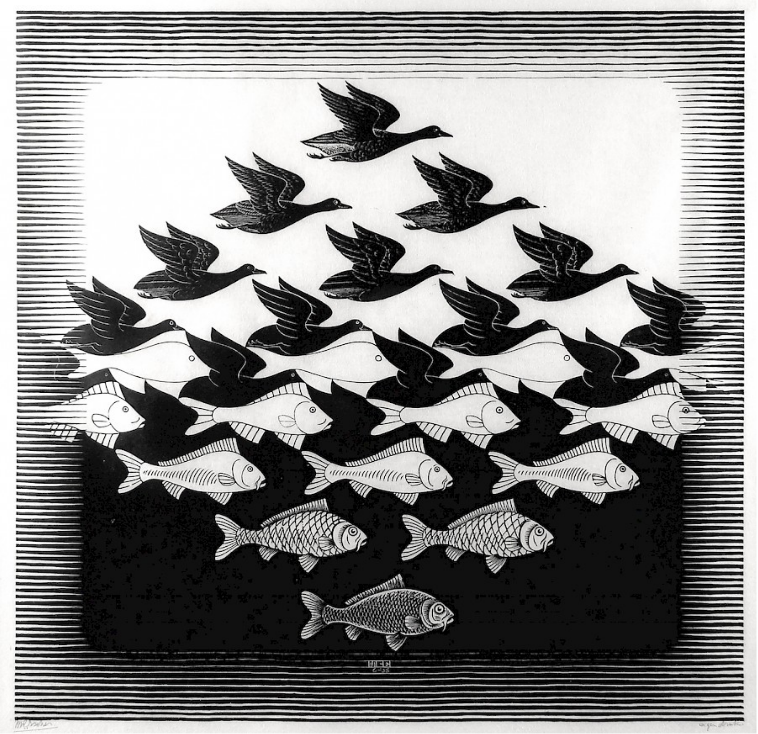
Adventures in Quasi-Dynamical Symmetries:

through the transformative lens of the similarity renormalization group



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-FG02-96ER40985"

Simplicity, Symmetry, and Beauty in Nuclei/ Shanghai / Sept 2018

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Our theme:

"Simplicity, symmetry, and beauty...
... in atomic nuclei"

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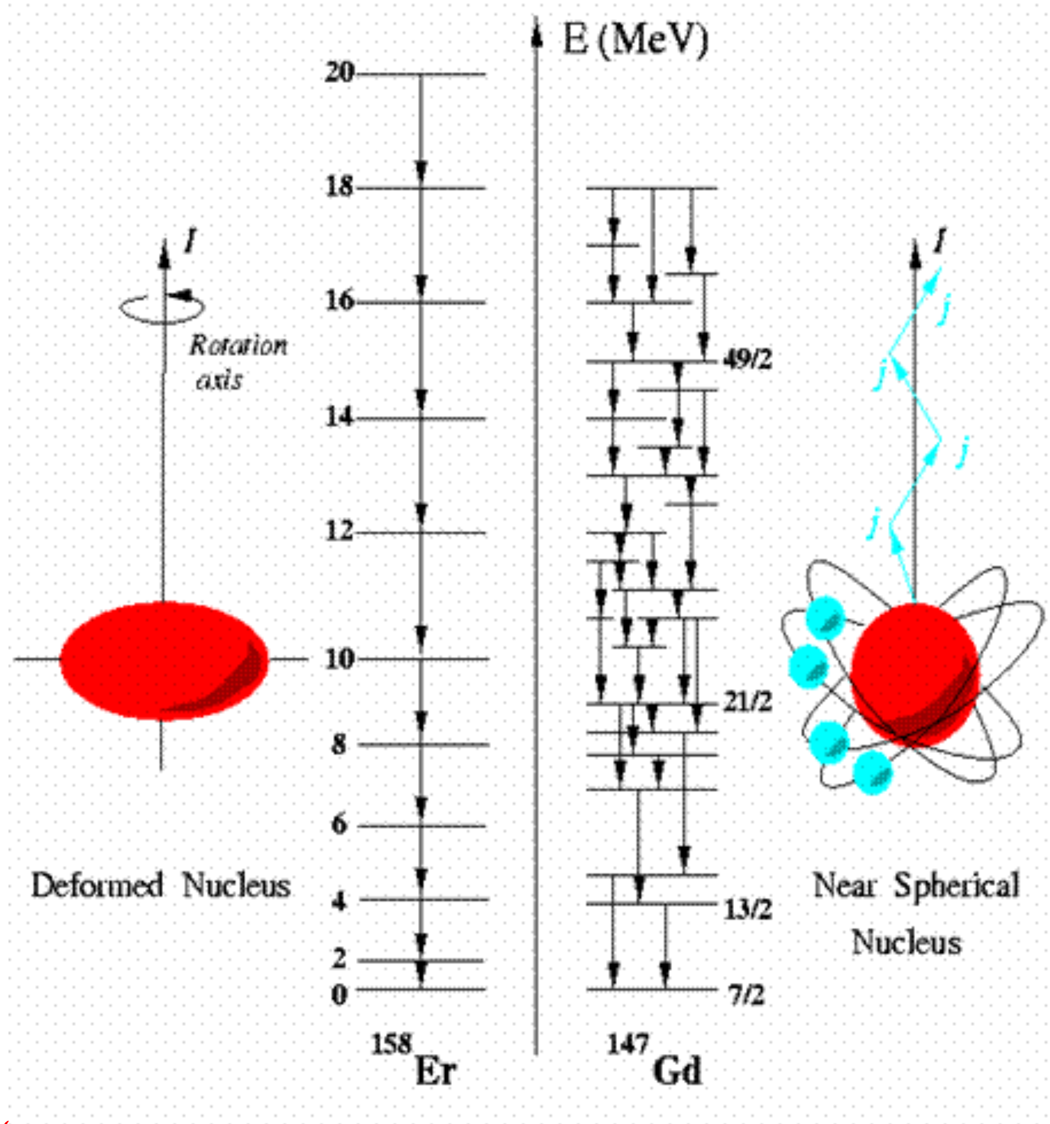
Nuclear spectra often
show remarkable **simplicity**



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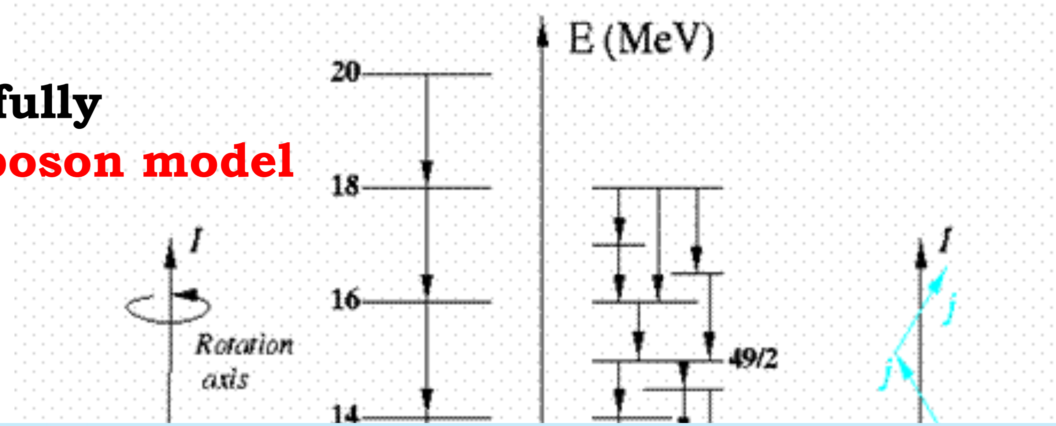
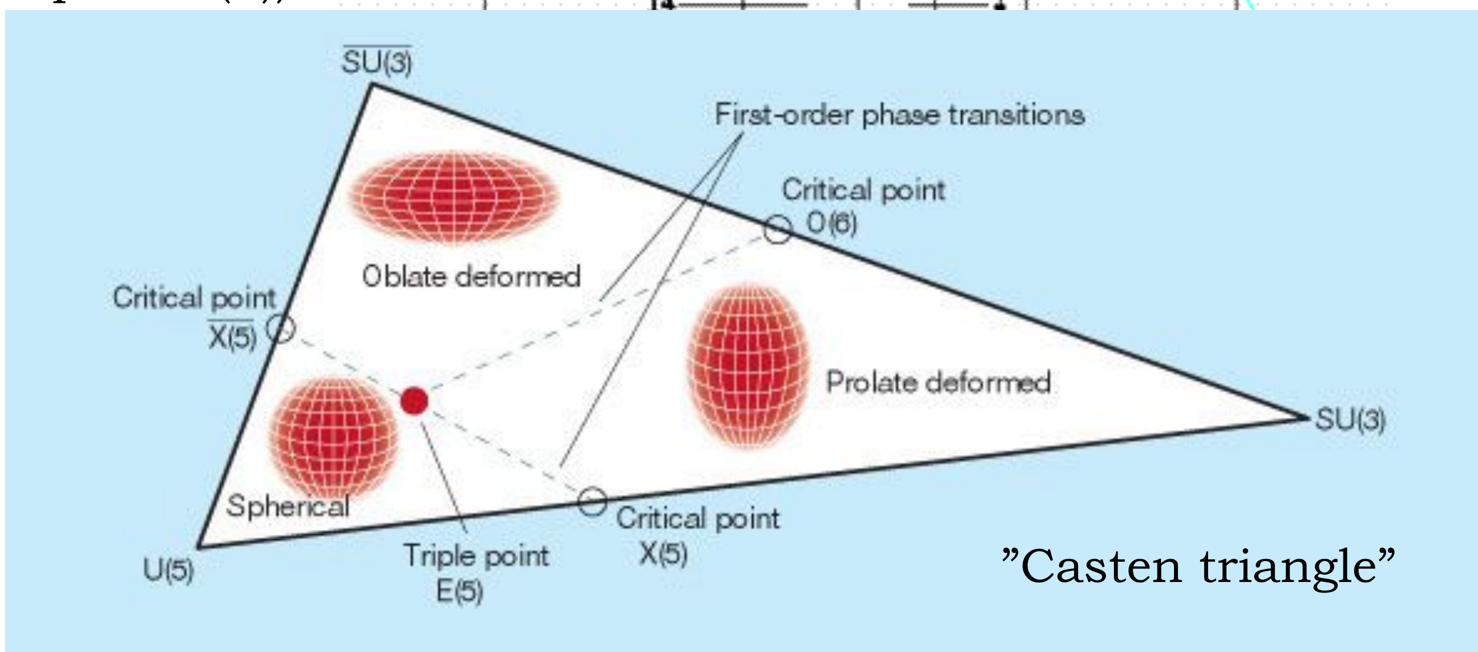
Nuclear spectra often show remarkable **simplicity**

These simplicities are **beautifully** modeled by the **interacting boson model**

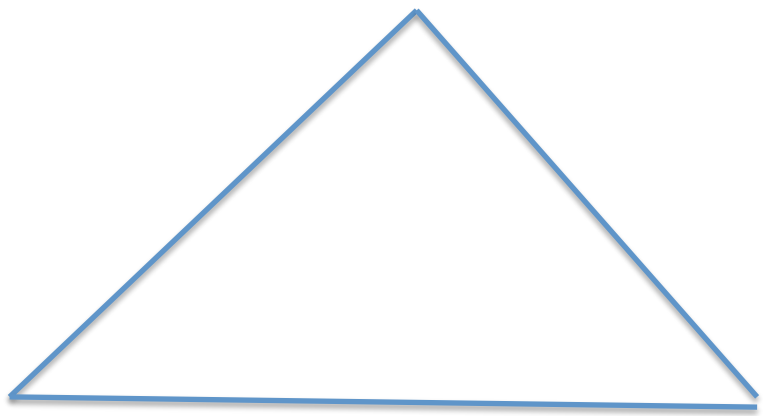
Each corner represents an exact **symmetry** group (each are subgroups of U(6))





"Casten triangle"

This talk has its own triangle:



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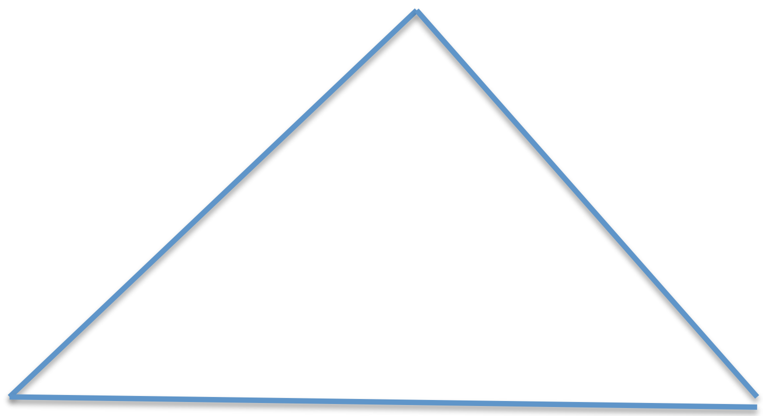
This talk has its own triangle:

Decomposing shell model
wave functions by group irreps
-> *quasi-dynamical symmetries*



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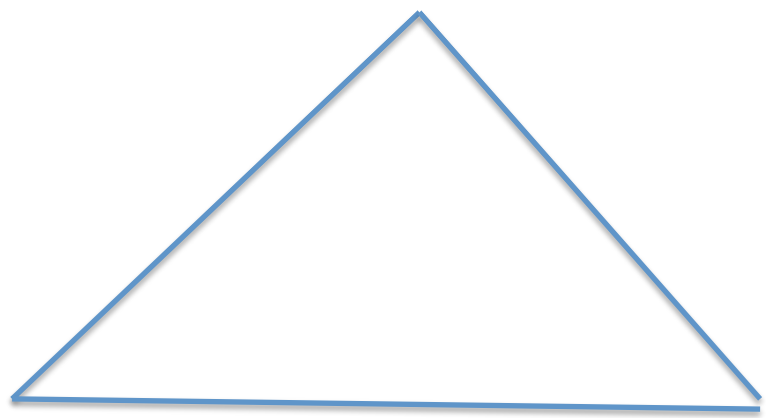

SRG: the similarity
renormalization group:
-> *unitary*
transformations back
to ***dynamical*** *symmetry*

This talk has its own triangle:

Decomposing shell model
wave functions by group irreps
-> *quasi-dynamical symmetries*

Spectral distribution theory, a metric on the space of Hamiltonians
-> *a new way to look at SRG and a new SRG*

SRG: the similarity renormalization group:
-> *unitary transformations back to* ***dynamical*** *symmetry*

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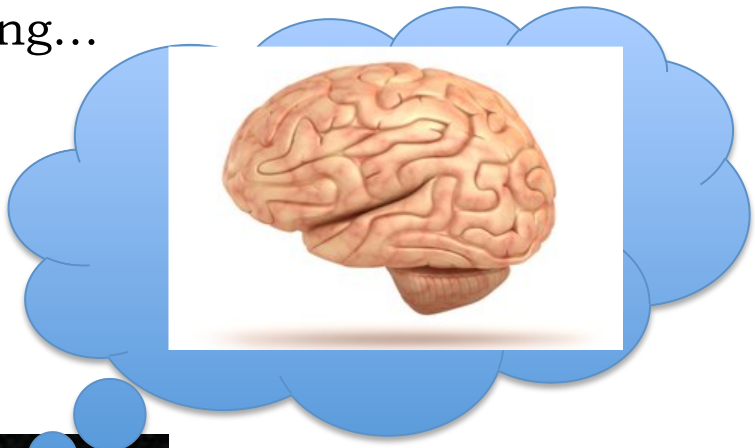
While the interacting boson model and similar **beautiful** and **simple** models can describe a lot of nuclear data

today we have moved away from thinking…



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While the interacting boson model and similar **beautiful** and **simple** models can describe a lot of nuclear data

…to supercomputing!

today we have moved away from thinking…

For example….

