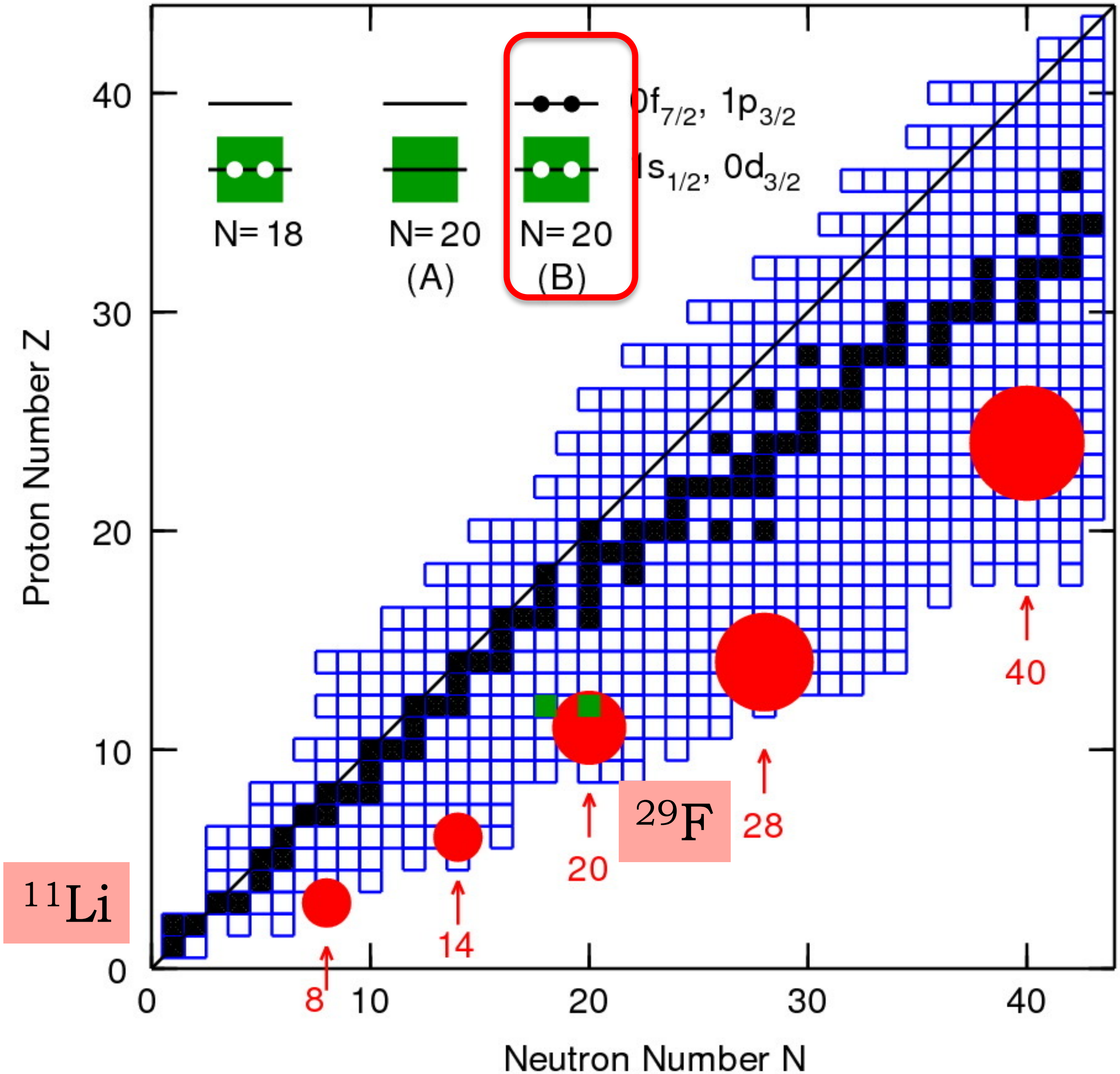


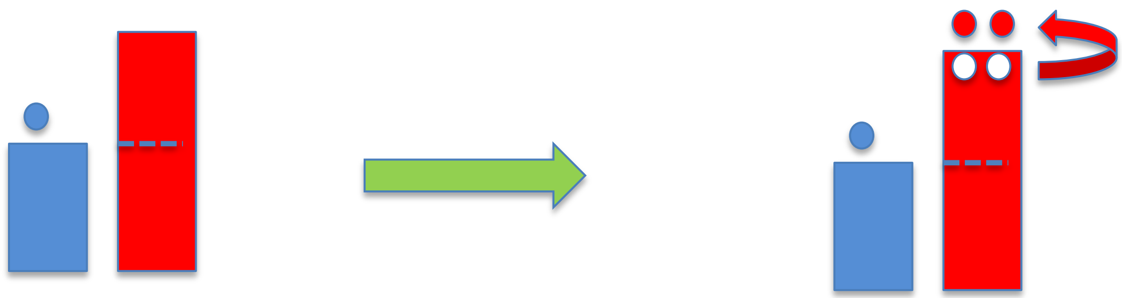
Figure:
Alex Brown

Case study: ^{11}Li

^{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



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

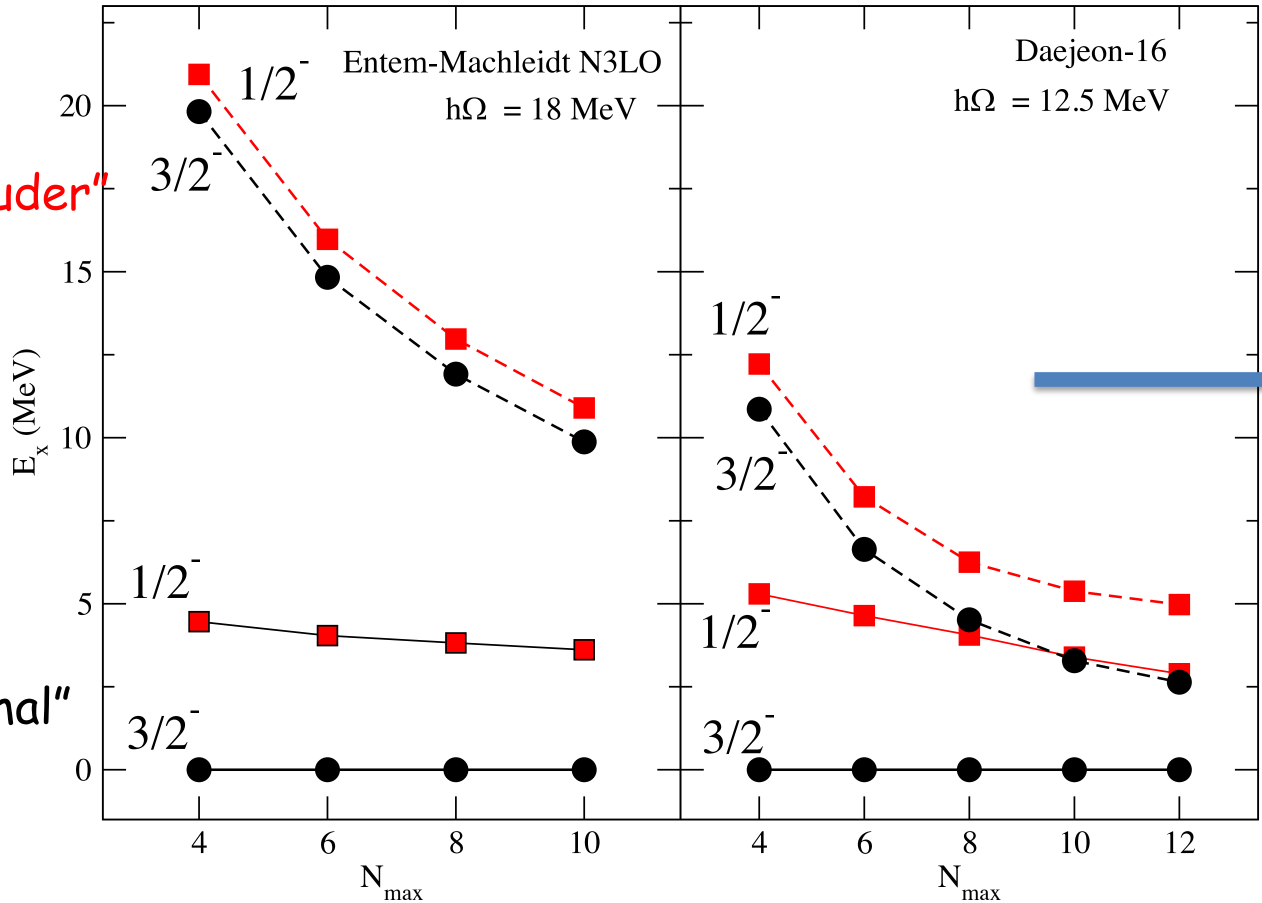
^{11}Li makes for an excellent case study

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

CASE STUDY: ^{11}LI

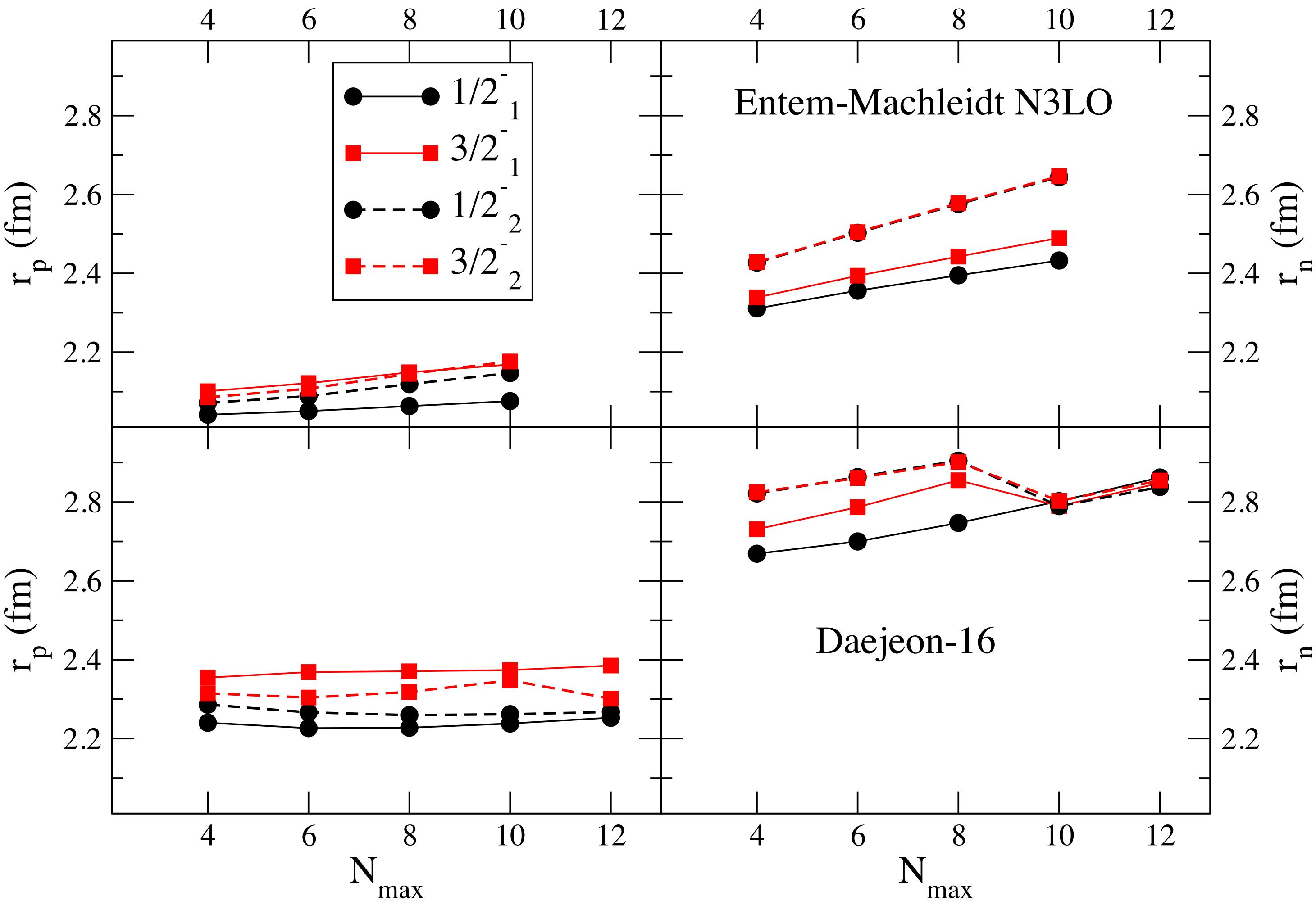
"intruder"