In configuration-interaction method
(a.k.a. shell model diagonalization):

we use the matrix formalism

Maria Mayer

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

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

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

For example....

In configuration-interaction method (a.k.a. shell model diagonalization):

we use the matrix formalism


Maria Mayer

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

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

Largest (?) known M-scheme calculation
^{6}Li, N_{max}=22, **25 billion basis states**
(Forssen *et al*, arXiv:1712.09951 with pANTOINE)

For example

In configurati

(a.k.a. shell m

w

"The purpose of computing is insight, not numbers"
--Richard Hamming

$\mathbf{H}$

$c_\alpha |\alpha\rangle$

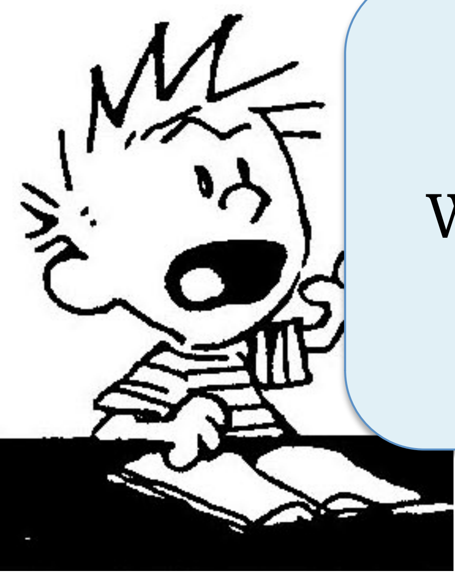
$$H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} | \beta \rangle$$

Largest (?) known M-scheme calculation
^{6}Li, N_{max}=22, **25 billion basis states**
(Forssen *et al*, arXiv:1712.09951 with pANTOINE)

FOR EXAMPLE

In configurati
(a.k.a. shell m
w

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



We can use group theory!

Largest (?) known M-scheme cal
^{6}Li, N_{max}=22, **25 billion basis s**
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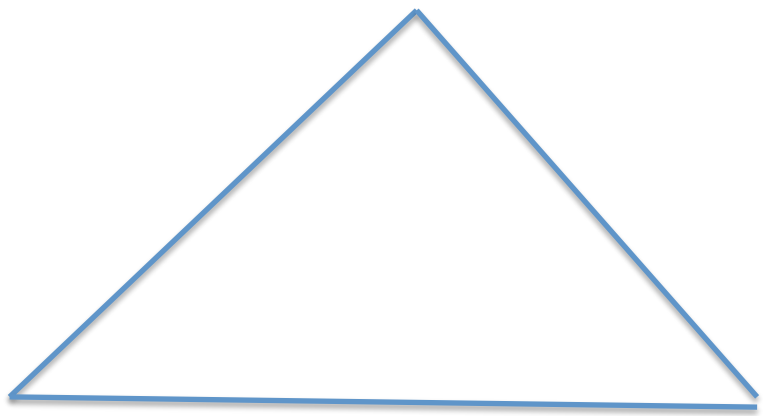
Decomposing shell model wave functions by group irreps -> *quasi-dynamical symmetries*



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

Casimir

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

In particular, 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*)

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Casimir

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

In particular, if the Casimir(s) commute(s) with the Hamiltonian,

$$\left[\hat{H},\hat{C}\right]=0$$

This is known as *dynamical symmetry*

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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*

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

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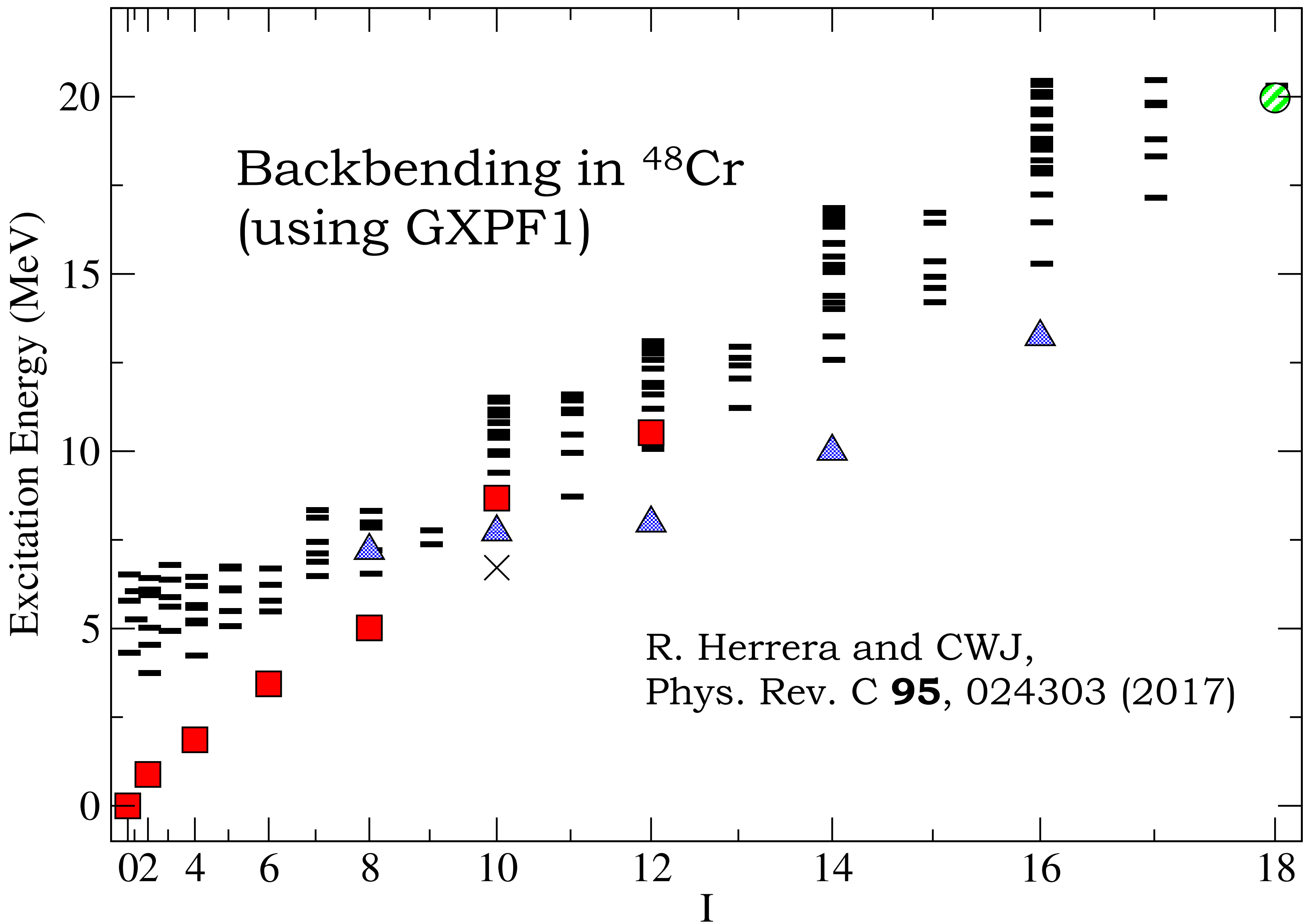
Casimir

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

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

For ... he
the ... *irrep*

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

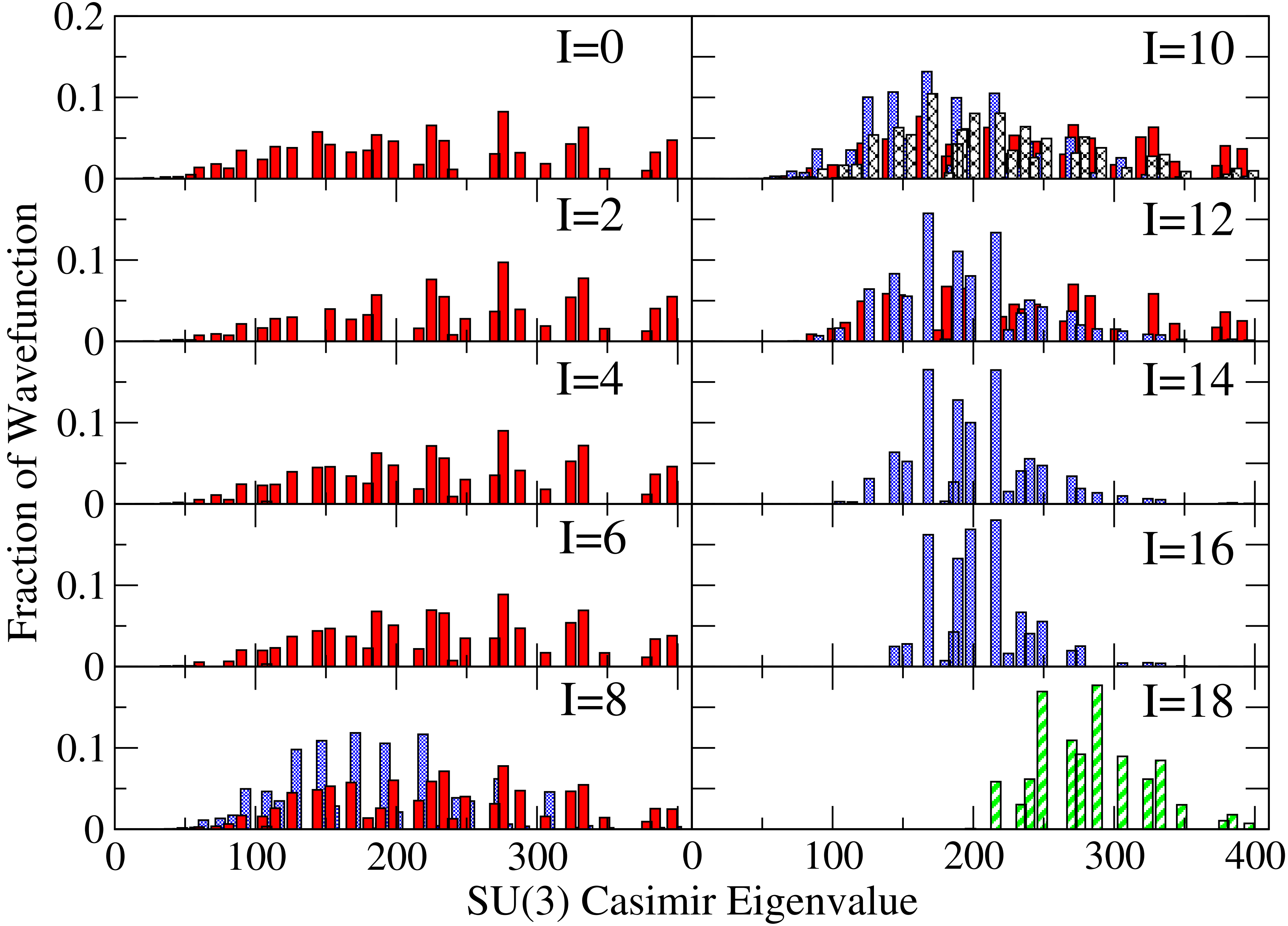

Backbending in ^{48}Cr
(using GXPF1)
R. Herrera and CWJ,
Phys. Rev. C **95**, 024303 (2017)
Excitation Energy (MeV)
I
0
5
10
15
20
02
4
6
8
10
12
14
16
18

Backbending in ^{48}Cr (using GXPF1)

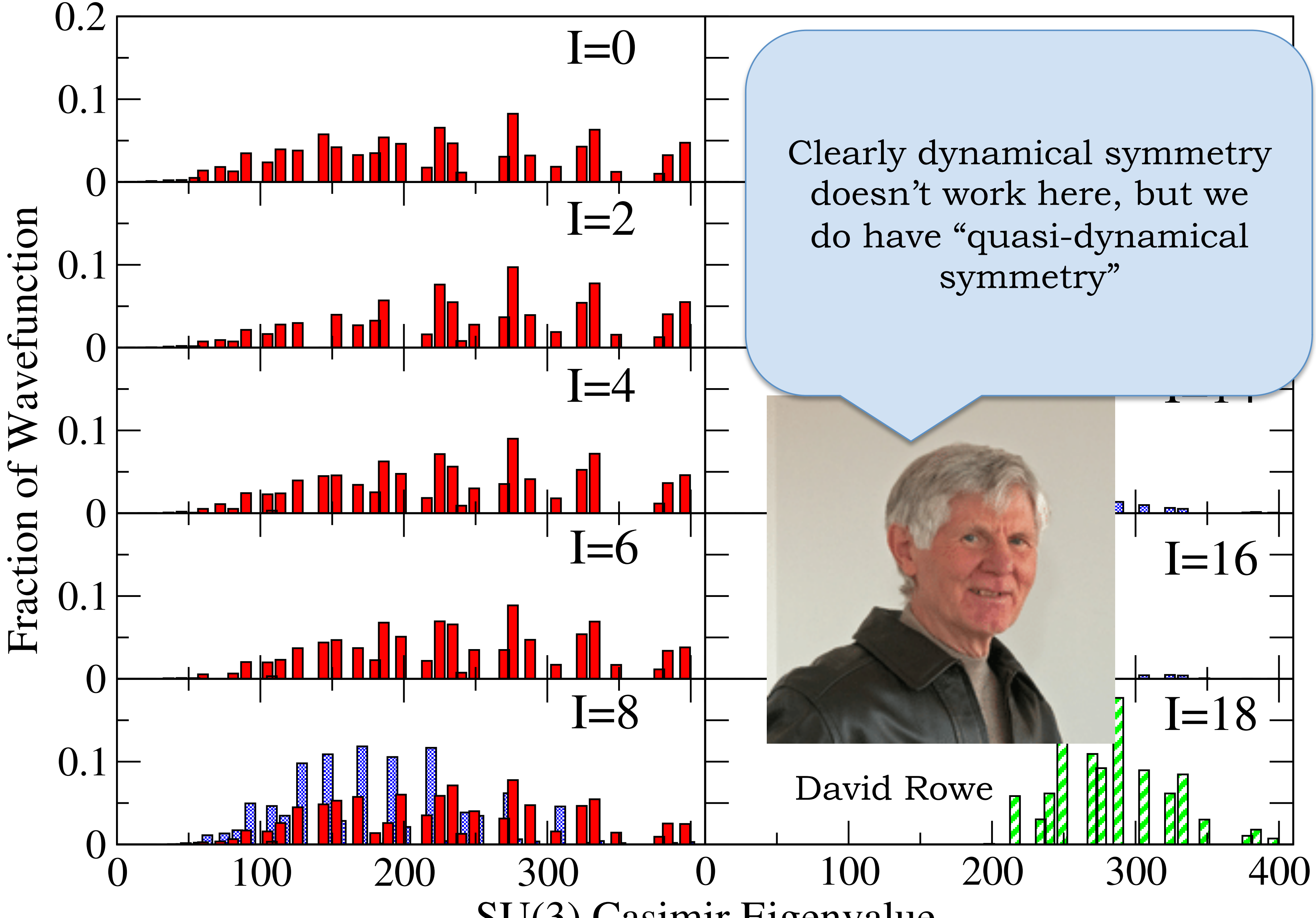
Wave functions computed in interacting shell model* using GXPF1 interaction; then SU(3) 2-body Casimir read in and decomposition done with Lanczos

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

*BIGSTICK shell model code: github/cwjsdsu/BigstickPublick
CWJ, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761-2774 (2013)
CWJ, Ormand, McElvain, and Shan arXiv:1801:08432

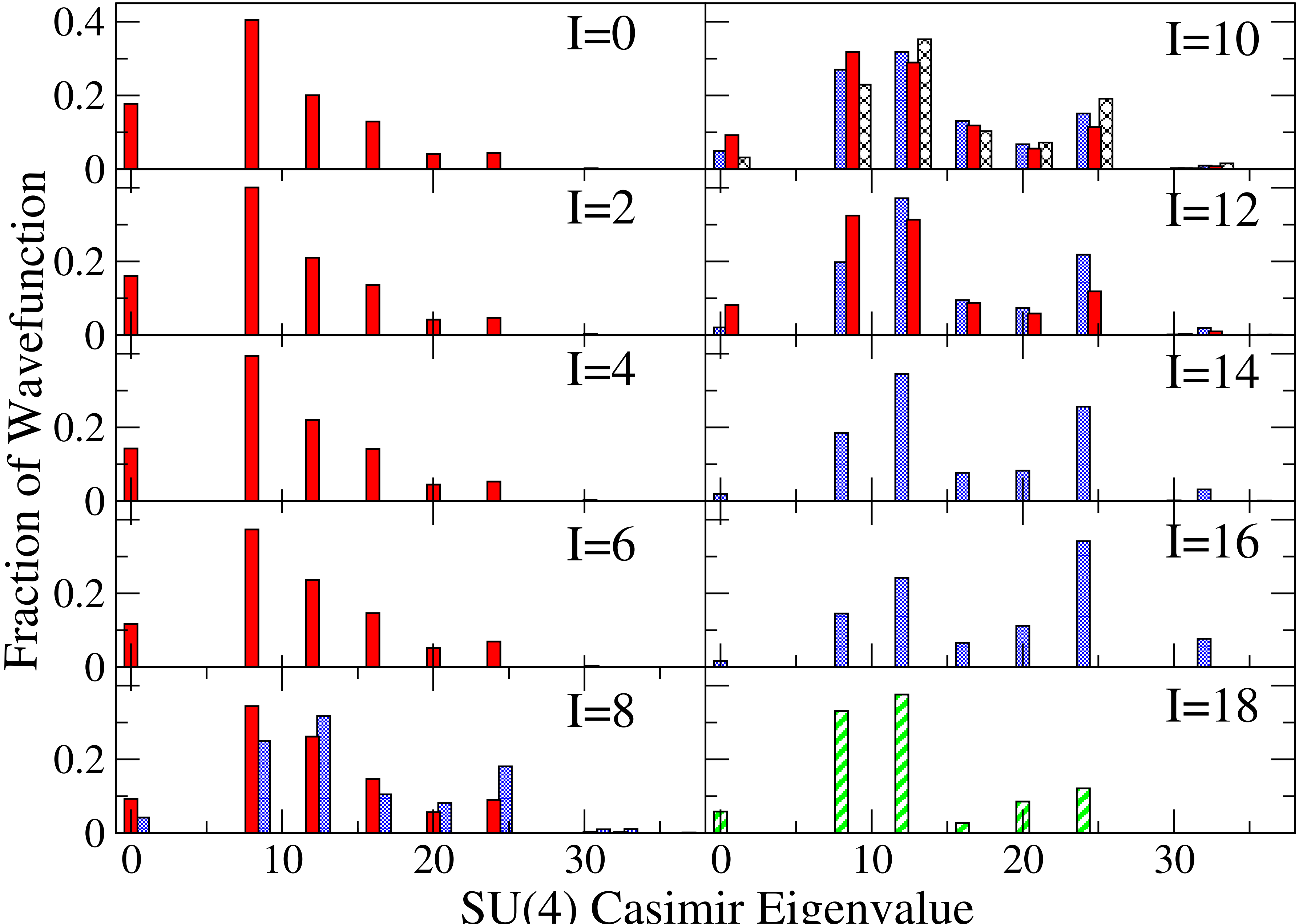


I=0
I=2
I=4
I=6
I=8
I=10
I=12
I=14
I=16
I=18
0.2
0.1
0
0
100
200
300
400
Fraction of Wavefunction
SU(3) Casimir Eigenvalue


Fraction of Wavefunction
0.2
0.1
0
I=0
I=2
I=4
I=6
I=8
I=16
I=18
0
100
200
300
400
SU(3) Casimir Eigenvalue
Clearly dynamical symmetry doesn't work here, but we do have "quasi-dynamical symmetry"
David Rowe

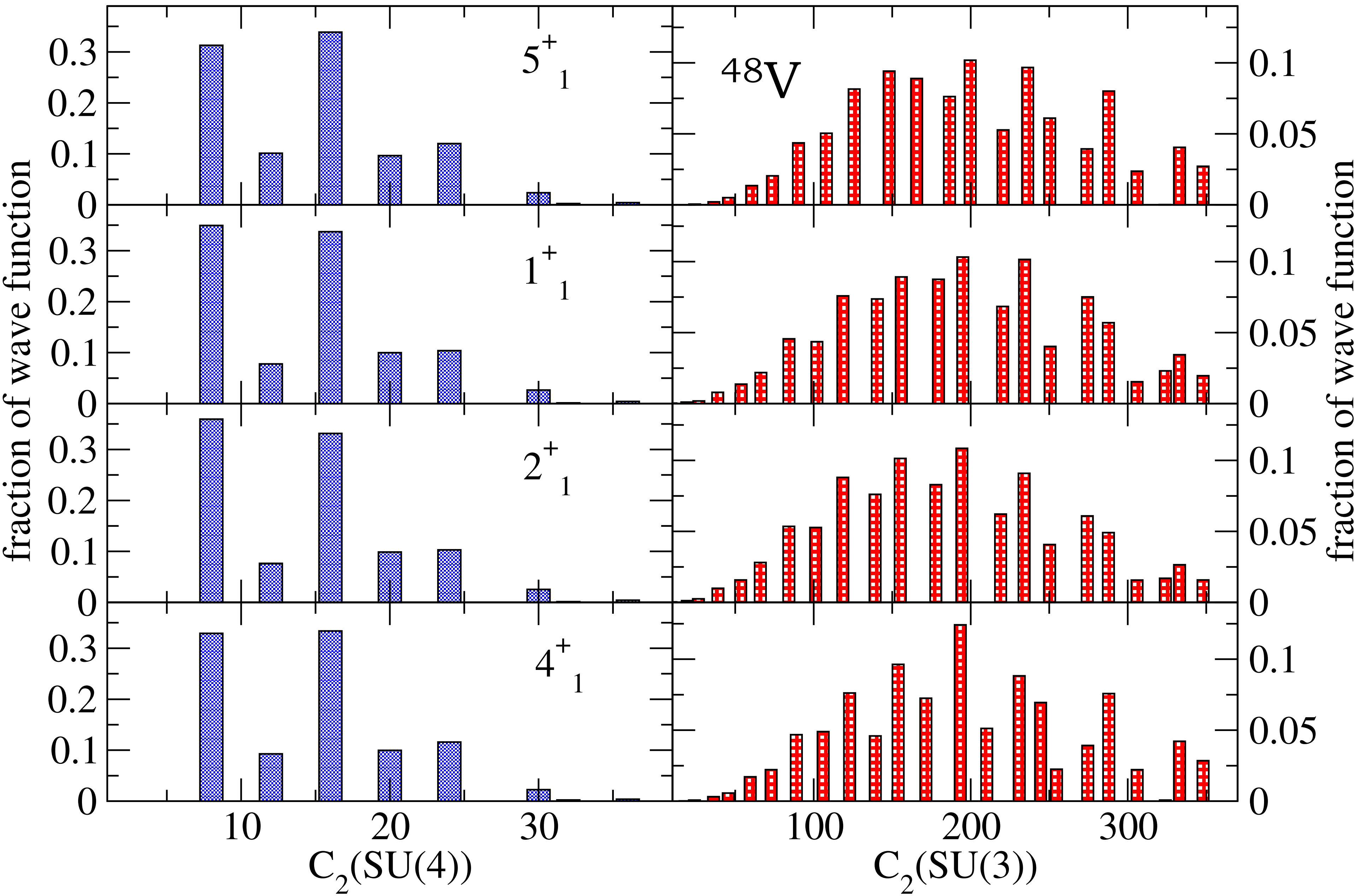
What about other groups?

Eugene Wigner

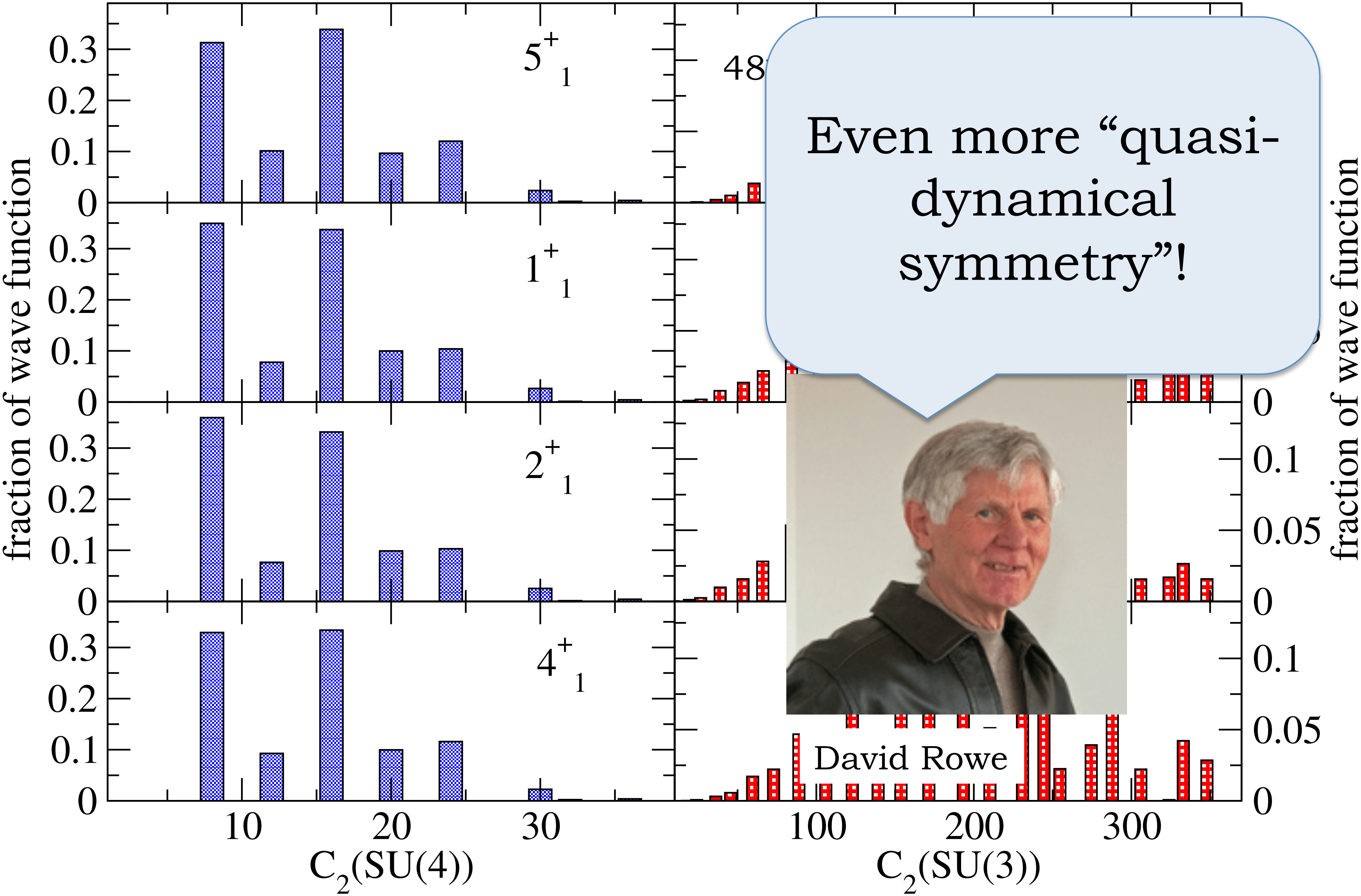

Fraction of Wavefunction
0.4
0.2
0
I=0
I=2
I=4
I=6
I=8
I=10
I=12
I=14
I=16
I=18
0
10
20
30
SU(4) Casimir Eigenvalue

What about non-rotational nuclei?

Eugene Wigner



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



fraction of wave function
0.3
0.2
0.1
0
5+ 1
1+ 1
2+ 1
4+ 1
10
20
30
C2(SU(4))
100
200
300
C2(SU(3))
0.1
0.05
fraction of wave function
Even more “quasi-dynamical symmetry”!
David Rowe

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Is there some way to turn a *quasi*-dynamical symmetry into a *dynamical* symmetry? Like a unitary transformation?

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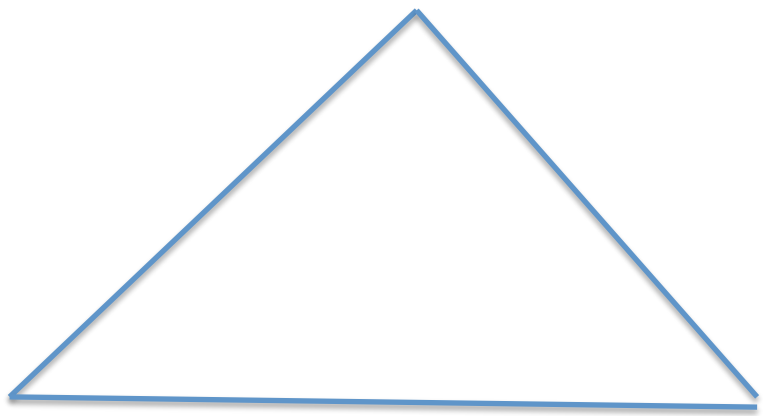
Decomposing shell model
wave functions by group irreps
-> *quasi-dynamical symmetries*



SRG: the similarity
renormalization group:
-> *unitary transformations back to **dynamical** symmetry*

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Is there some way to turn a *quasi*-dynamical symmetry into a *dynamical* symmetry? Like a unitary transformation?

Sure! Why not use the *similarity renormalization group (SRG)?*

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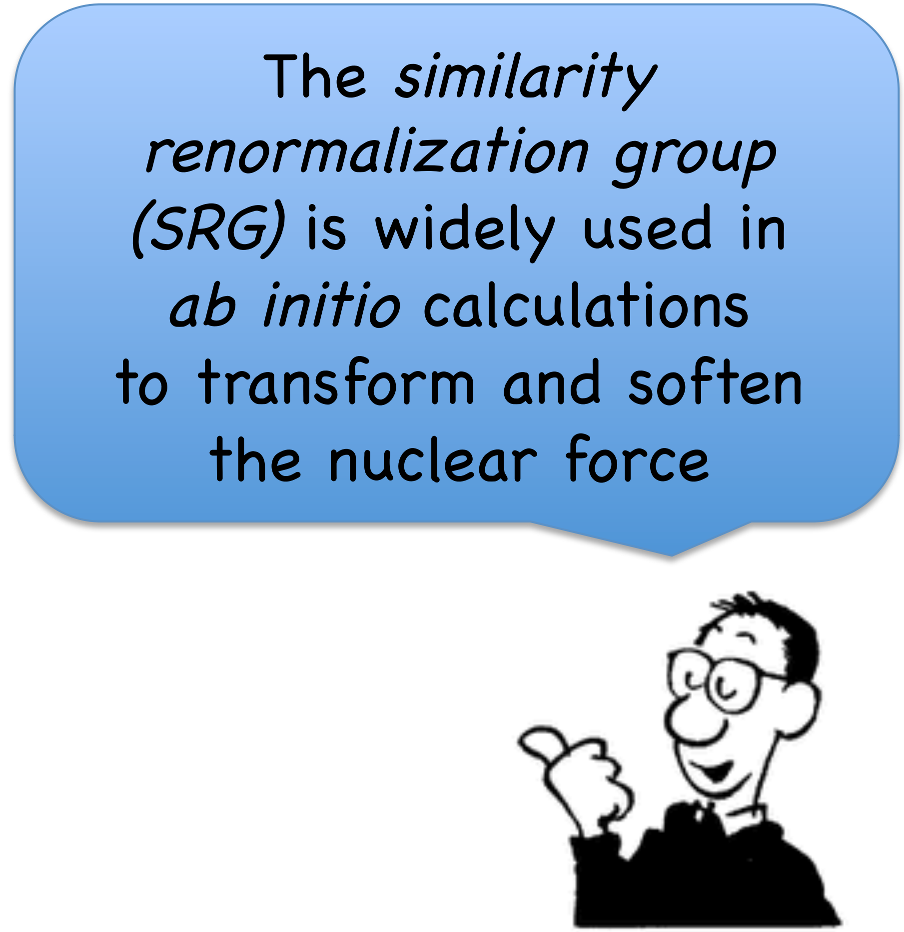

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$$H(s) = U(s)H(0)U^{\dagger}(s)$$

$$U(s) = e^{\eta}$$

$$\frac{dH(s)}{ds} = \left[\eta, H(s)\right]$$

The *similarity renormalization group (SRG)* is widely used in *ab initio* calculations to transform and soften the nuclear force

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$$H(s) = U(s) H(0) U^{\dagger}(s)$$

$$U(s) = e^{\eta}$$

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Typically, η = [G,H]
where G is the *generator* .
SRG drives H(s) to be “more like” G.
(More on this soon).