"normal"

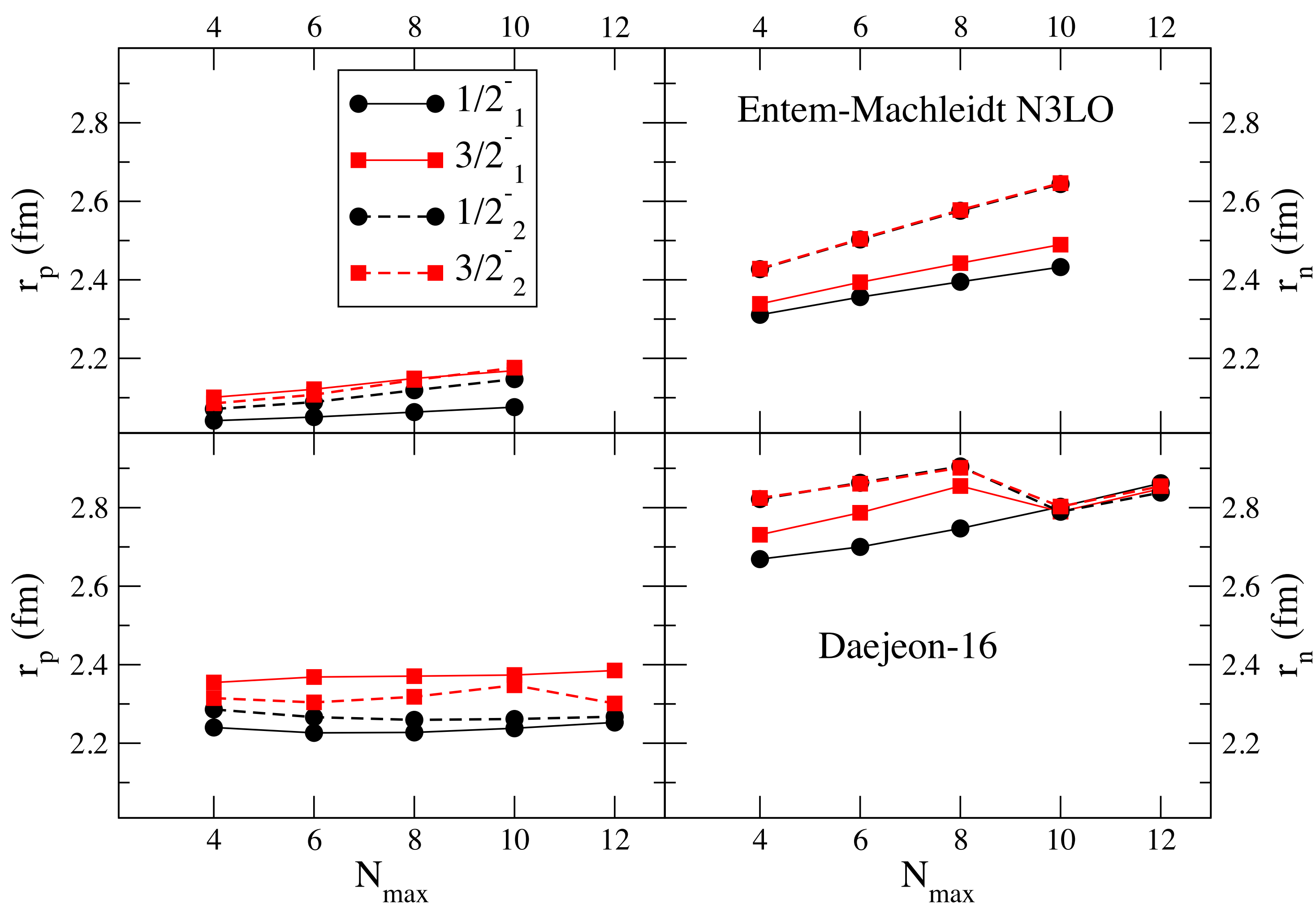


Mark Caprio

CASE STUDY: ^{11}LI



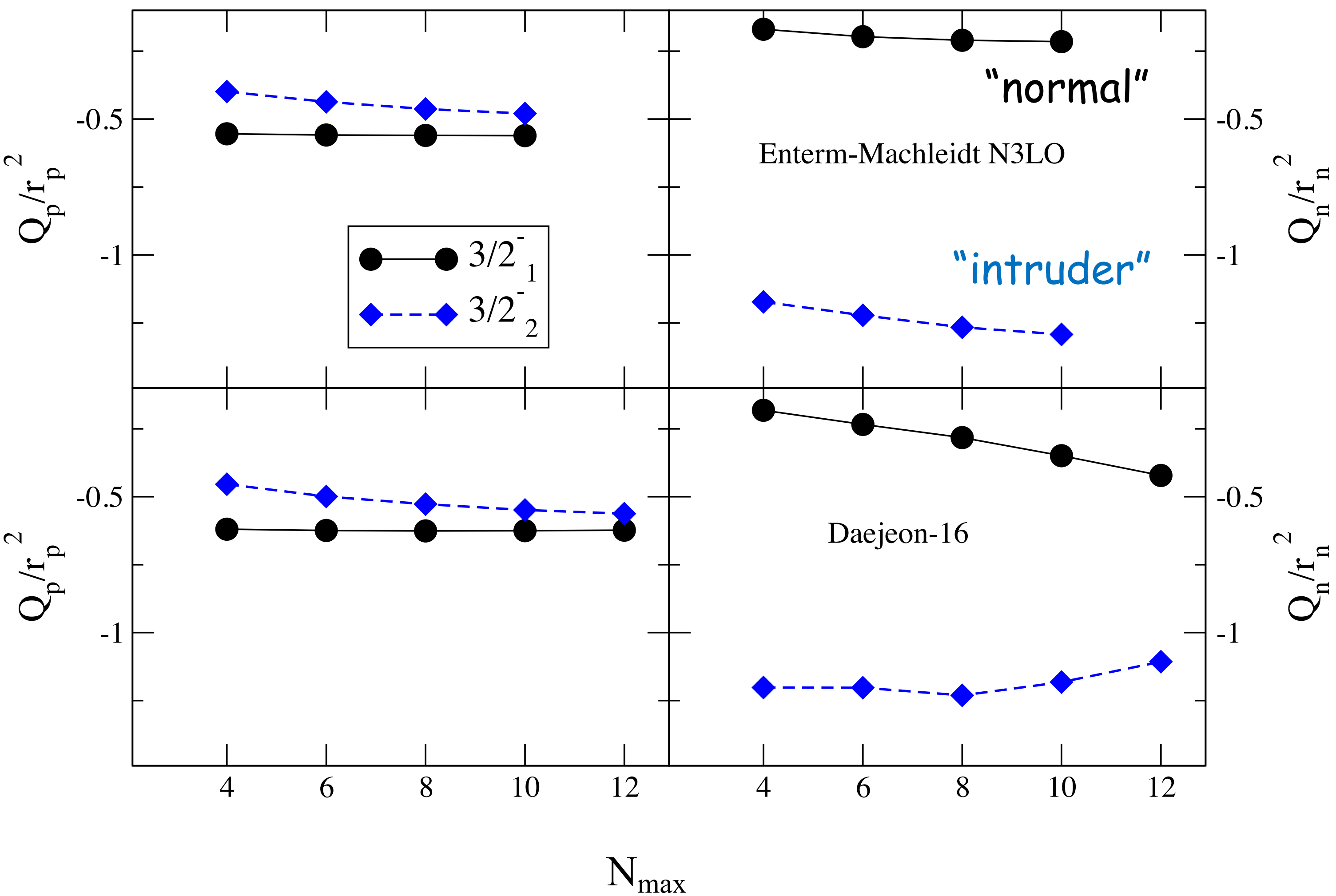
Case study: ^{11}Li



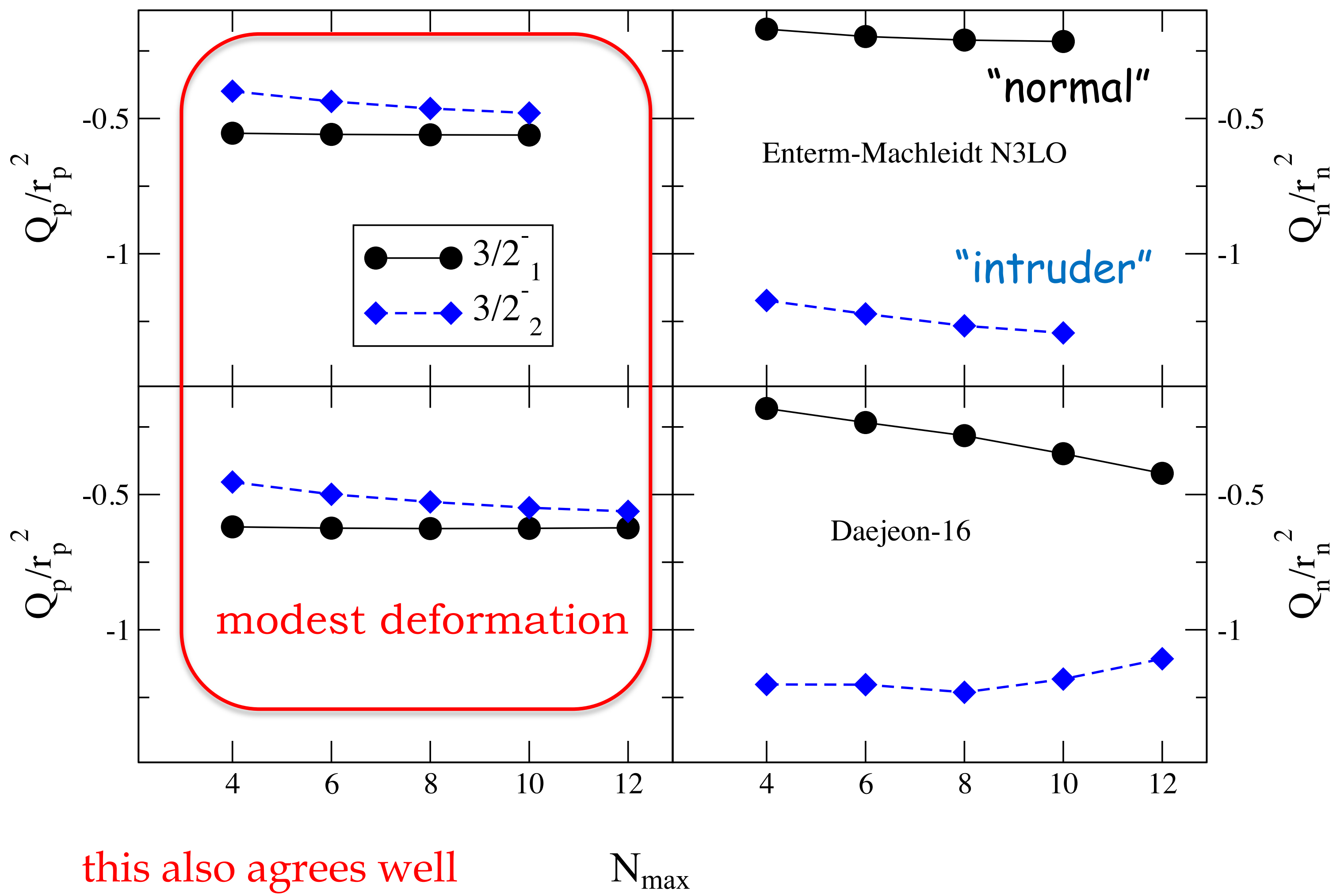
Radii are notorious difficult to get right

Mark Caprio

CASE STUDY: ^{11}LI

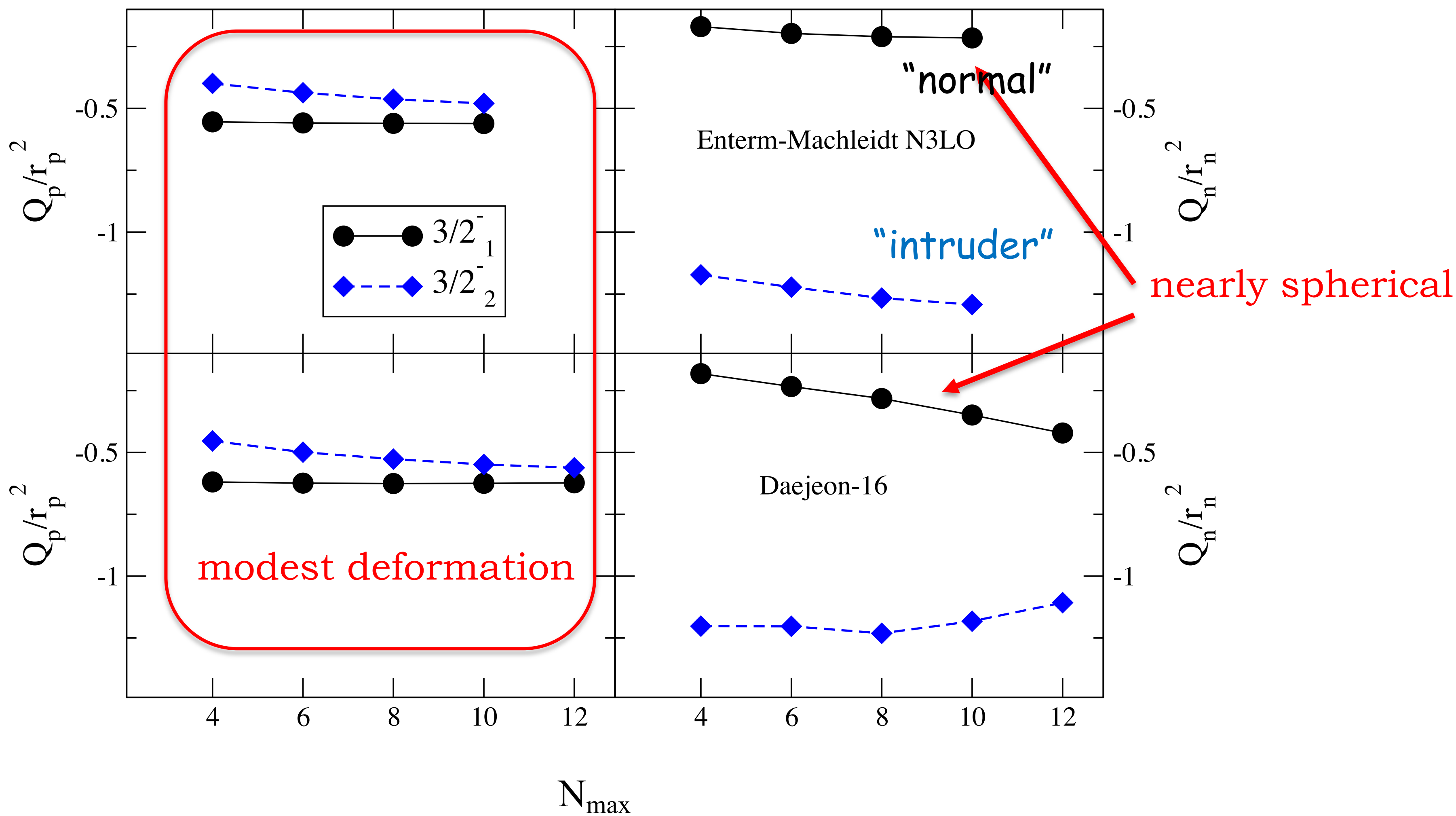


CASE STUDY: ^{11}LI

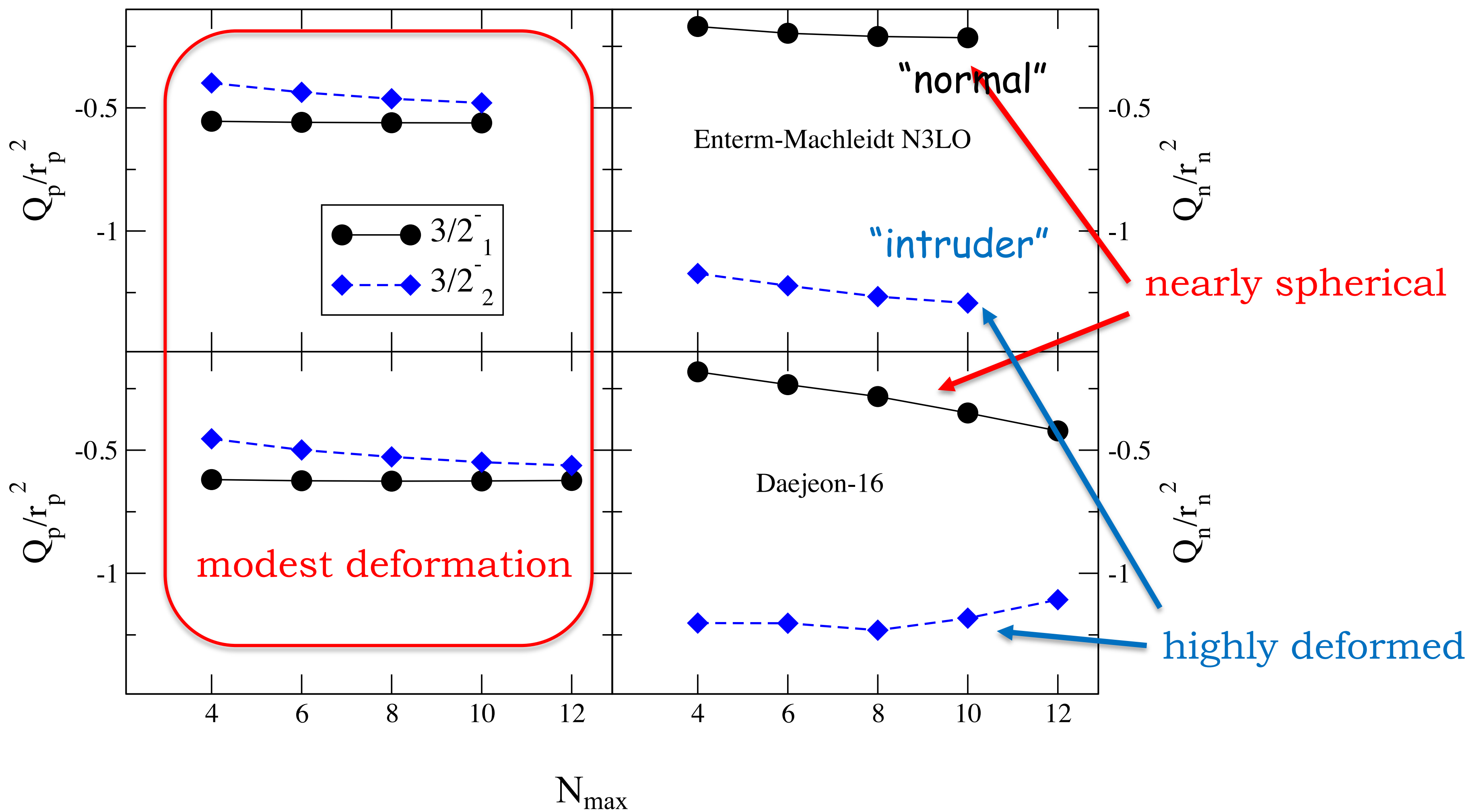


this also agrees well with experiment

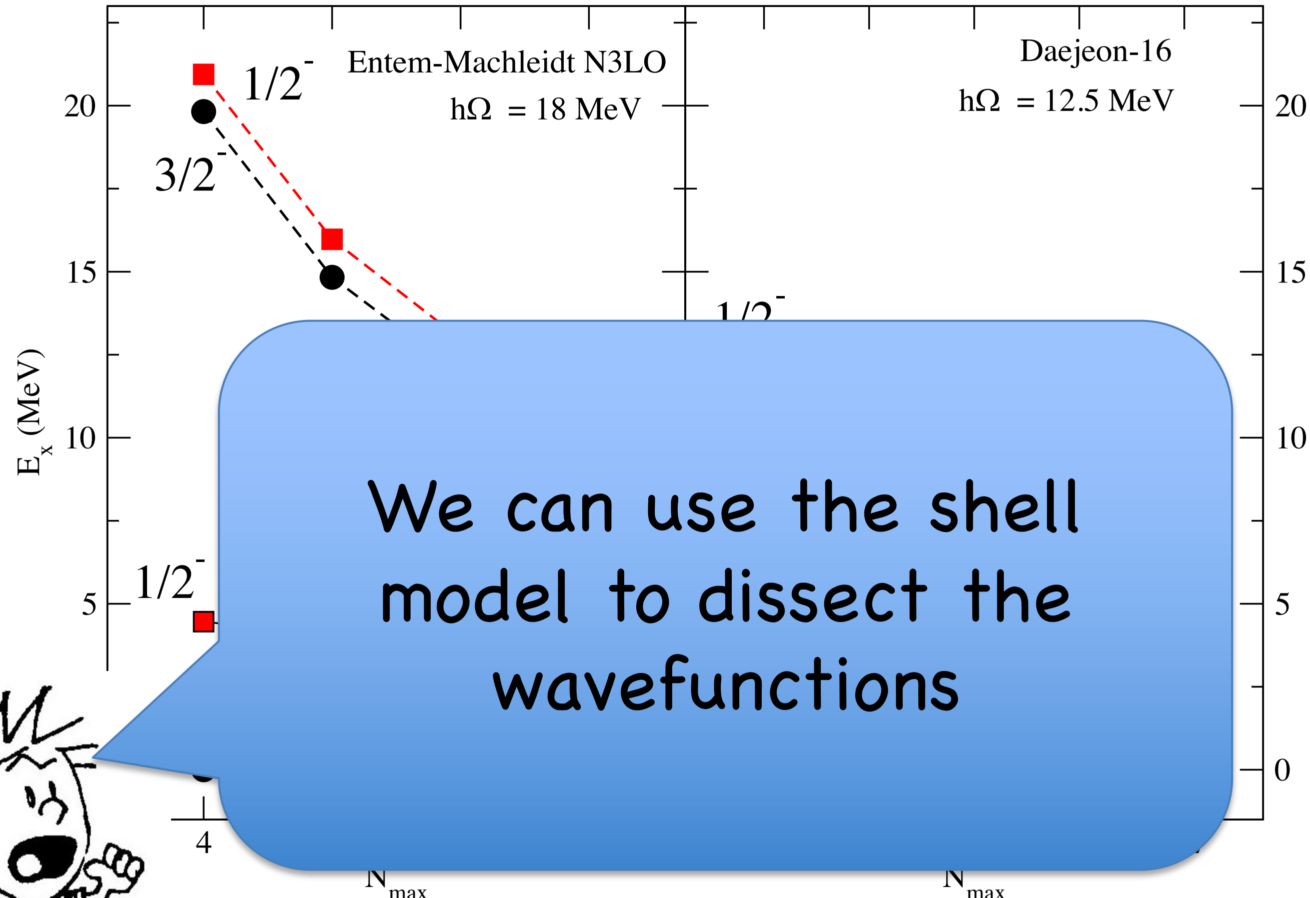