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Typically, η = [G,H]
where G is the *generator* .
SRG drives H(s) to be "more like" G.
(More on this soon).

A common choice is the kinetic energy,
but I'll use the SU(3) Casimir operator

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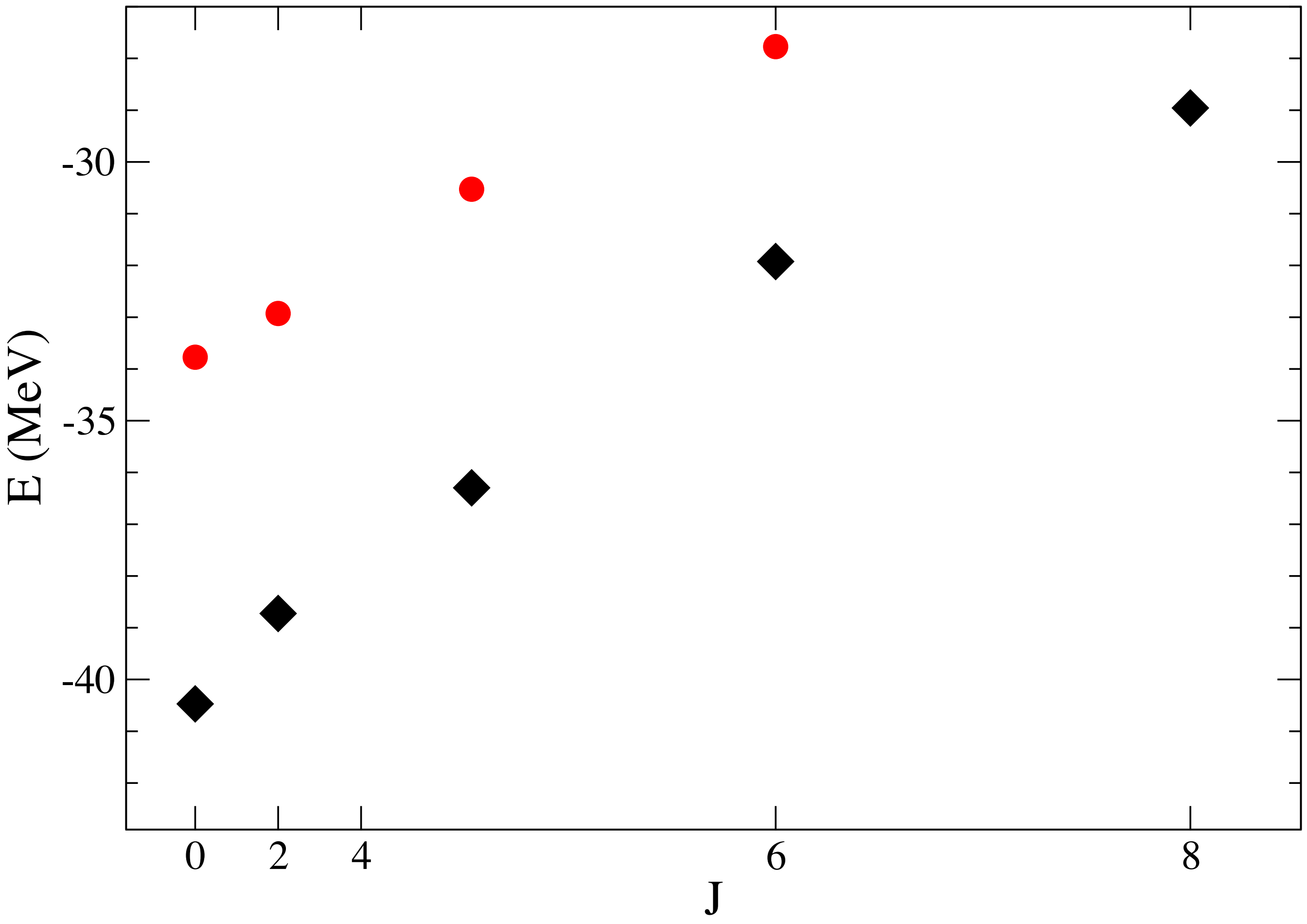

^{20}Ne

USDB interaction

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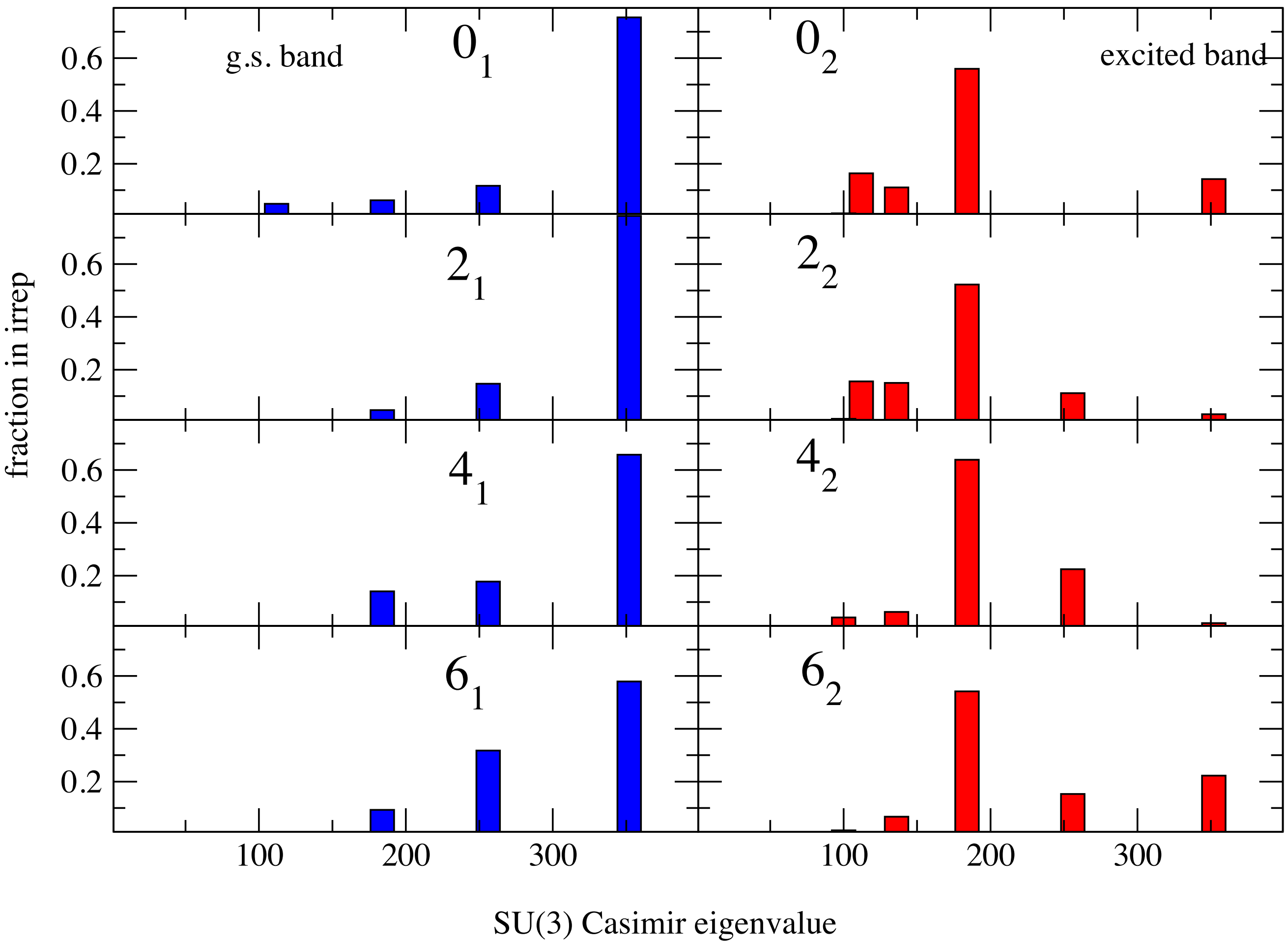

^{20}Ne

USDB interaction

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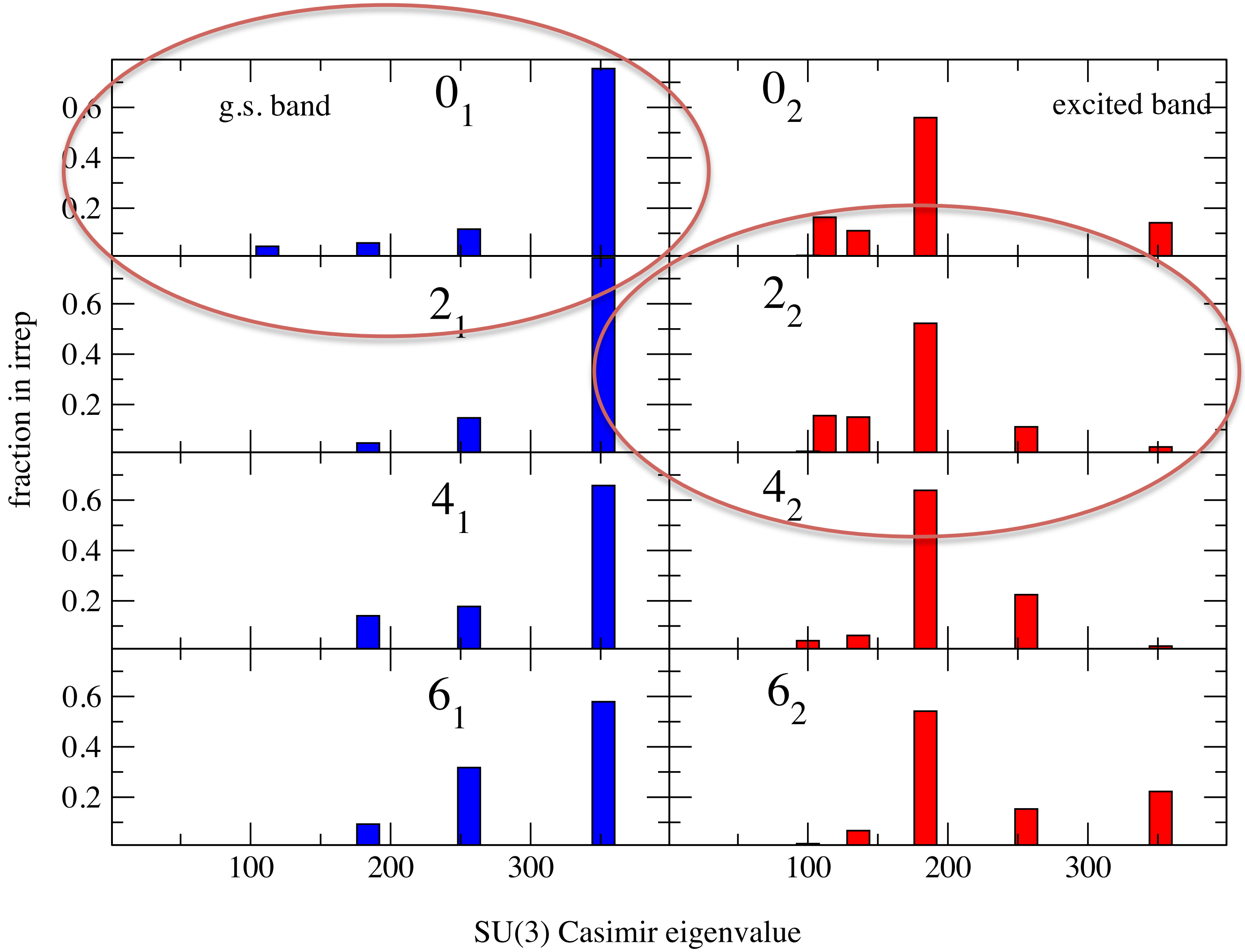

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USDB interaction

dimension = 640

$$\frac{dH(s)}{ds} = \left[\left[G, H(s)\right], H(s)\right]$$

G = SU(3) Casimir operator

Calculations done on the many-body matrix directly

I transform **H** and diagonalize, but decompose using the untransformed Casimir.