Case study: ^{11}Li



Case study: ^{11}Li

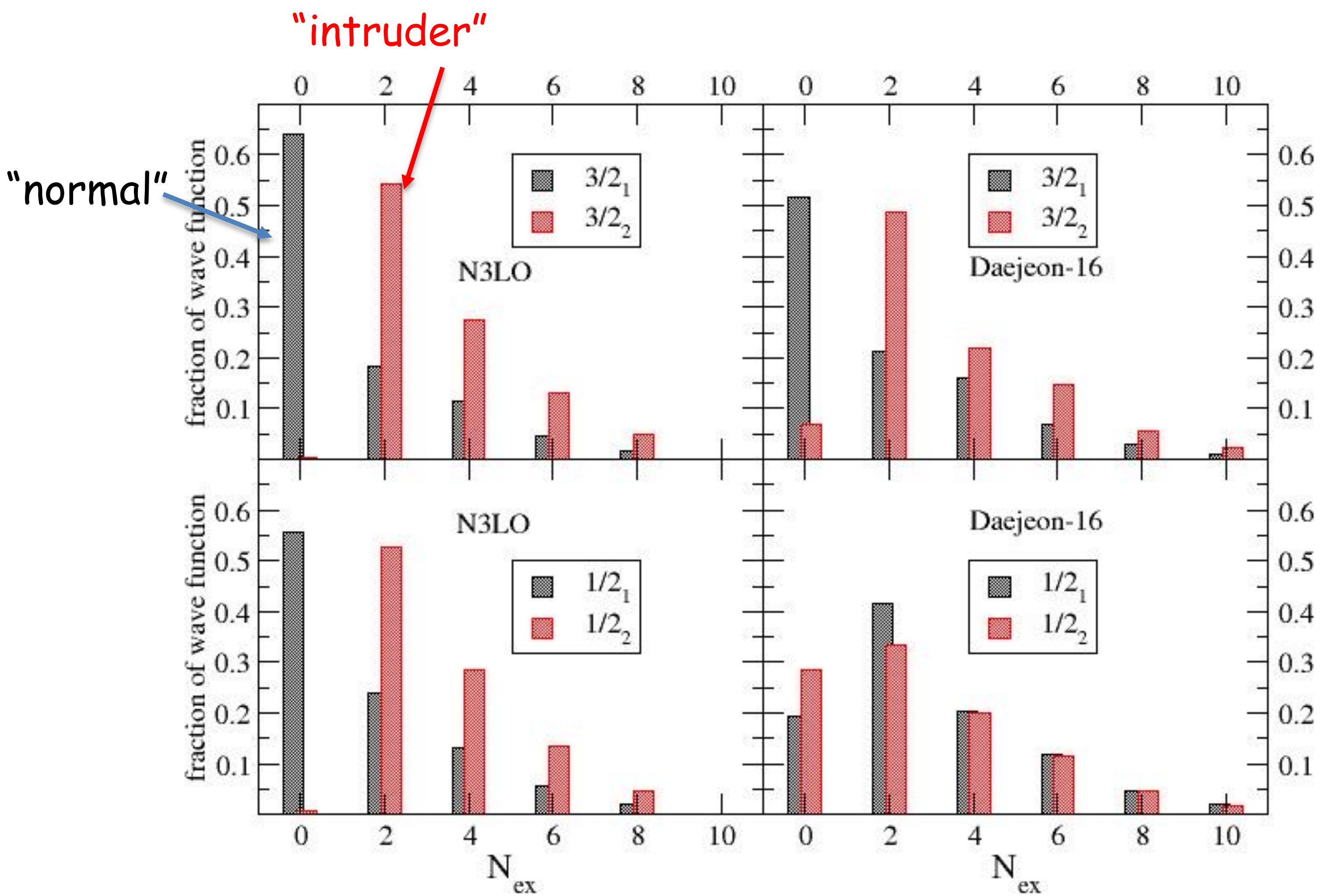


CASE STUDY: ^{11}LI



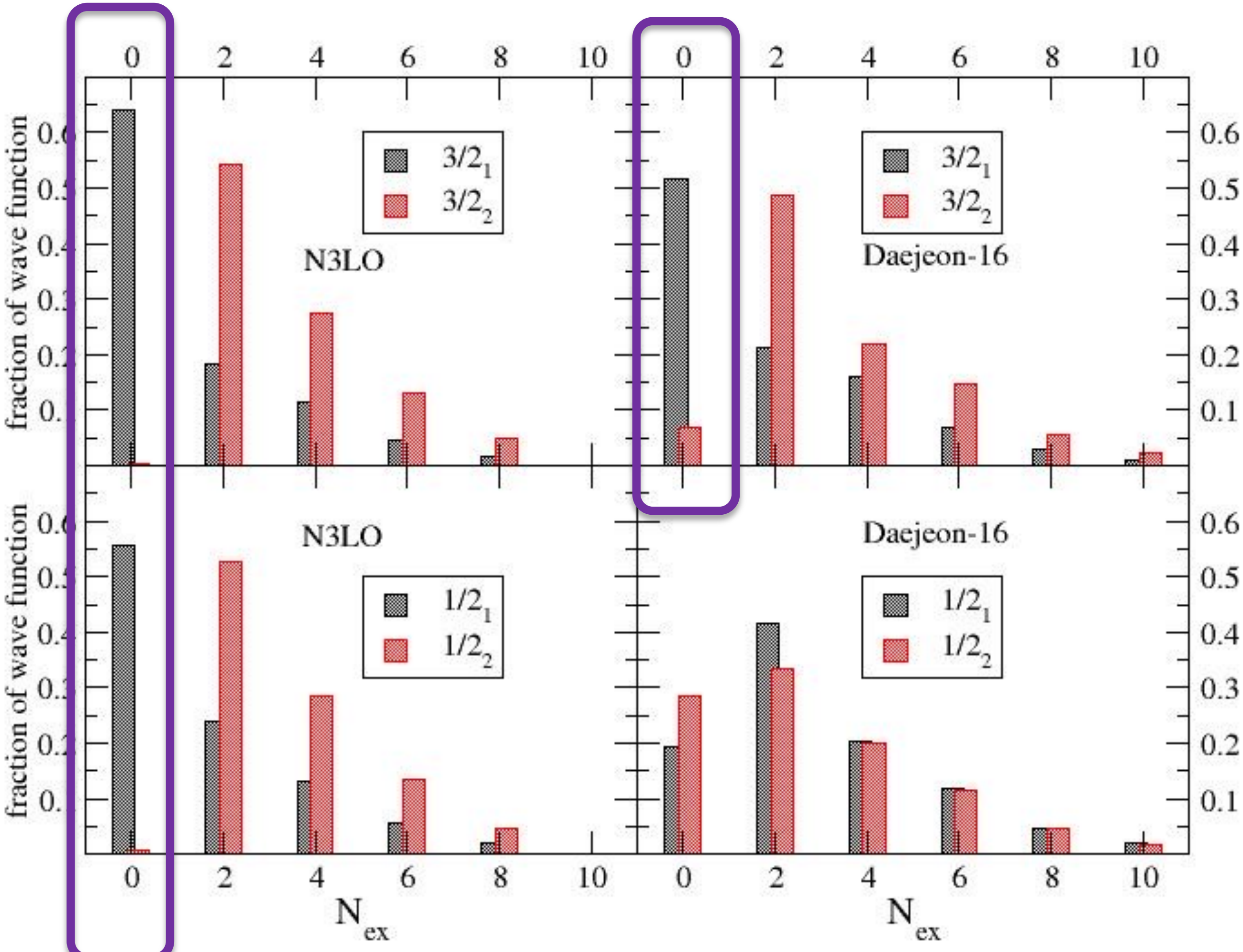
We can use the shell model to dissect the wavefunctions