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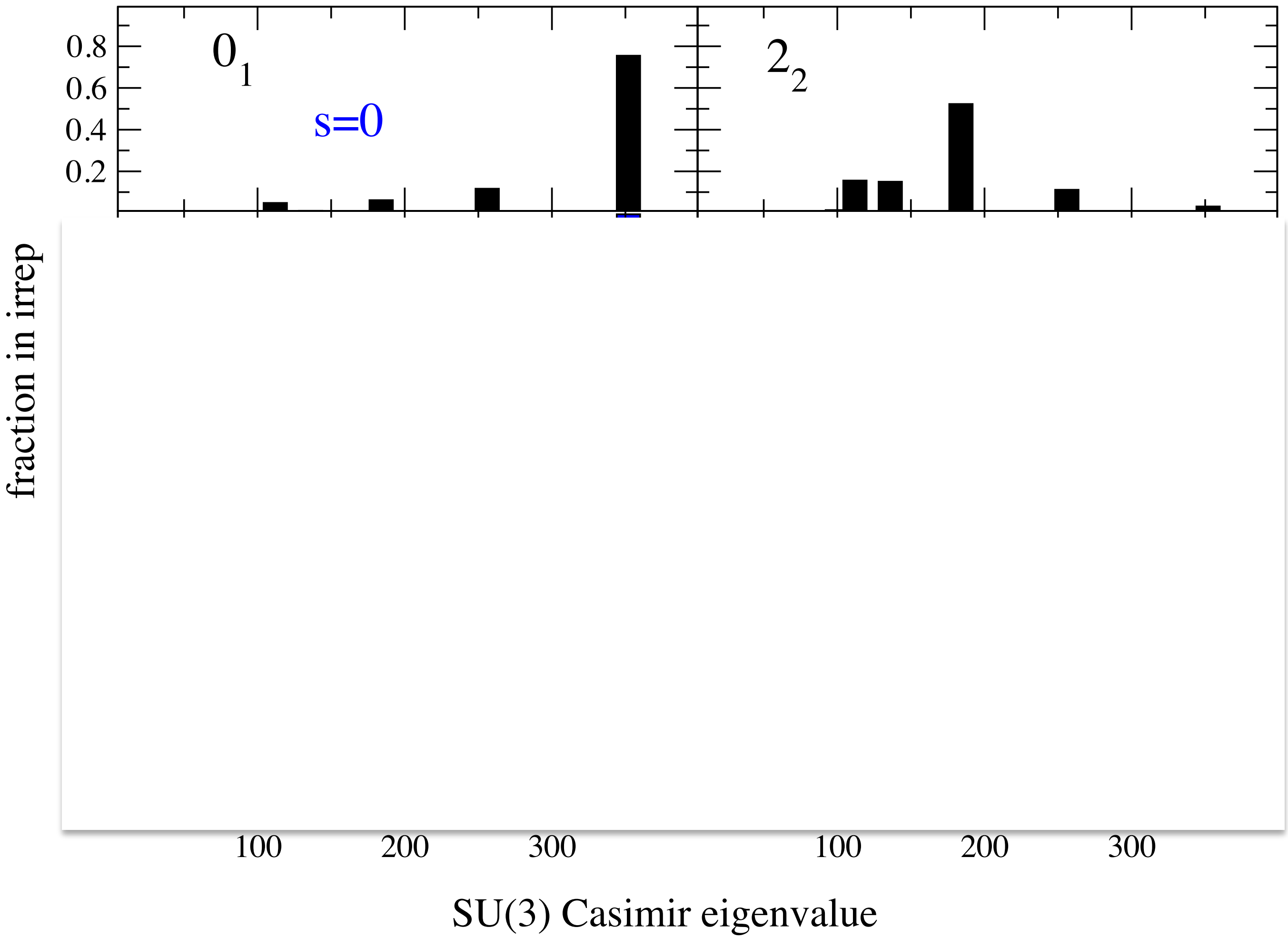

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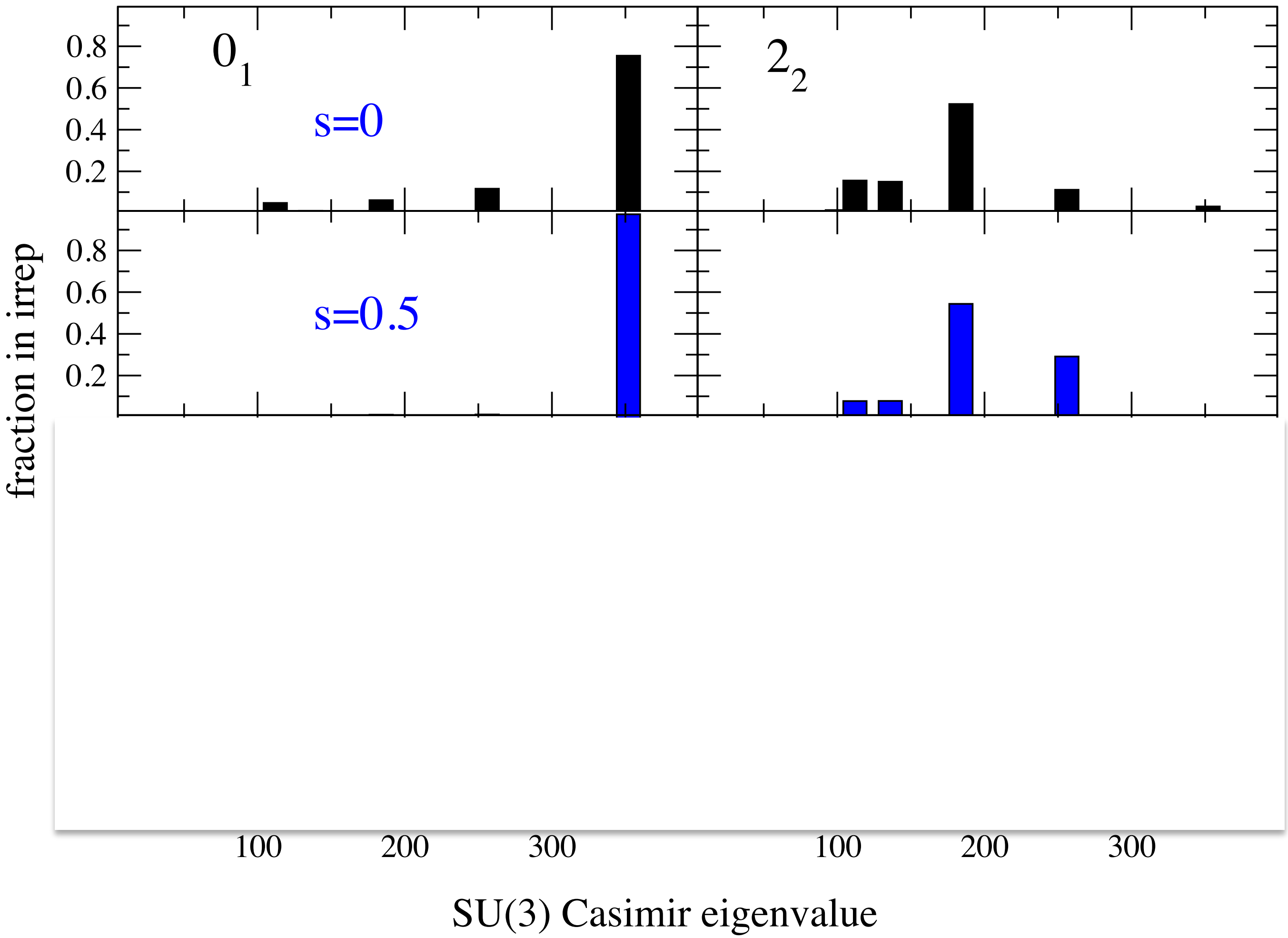

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USDB interaction

Increasing evolution

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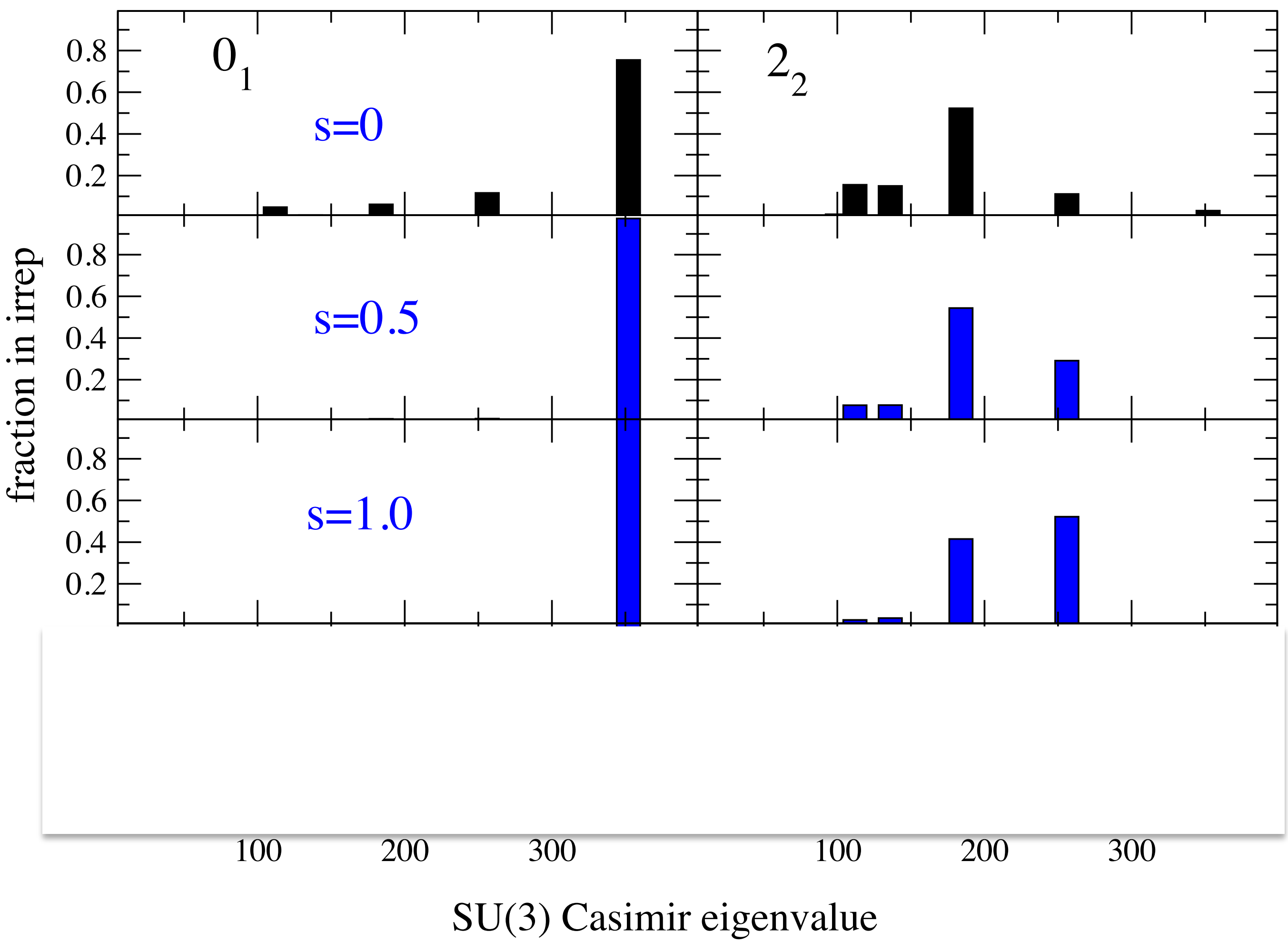

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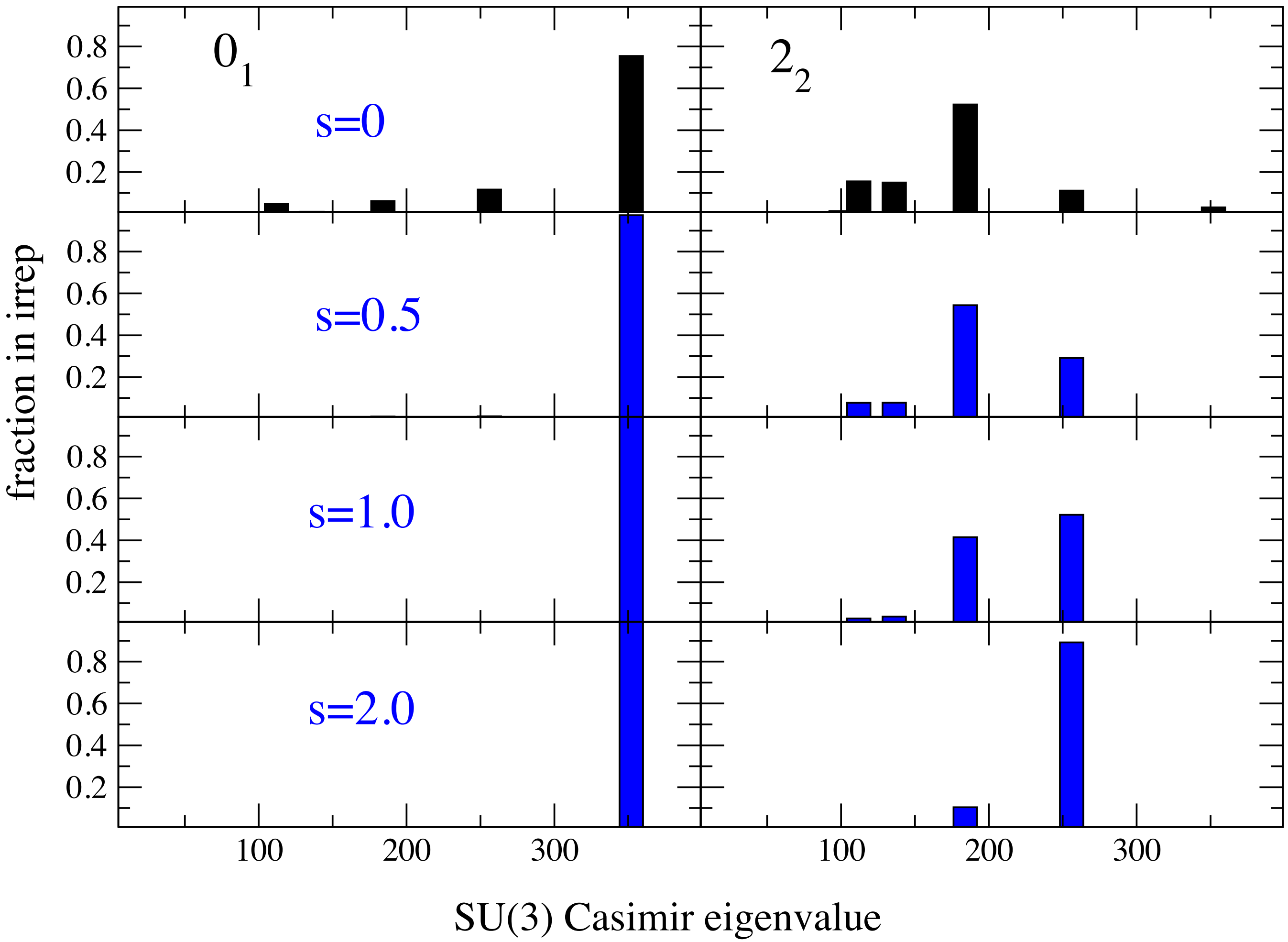
Increasing evolution

San Diego State University



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USDB interaction

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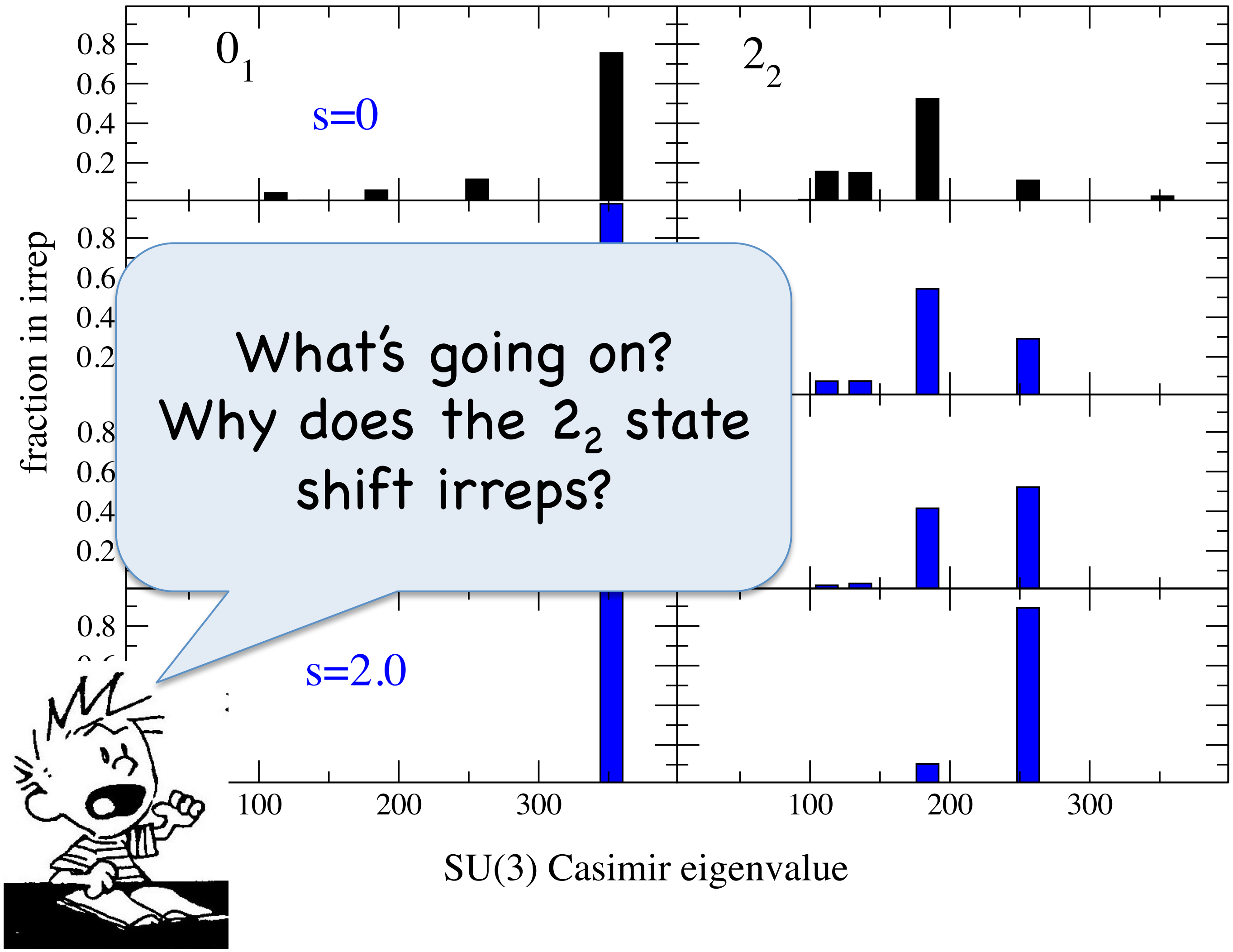

^{20}Ne

USDB interaction

Increasing evolution

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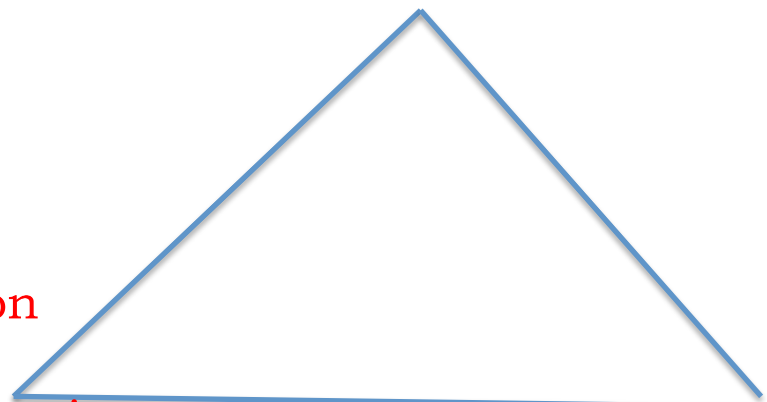
Decomposing shell model wave functions by group irreps
-> *quasi-dynamical symmetries*



Spectral distribution theory, a metric on the space of Hamiltonians
-> *a new way to look at SRG and a new SRG*

SRG: the similarity renormalization group:
-> *unitary transformations back to **dynamical** symmetry*

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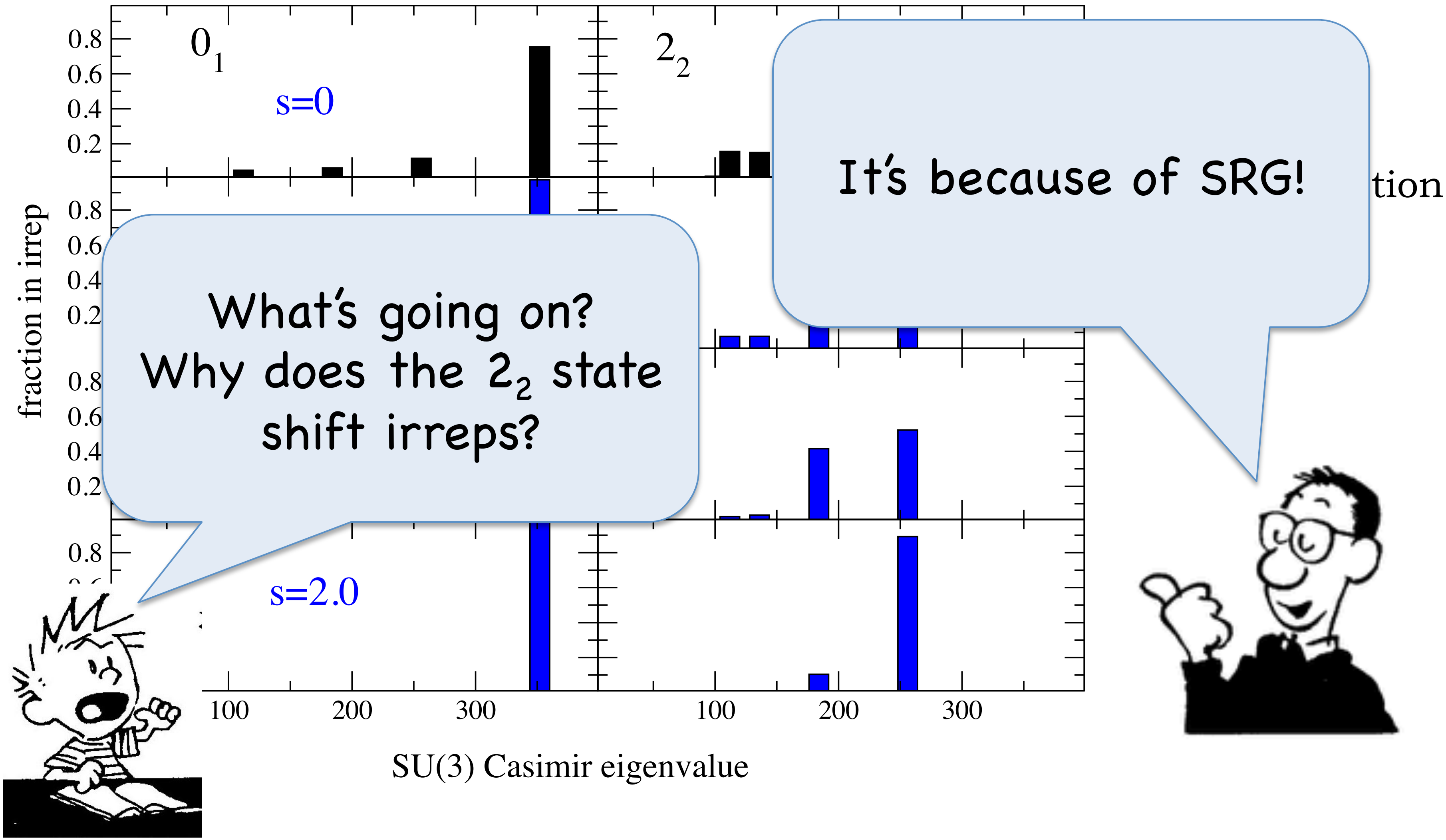

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It turns out one can re-derive SRG using *spectral distribution theory* (French, Ratcliffe, Wong, Draayer, many others)

One can define an *inner product* on matrices/Hamiltonian using traces:

(A,B) = tr AB*

*well, there are some subtleties that are not important here

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Suppose we want to transform H(s)

$$H(s) = U(s)H(0)U^{\dagger}(s)$$

so as to increase

tr (H(s) G)

(i.e., to make H more "parallel" to G)

It's because of SRG!

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Suppose we want to transform H(s)

$$H(s)=U(s)H(0)U^{\dagger}(s)$$

so as to increase

tr (H(s) G)

(i.e., to make H more "parallel" to G)

maximizing the derivative $\frac{d}{ds}tr\left(GH(S)\right)$

leads to standard SRG

$$\frac{dH(s)}{ds}=\left[\left[G,H(s)\right],H(s)\right]$$

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Suppose we want to transform H(s)

$$H(s) = U(s) H(0) U^{\dagger}(s)$$

so as to increase

tr (H(s) G)

(i.e., to make H more "parallel" to G)

maximizing the derivative $\frac{d}{ds} tr\left(GH(S)\right)$

leads to standard SRG

$$\frac{dH(s)}{ds} = \left[\left[G, H(s)\right], H(s)\right]$$

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Suppose instead we want to transform H(s)

$$H(s) = U(s) H(0) U^{\dagger}(s)$$

so as to **decrease** tr $[H(s),G]^2$

(i.e., to make H "commute more" with G)

so maximizing the derivative $-\frac{d}{ds} tr \left[G, H(s) \right]^2$
leads to "new" SRG:

$$\frac{dH}{ds} = \left[\left[\left[\left[G, H \right], G \right], H \right], H \right]$$

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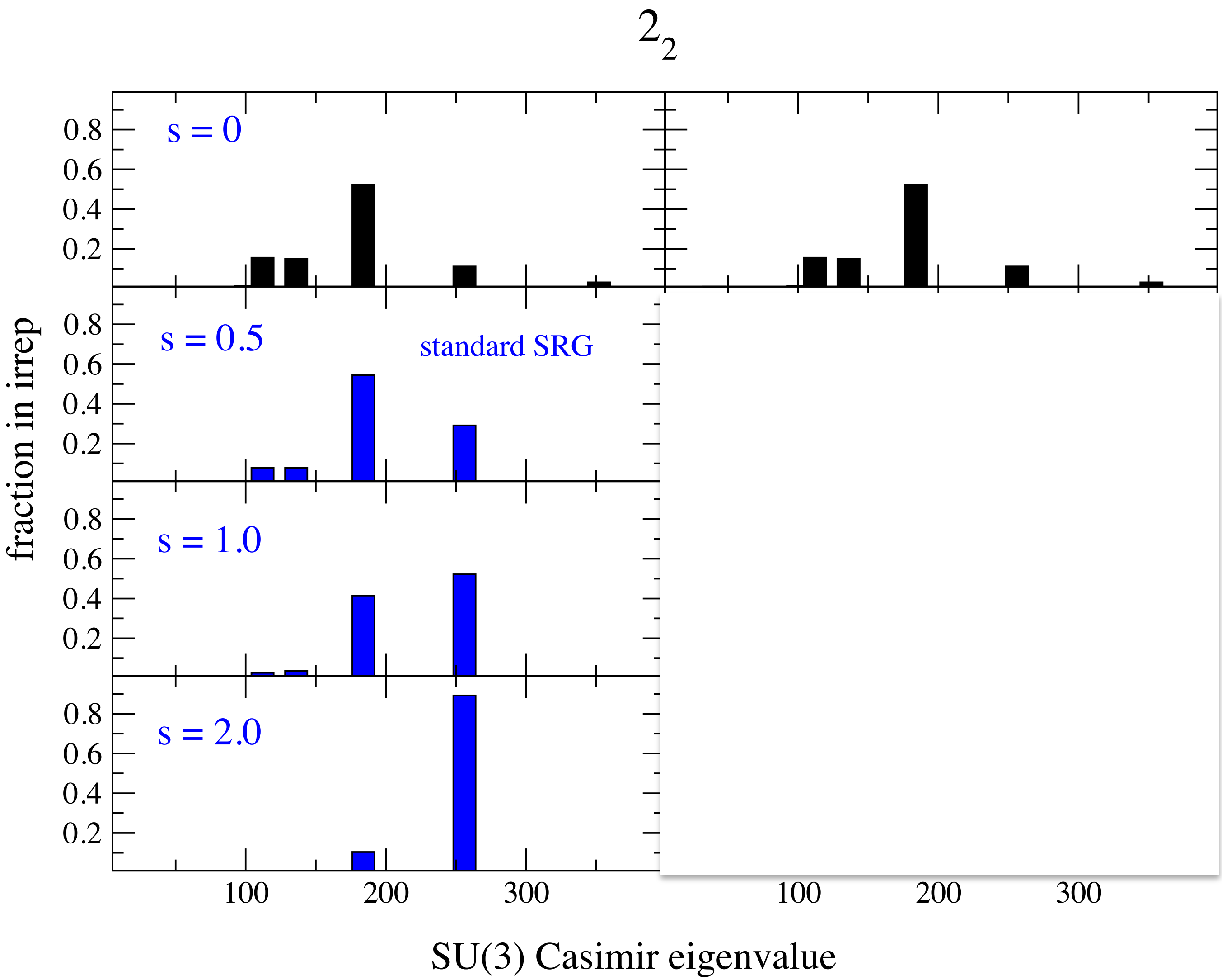

^{20}Ne

USDB interaction

Increasing evolution

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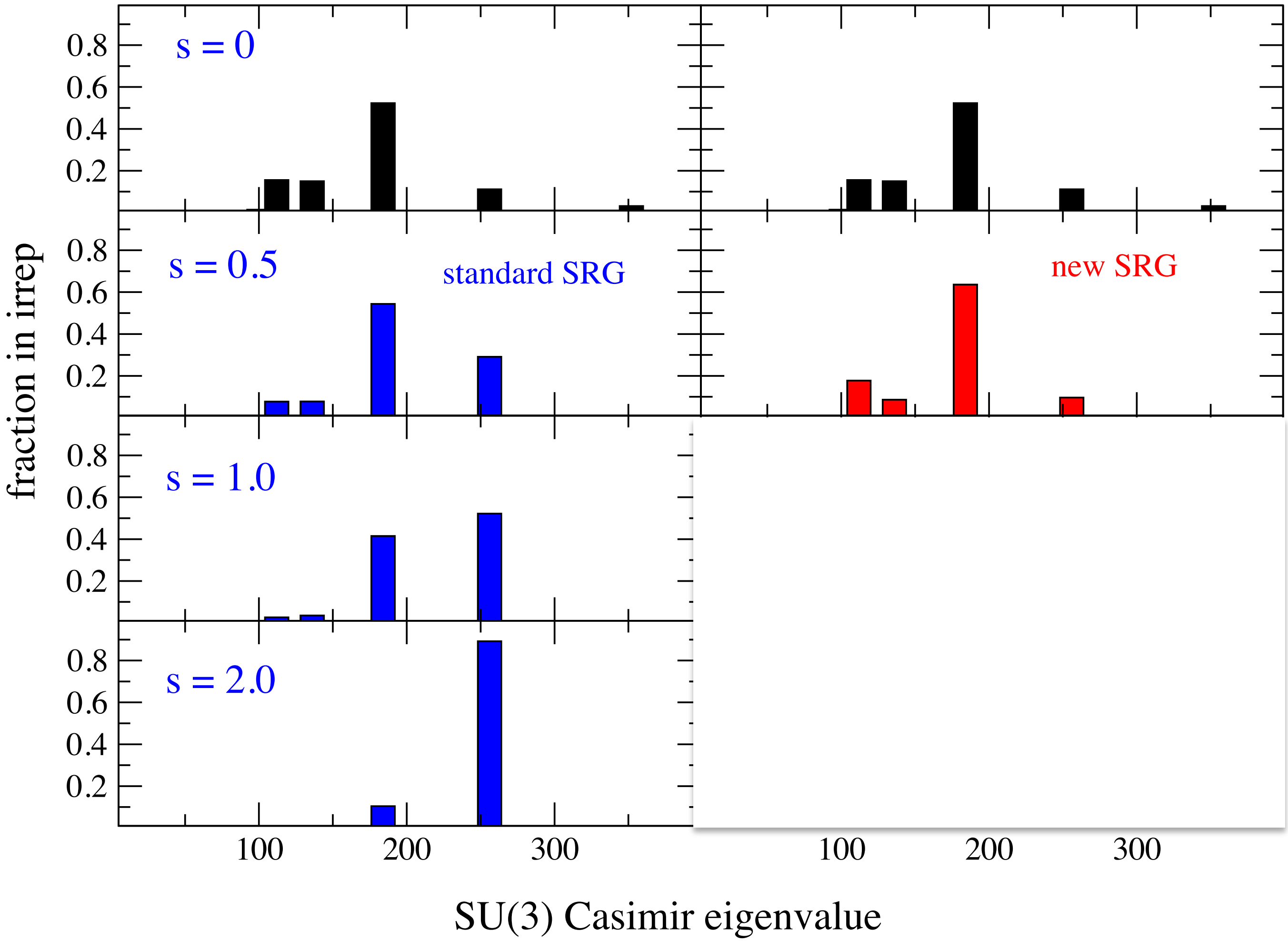
2_2