Case study: ^{11}Li



CASE STUDY: ^{11}LI

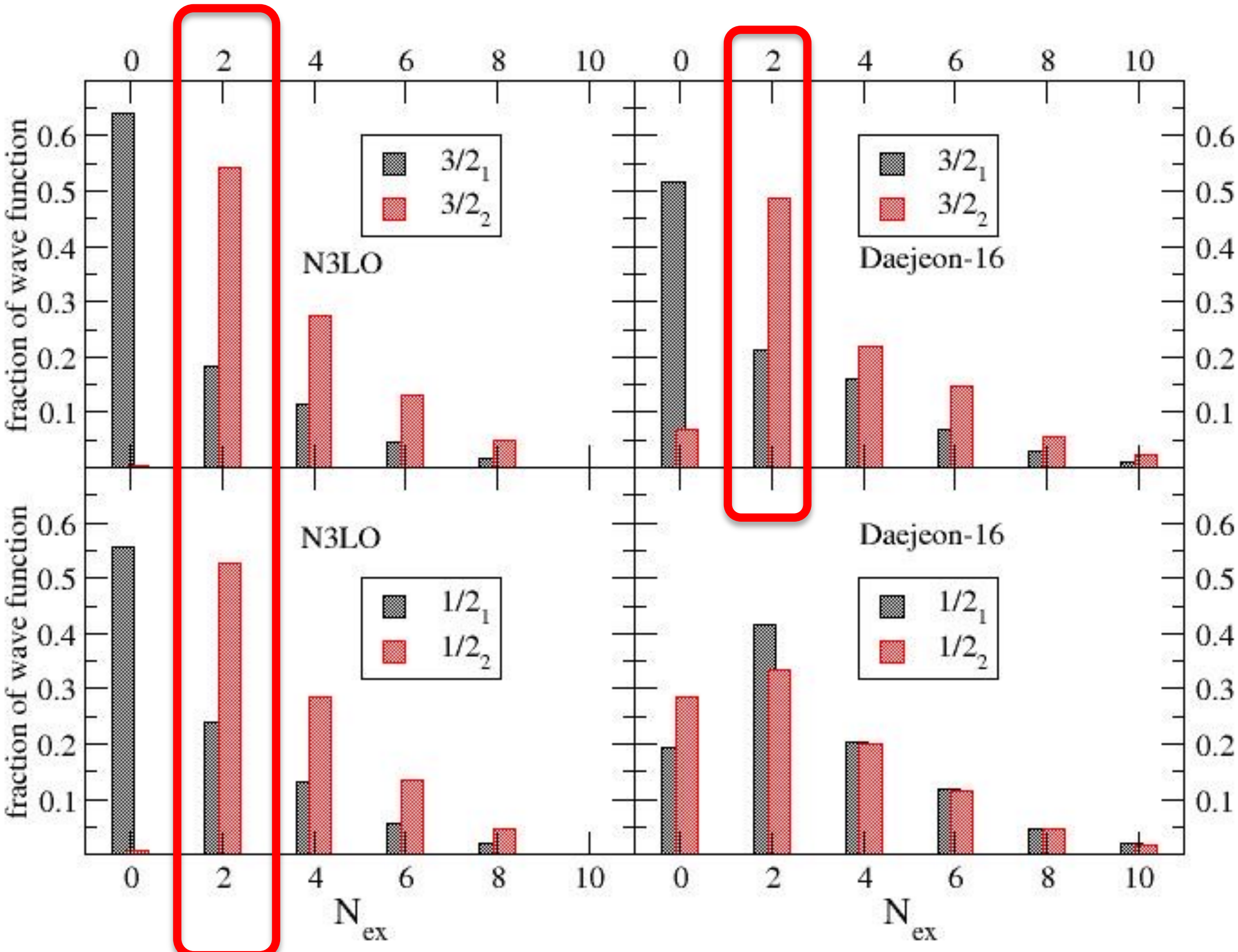
Primarily valence space



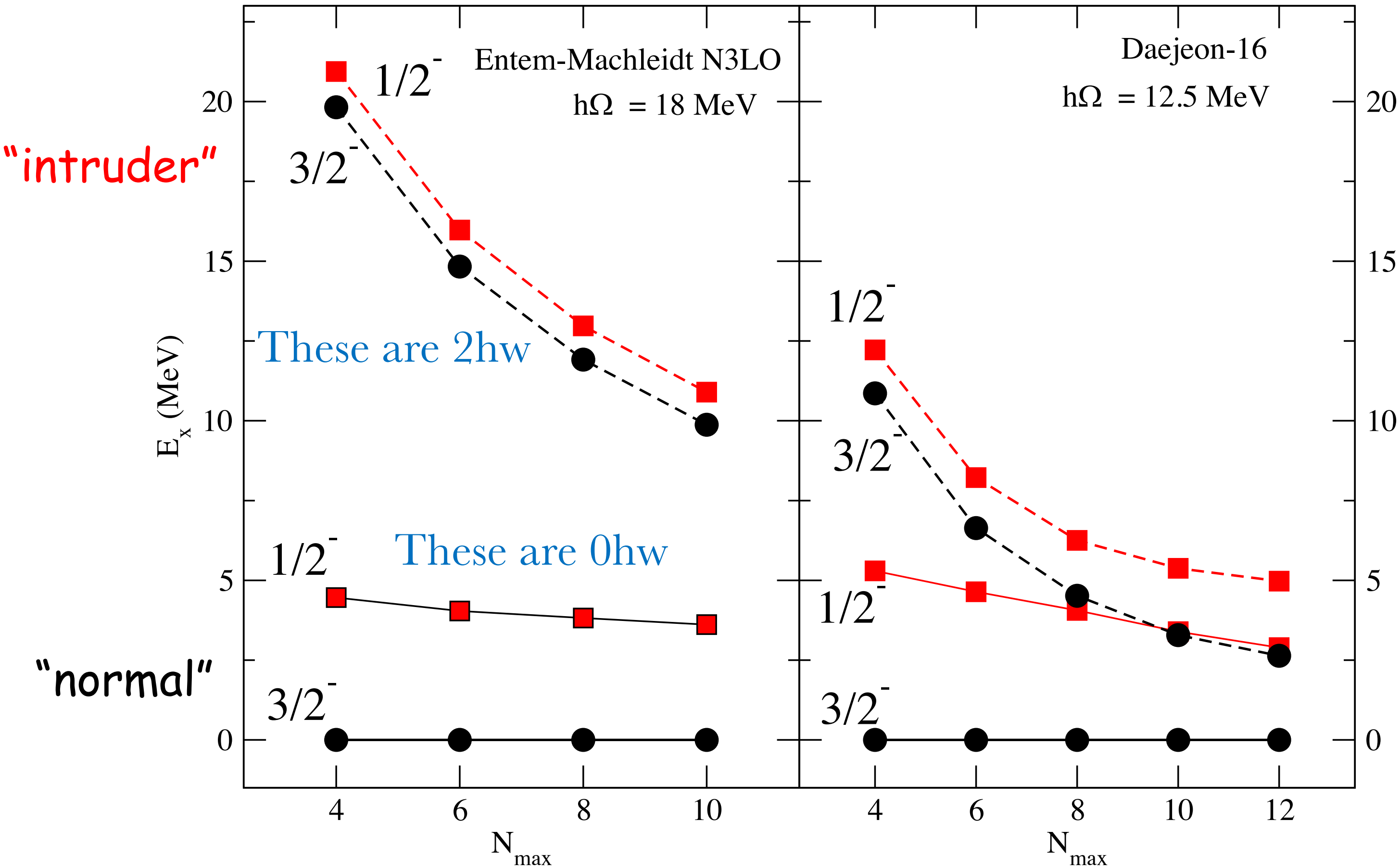
CASE STUDY: ^{11}LI

"intruder"

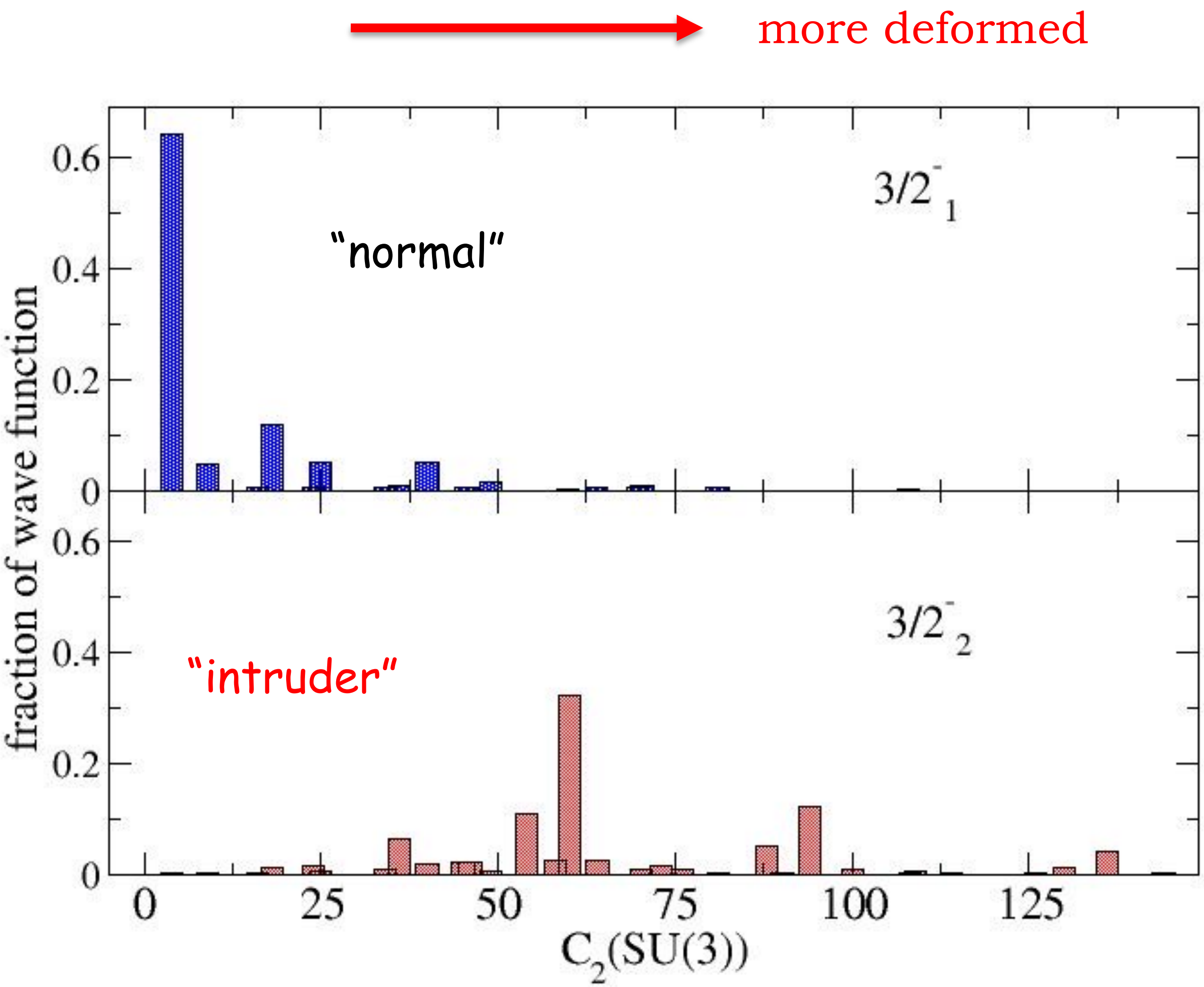
Primarily 2p-2h



CASE STUDY: ^{11}LI



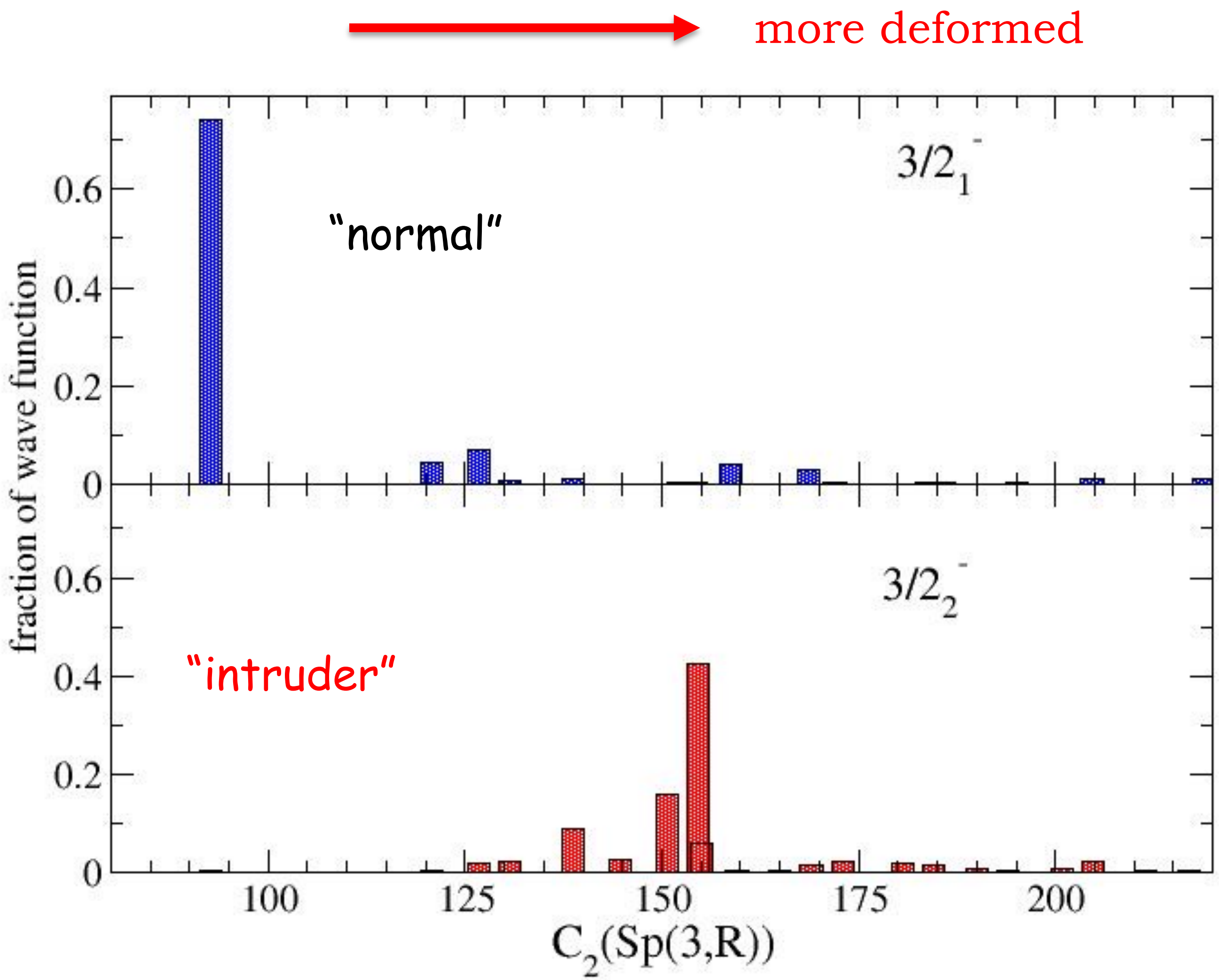
CASE STUDY: ^{11}LI



Group-theoretical Decomposition

Elliot SU(3)

CASE STUDY: ^{11}LI

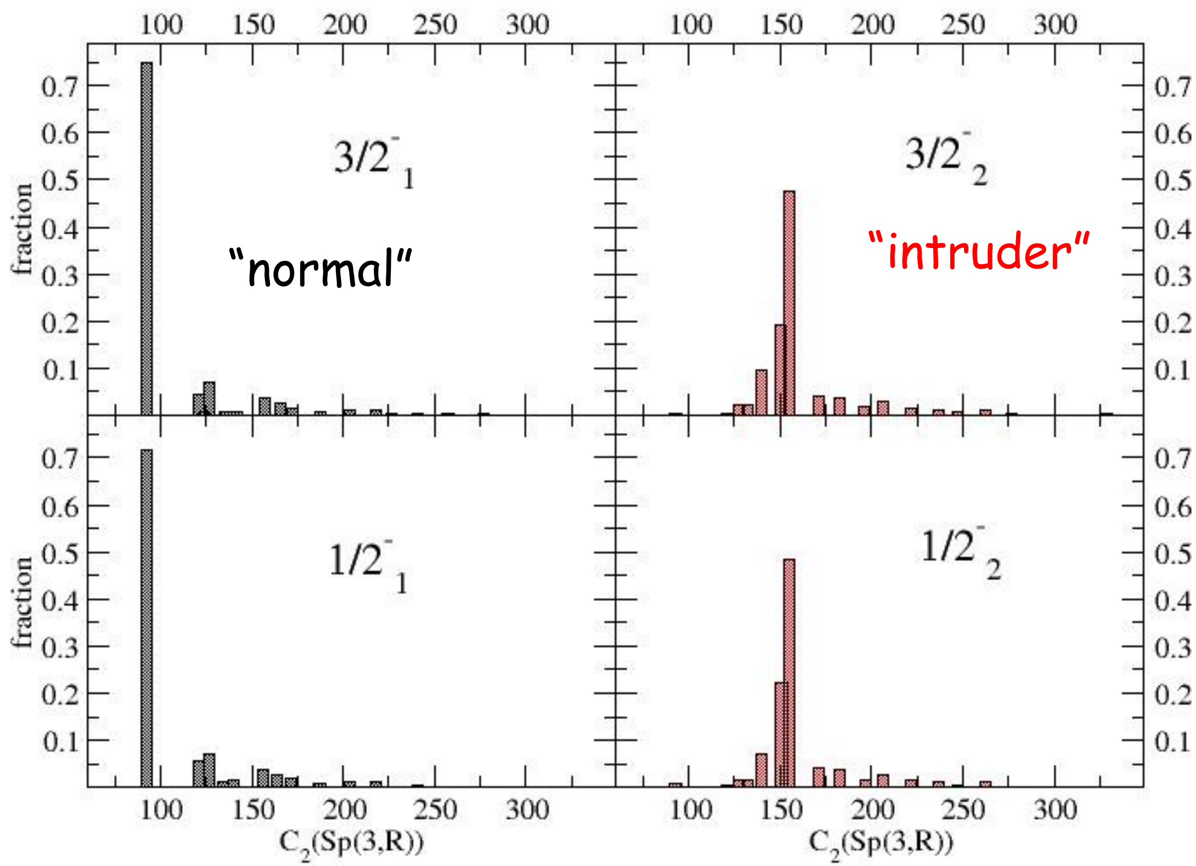


Group-theoretical Decomposition

Symplectic Sp(3,R)

CASE STUDY: ^{11}LI

more deformed

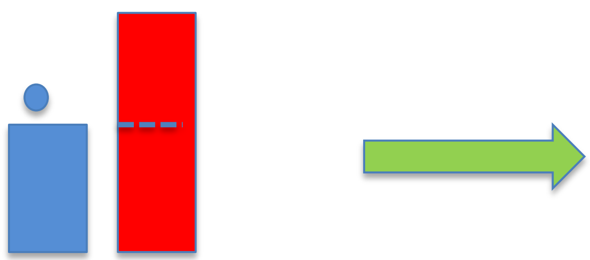


Group-theoretical Decomposition

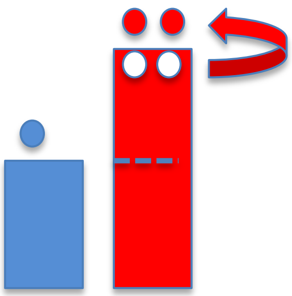
Symplectic Sp(3,R)

CASE STUDY: ^{29}F

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



One proton outside a filled shell
+ filled neutron shell

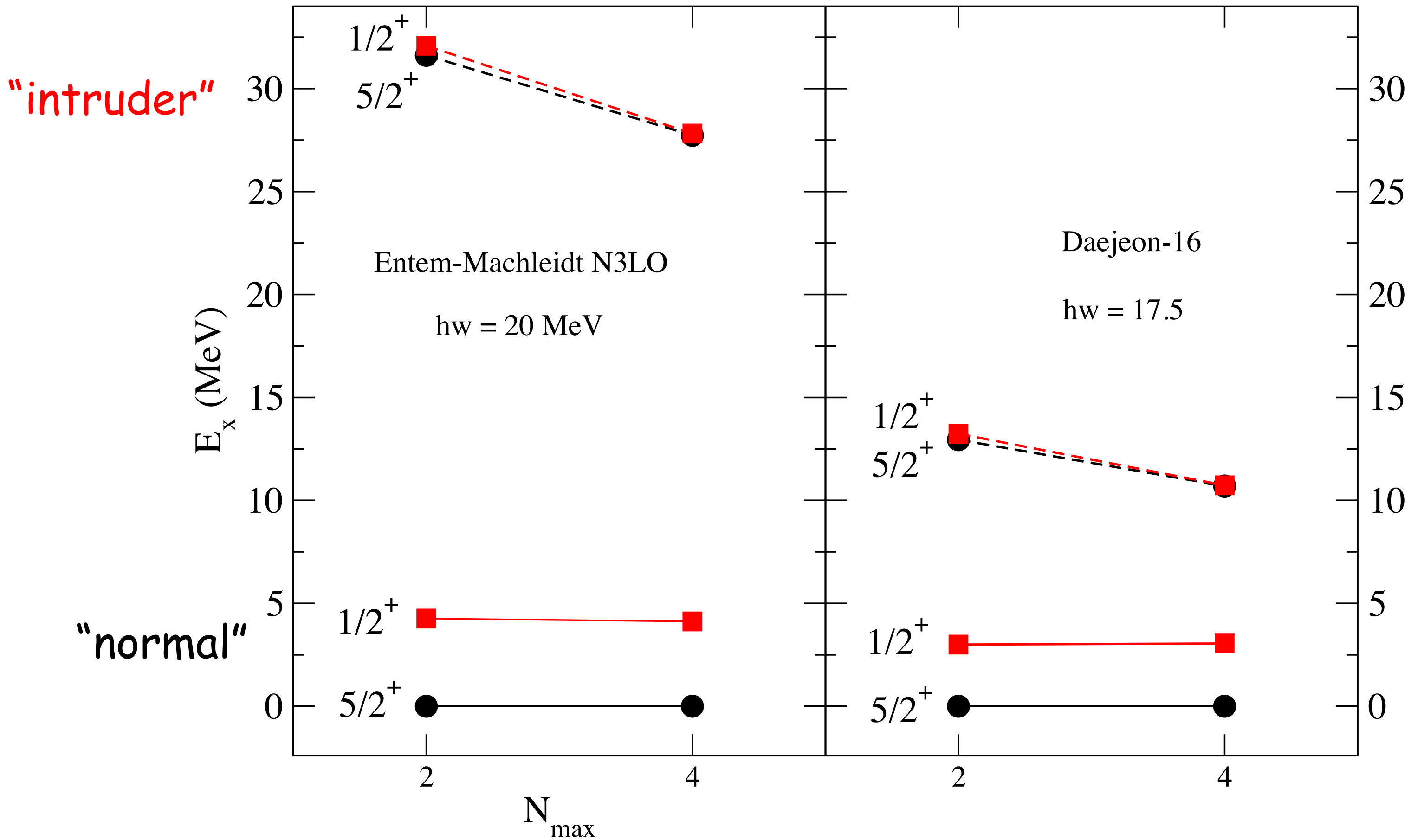


One proton outside a filled shell
+ neutron 2p-2h

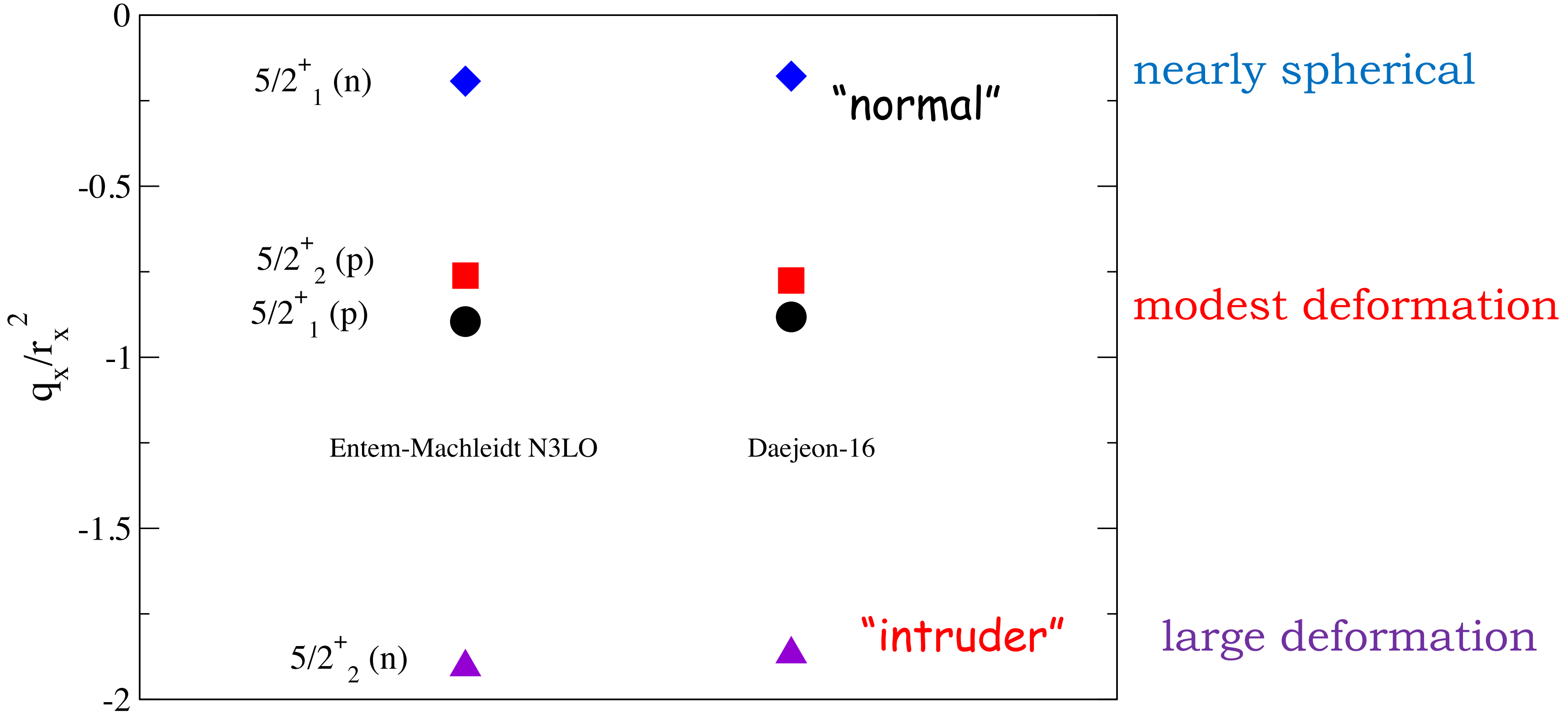
"island of inversion"