^{20}Ne

USDB interaction

Increasing evolution

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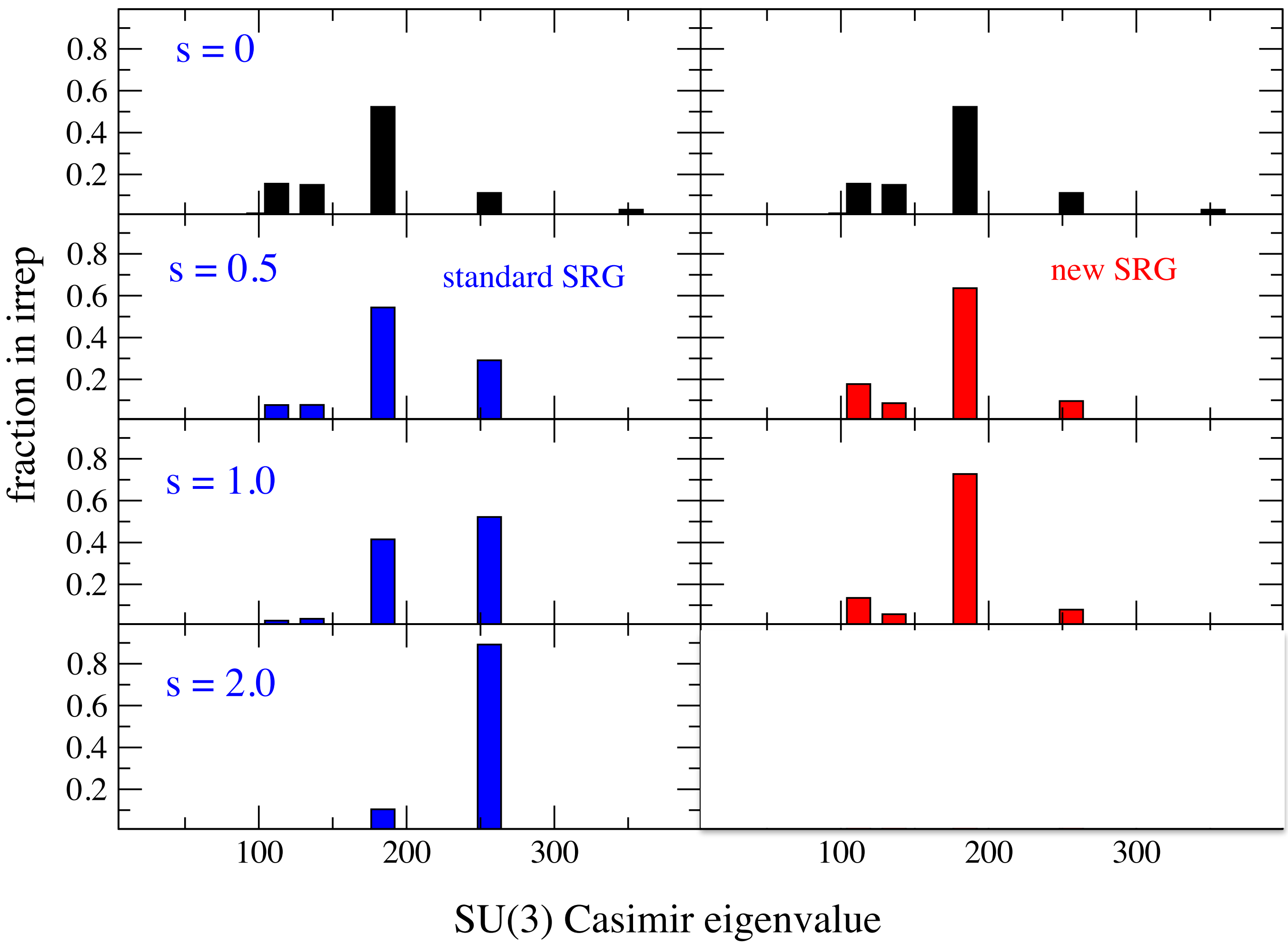
2_2



^{20}Ne

USDB interaction

Increasing evolution

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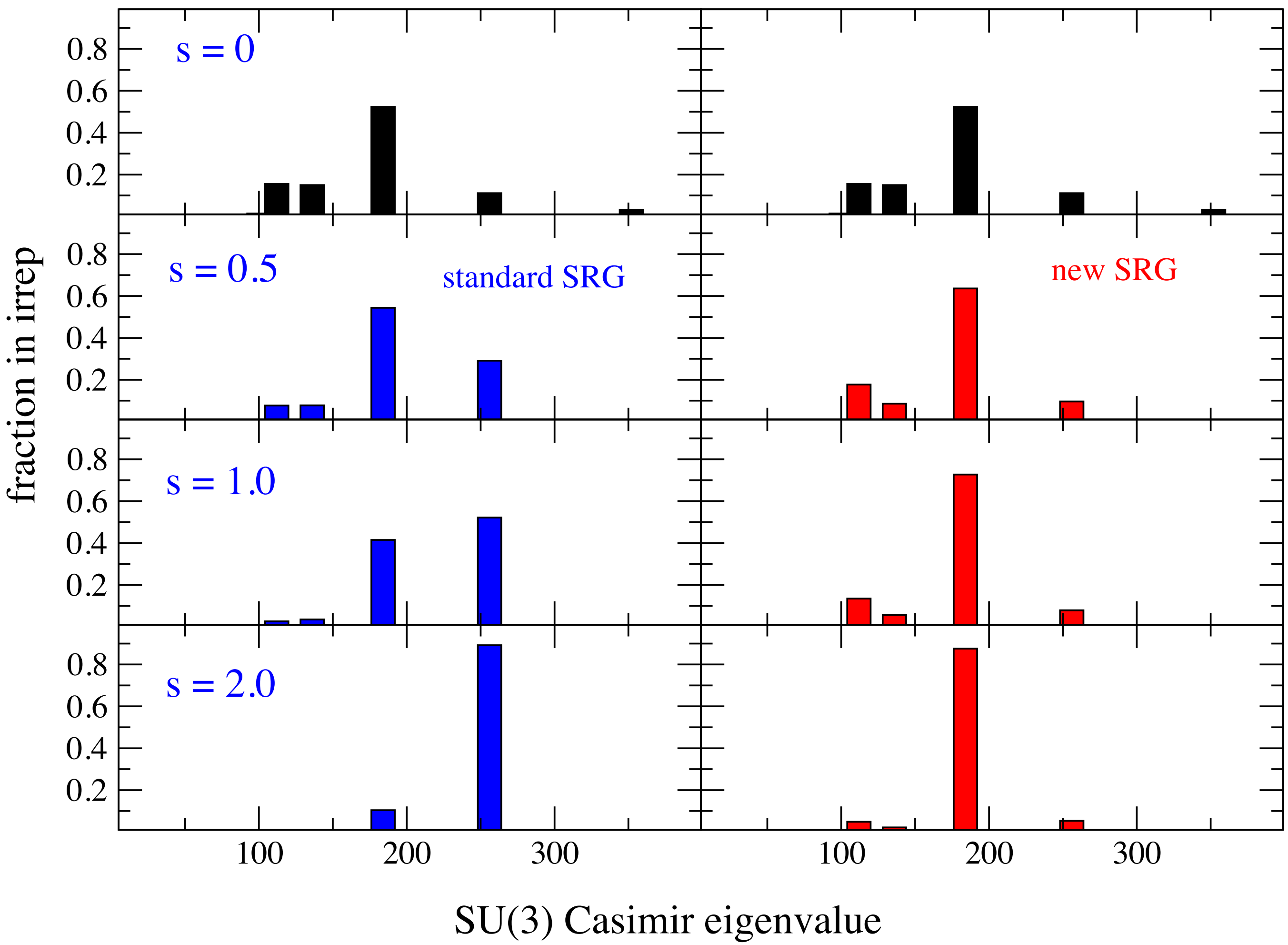
2_2



^{20}Ne

USDB interaction

Increasing evolution

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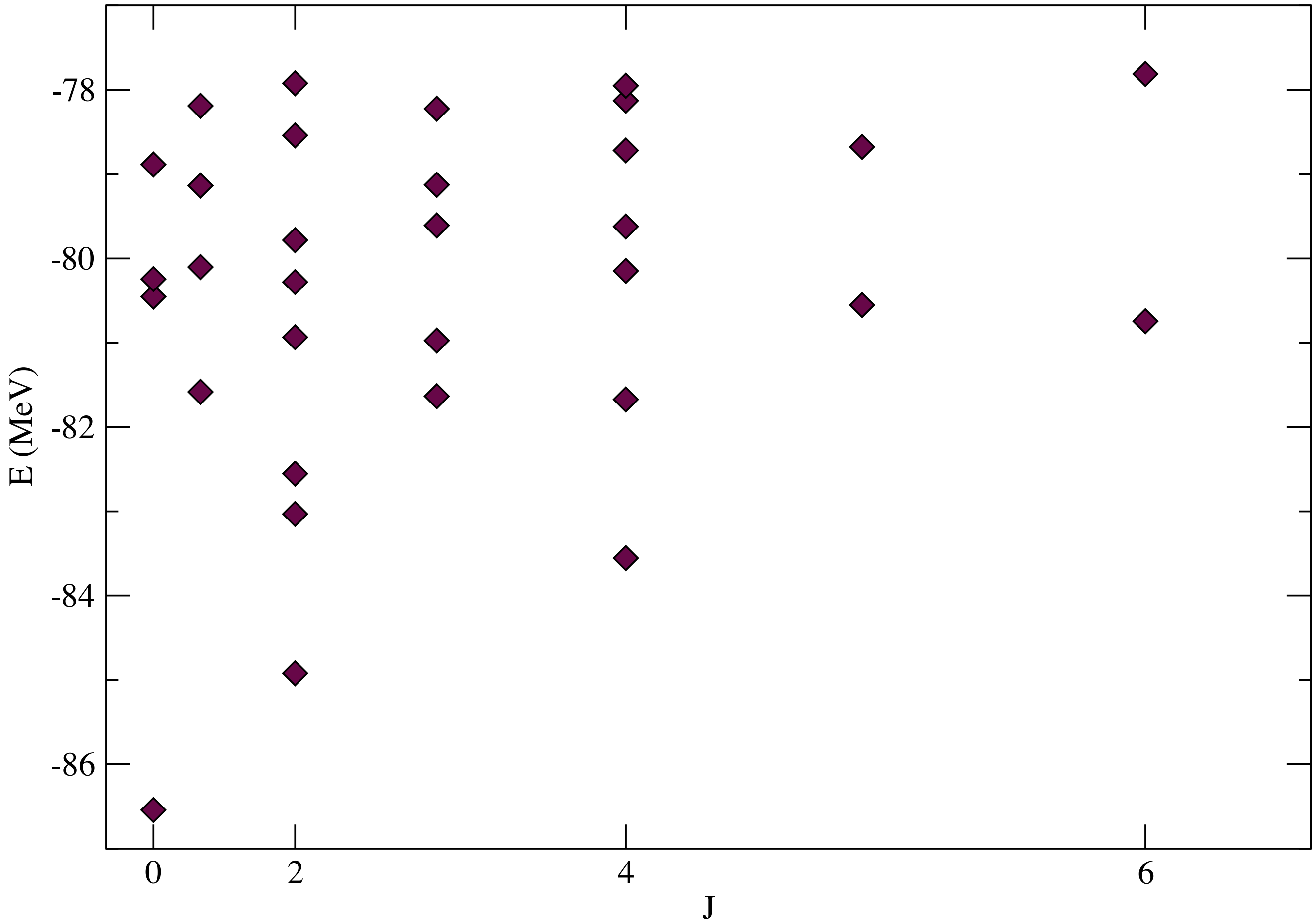

^{28}Ne

USDB interaction

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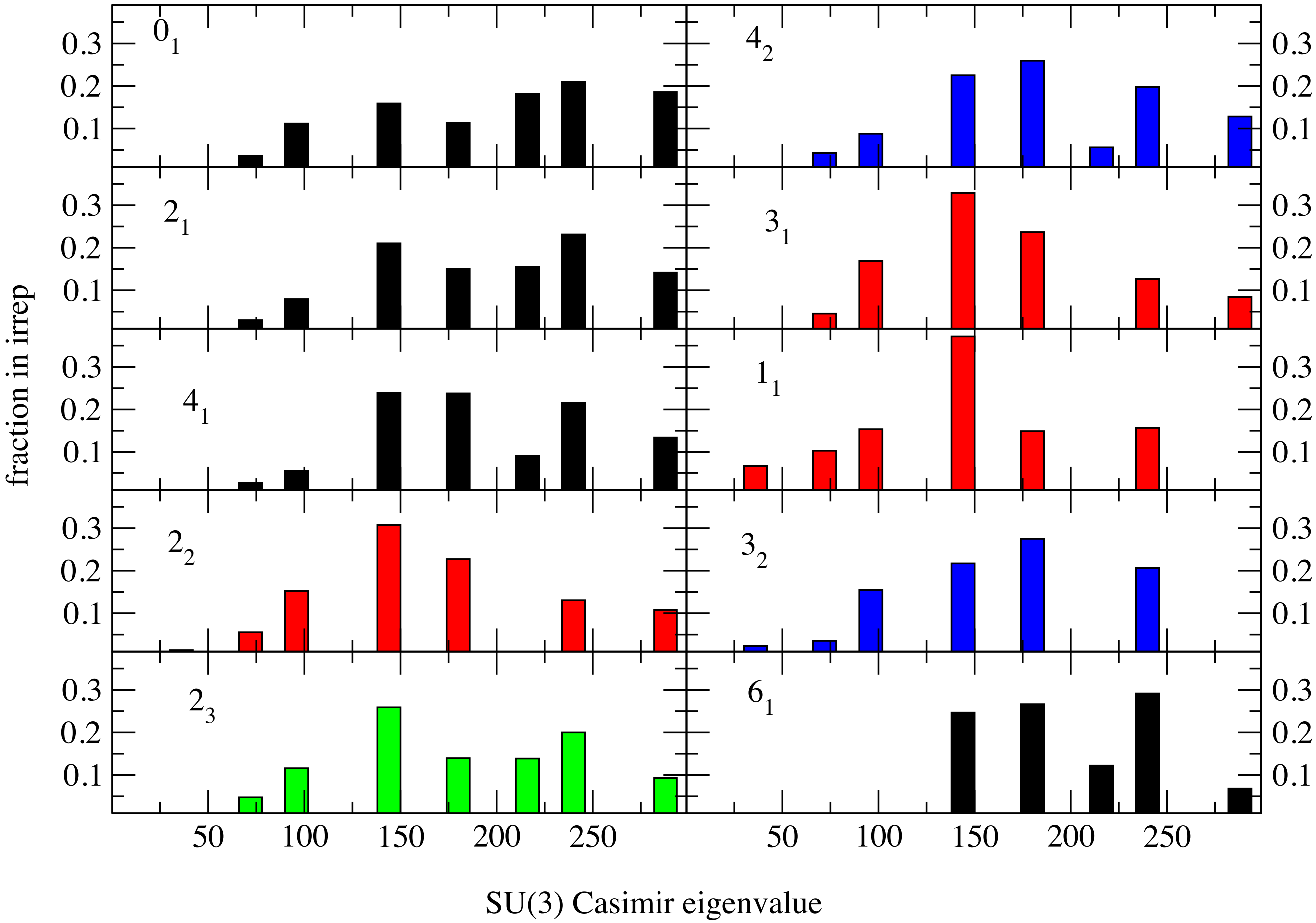