CASE STUDY: ^{29}F

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



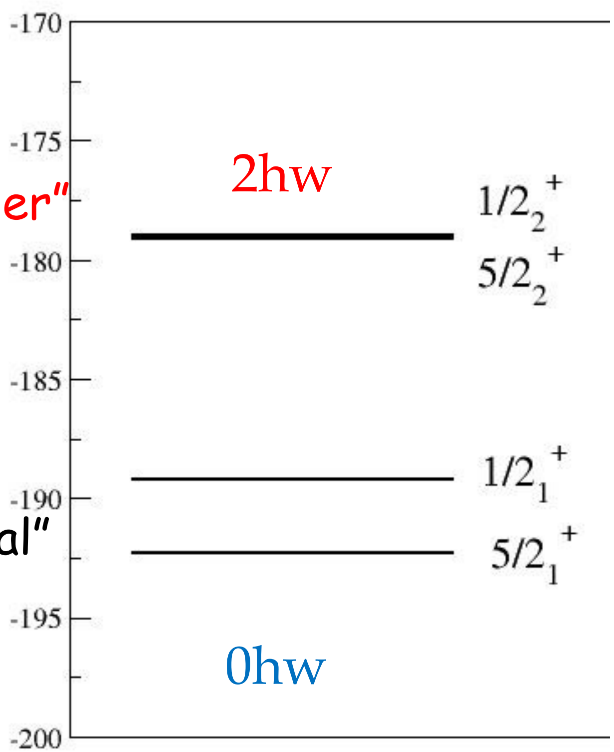
CASE STUDY: ^{29}F



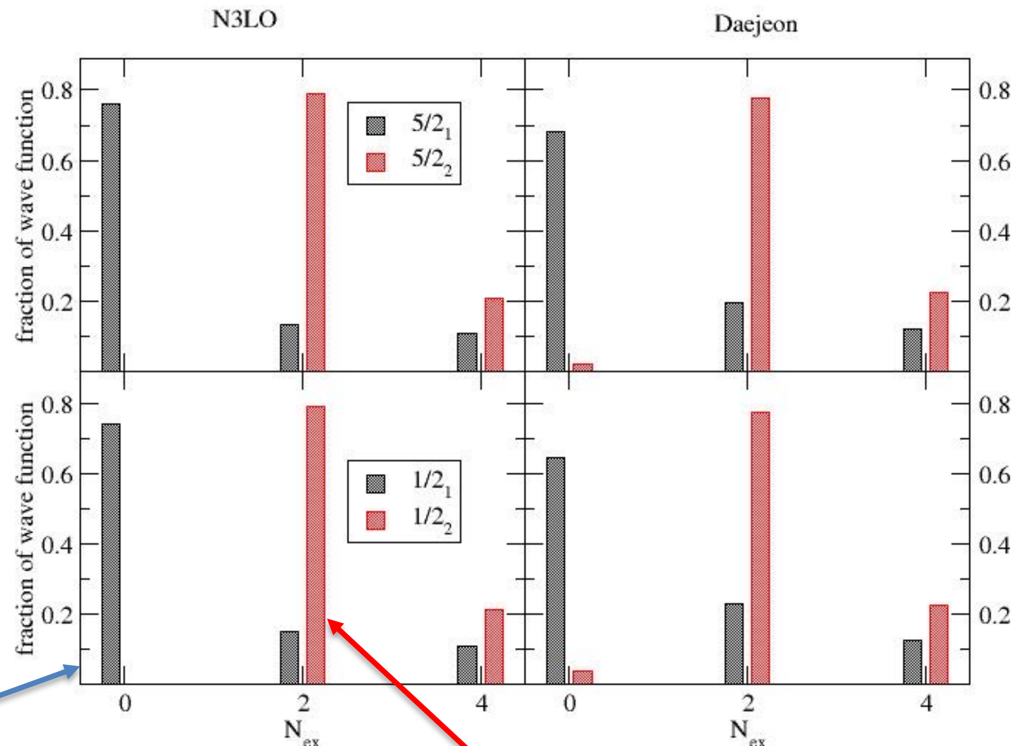
CASE STUDY: ^{29}F

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

“intruder”



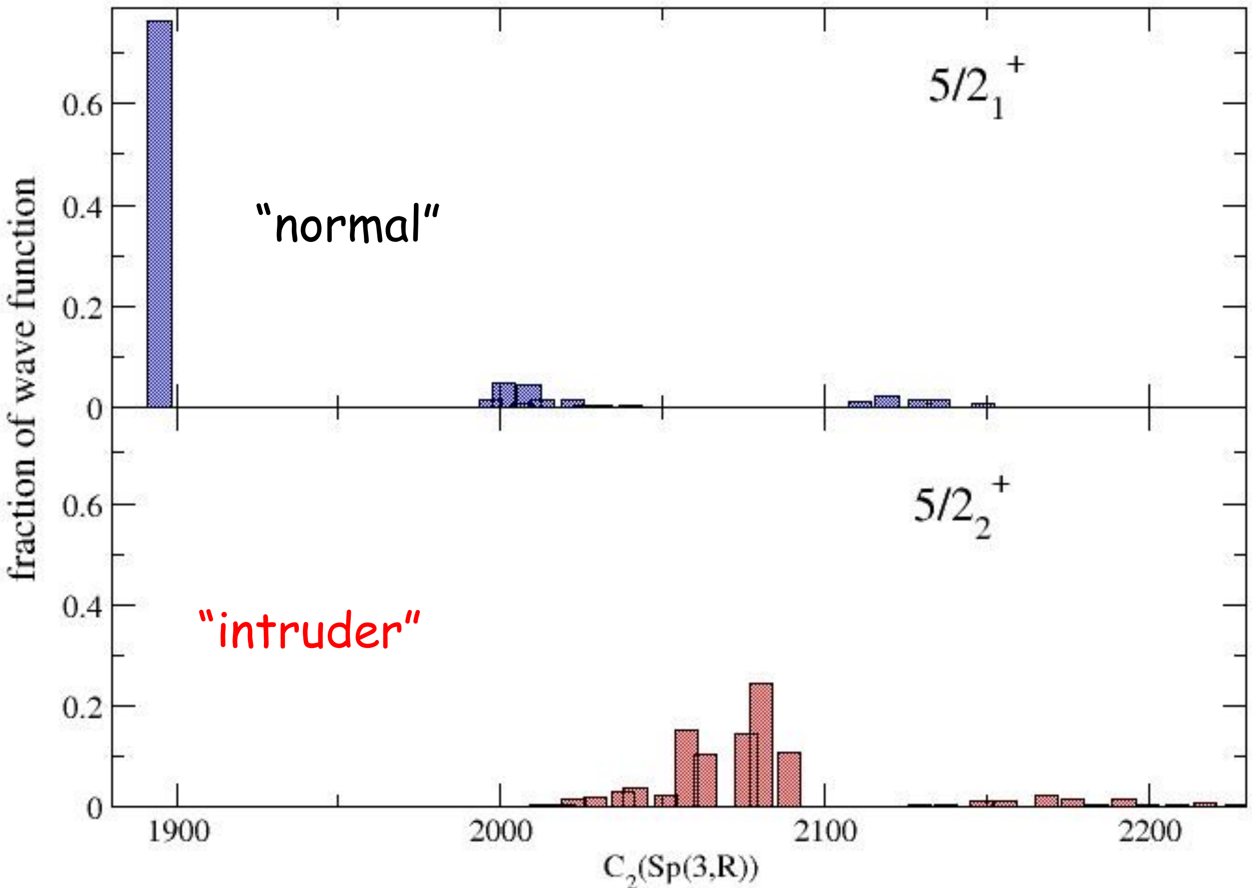
“normal”



“normal”

“intruder”

CASE STUDY: ^{29}F

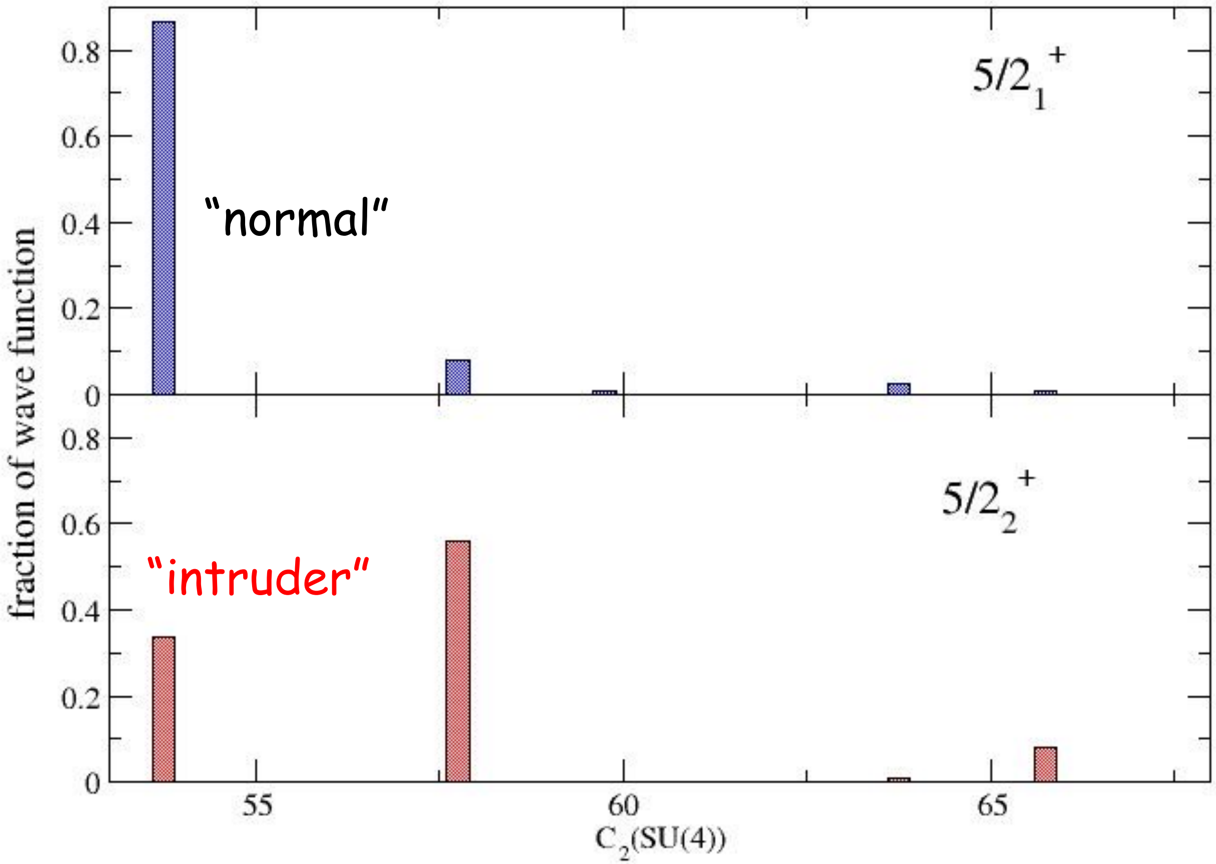


N_{max} = 4 (natural orbitals)

Group-theoretical Decomposition

Symplectic Sp(3,R)

CASE STUDY: ^{29}F

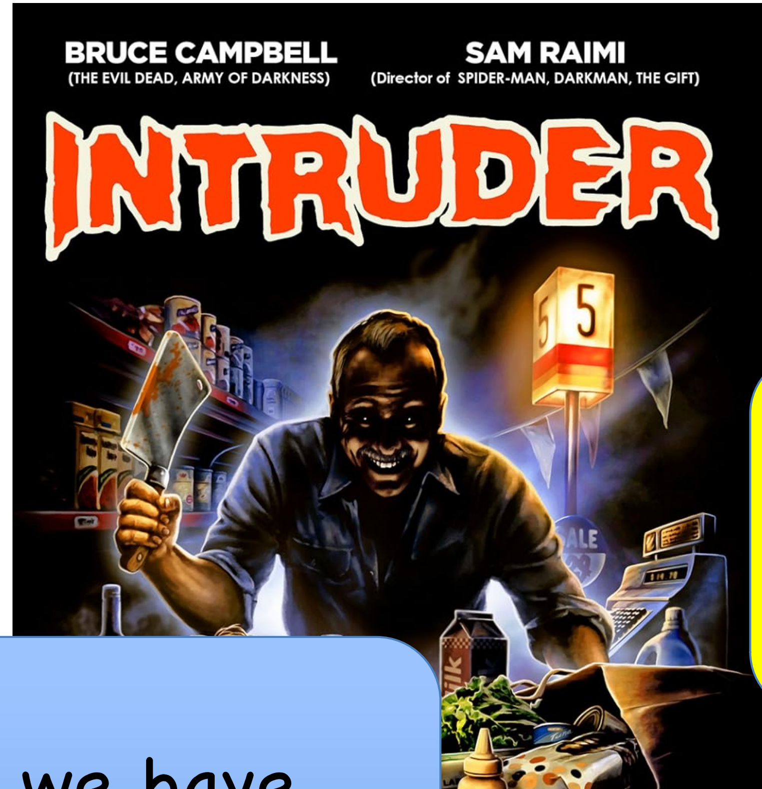


$N_{max} = 4$, natural orbitals

Group-theoretical decomposition

SU(4)

So basically we have intruders!



Yikes! Intruders are scary!

So basically we have intruders!

Summary

- Today we can perform huge configuration-interaction calculations, with billions of basis states—how do we understand all those numbers?

* We can turn to group theory to gain insight—even without understanding much group theory—and **see** band structure

- We can also use group decompositions to analyze the island of inversion, where we can see the states actually look quite 'simple'

- This suggests—without prior assumption—that group theory can indeed assist in tackling large problems.

Gracias!

Additional slides

for curious people

Some technical details

Casimir

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

For some wavefunction $| \Psi >$, we define the *fraction of the wavefunction in an irrep*

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

How are those decompositions calculated?

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For some wavefunction $|\Psi>$, we define the *fraction of the wavefunction in an irrep*

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

How are those decompositions calculated?

Naïve method: Solve eigenpair problems, e.g.

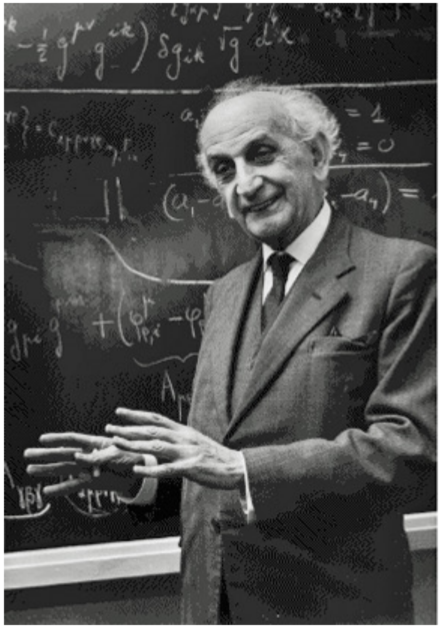
$$\mathbf{H} \mid \Psi_n > = E_n \mid \Psi_n >$$

and

$$\mathbf{L}^2 \mid l; \alpha > = l(l+1) \mid l; \alpha >$$

…and then take overlaps, $|< l; \alpha \mid \Psi_n >|^2$

PROBLEM: the spectrum of $\mathbf{L}^2$ is highly degenerate (labeled by α);
Need to sum over all α not orthogonal to $\mid \Psi_n >$!



$$\mathbf{A}\vec{v}_1 = \alpha_1\vec{v}_1 + \beta_1\vec{v}_2$$

$$\mathbf{A}\vec{v}_2 = \beta_1\vec{v}_1 + \alpha_2\vec{v}_2 + \beta_2\vec{v}_3$$

$$\mathbf{A}\vec{v}_3 = \beta_2\vec{v}_2 + \alpha_3\vec{v}_3 + \beta_3\vec{v}_4$$

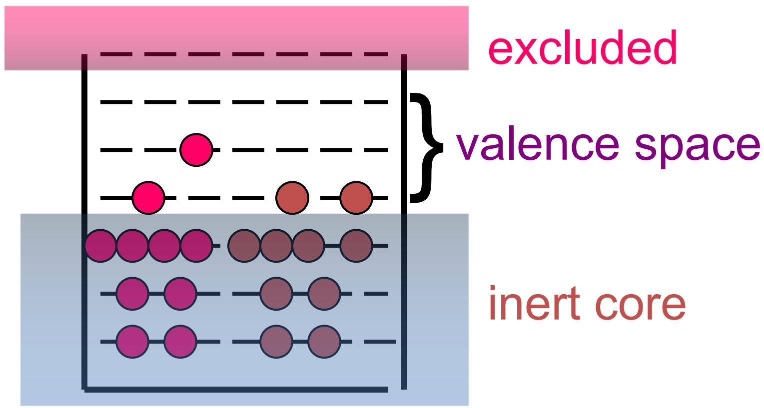
$$\mathbf{A}\vec{v}_4 = \beta_3\vec{v}_3 + \alpha_4\vec{v}_4 + \beta_4\vec{v}_5$$

Starting from some initial vector (the "pivot") v_1 , the Lanczos algorithm iteratively creates a new basis (a "Krylov space") in which to diagonalize the matrix **A**.

Eigenvectors are then expressed as a linear combination of the "Lanczos vectors": $|\psi\rangle = c_1 |v_1\rangle + c_2 |v_2\rangle + c_3 |v_3\rangle + \ldots$

There are roughly two kinds of shell model calculations

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



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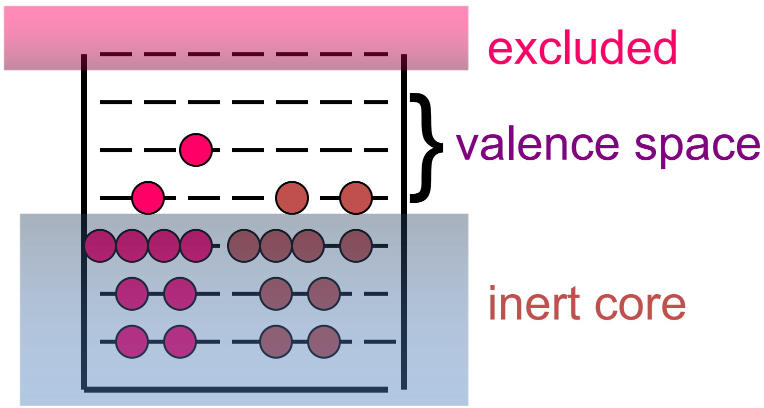
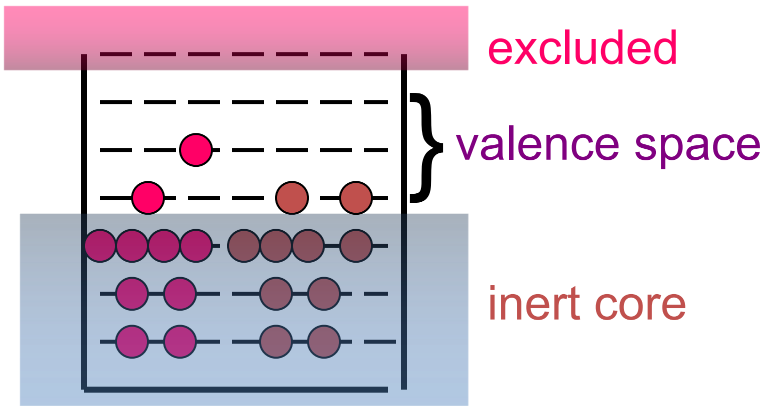


The interactions are fit to many-body spectra (e.g., to nuclear spectra between oxygen and calcium...)

Such interactions, however, are limited to a specific model space (e.g., the *sd* shell)



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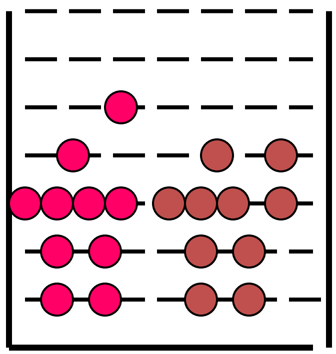
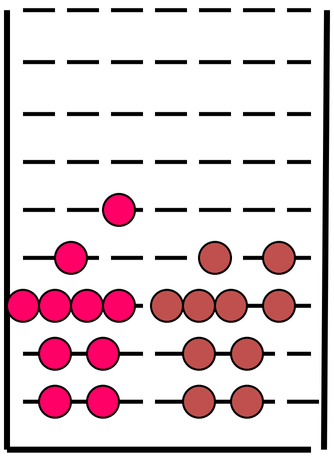


"No-core" shell model (NCSM) calculations do not have a fixed space

Instead they take the limit as the model space is increased



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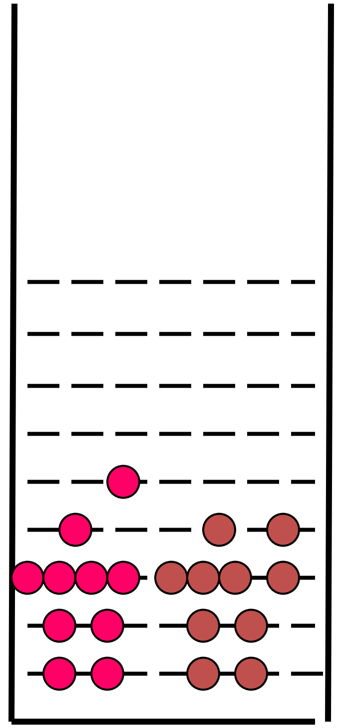

Instead they take the limit as the model space is increased

"No-core" shell model (NCSM) calculations do not have a fixed space

The interaction is calculated from an *ab initio* theory, such as chiral effective field theory

Nuclear force from, e.g., EFT breaking chiral symmetry

$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)\right)\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots) = E\Psi$$