^{28}Ne

USDB interaction

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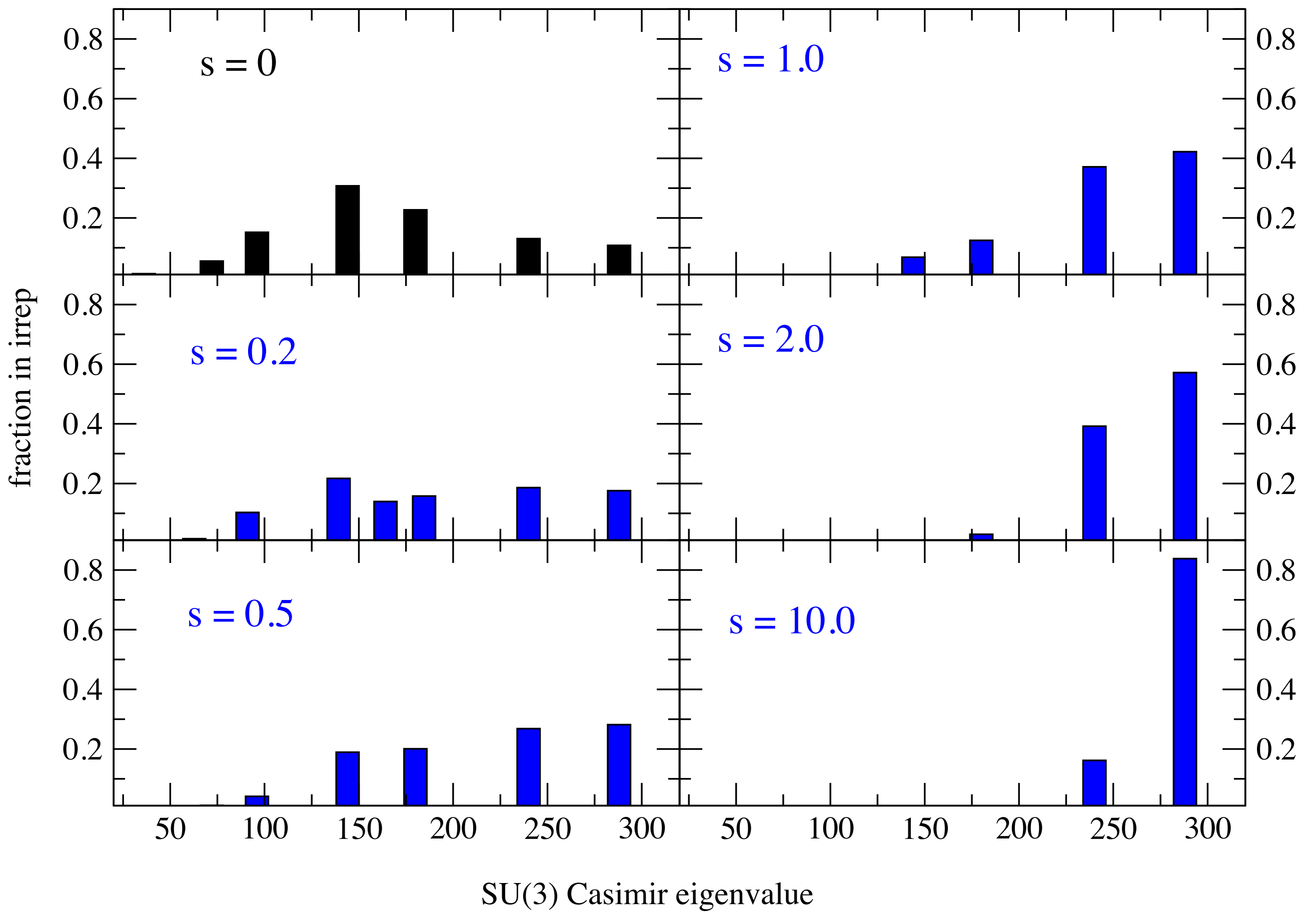

^{28}Ne

USDB interaction

2_2 state

standard SRG

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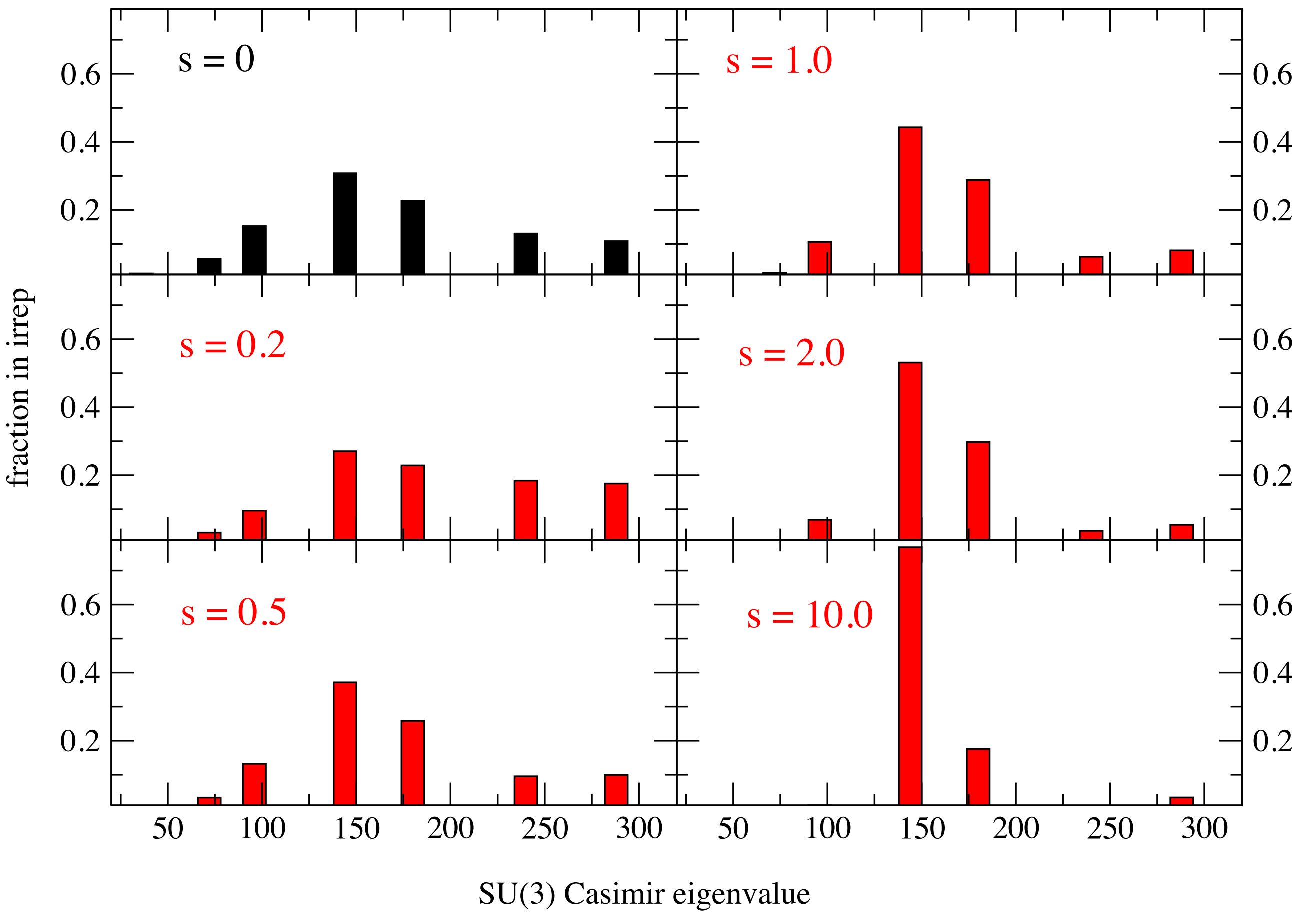

^{28}Ne

USDB interaction

2_2 state

new SRG

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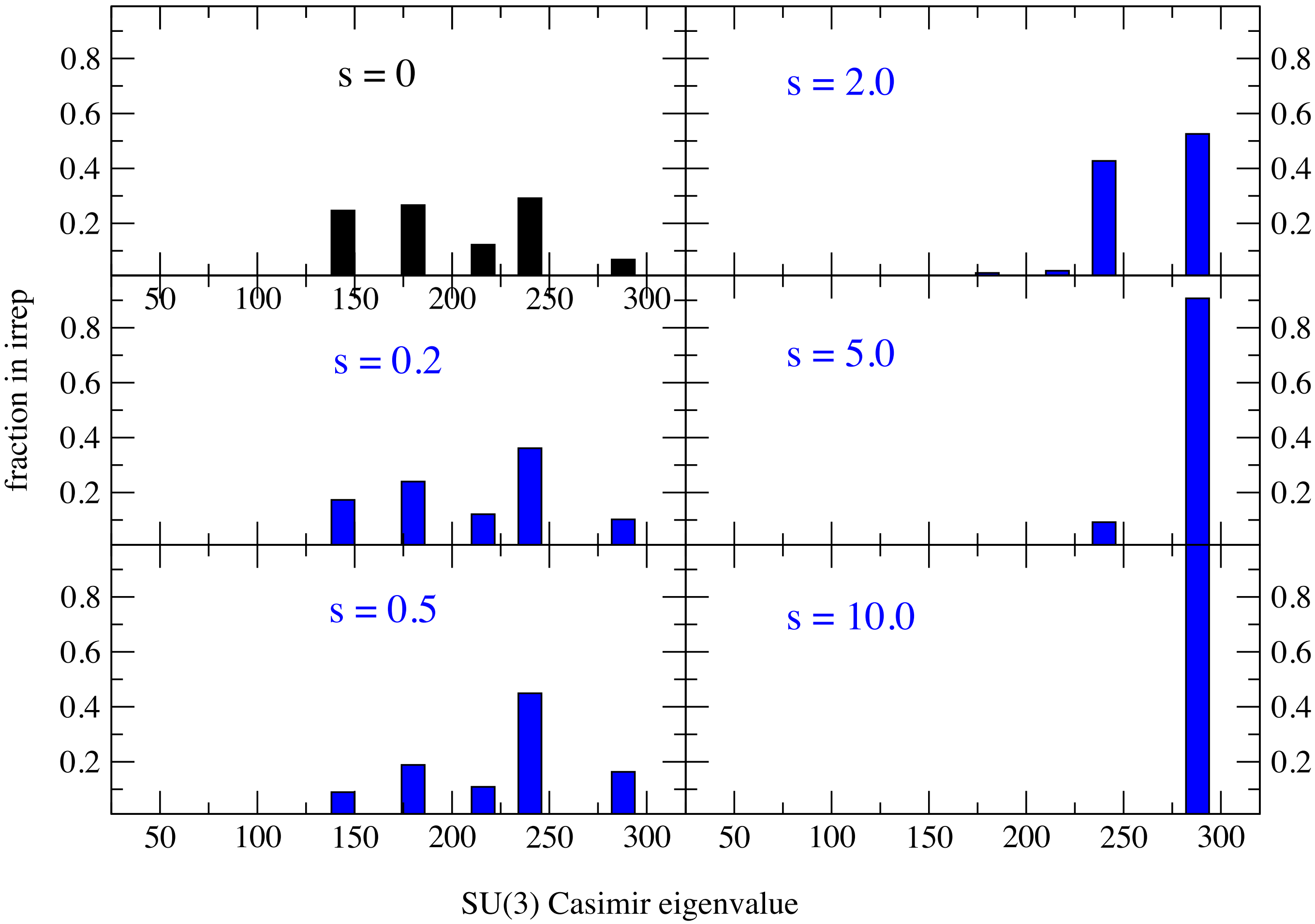

^{28}Ne

USDB interaction

6_1 state

standard SRG

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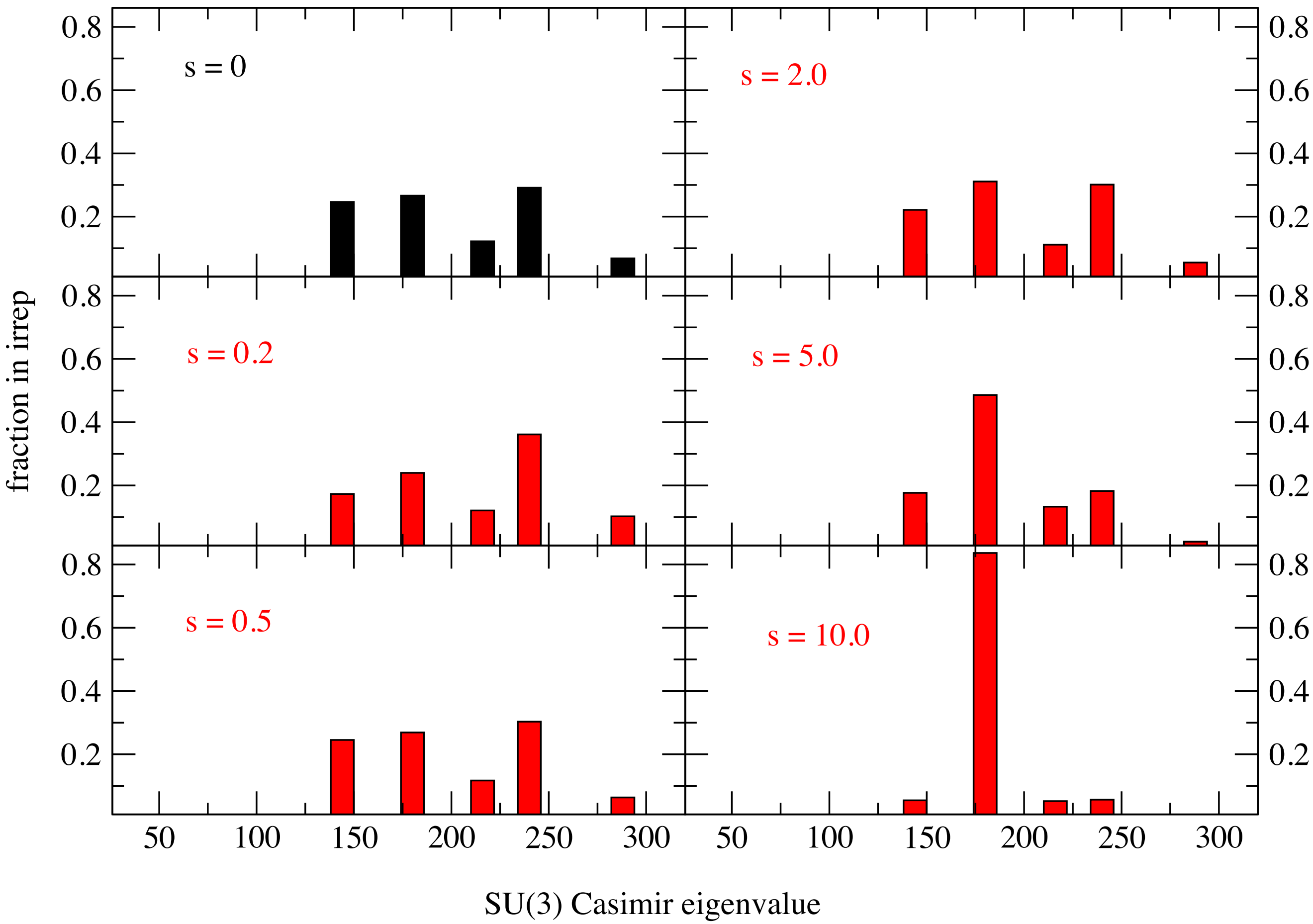


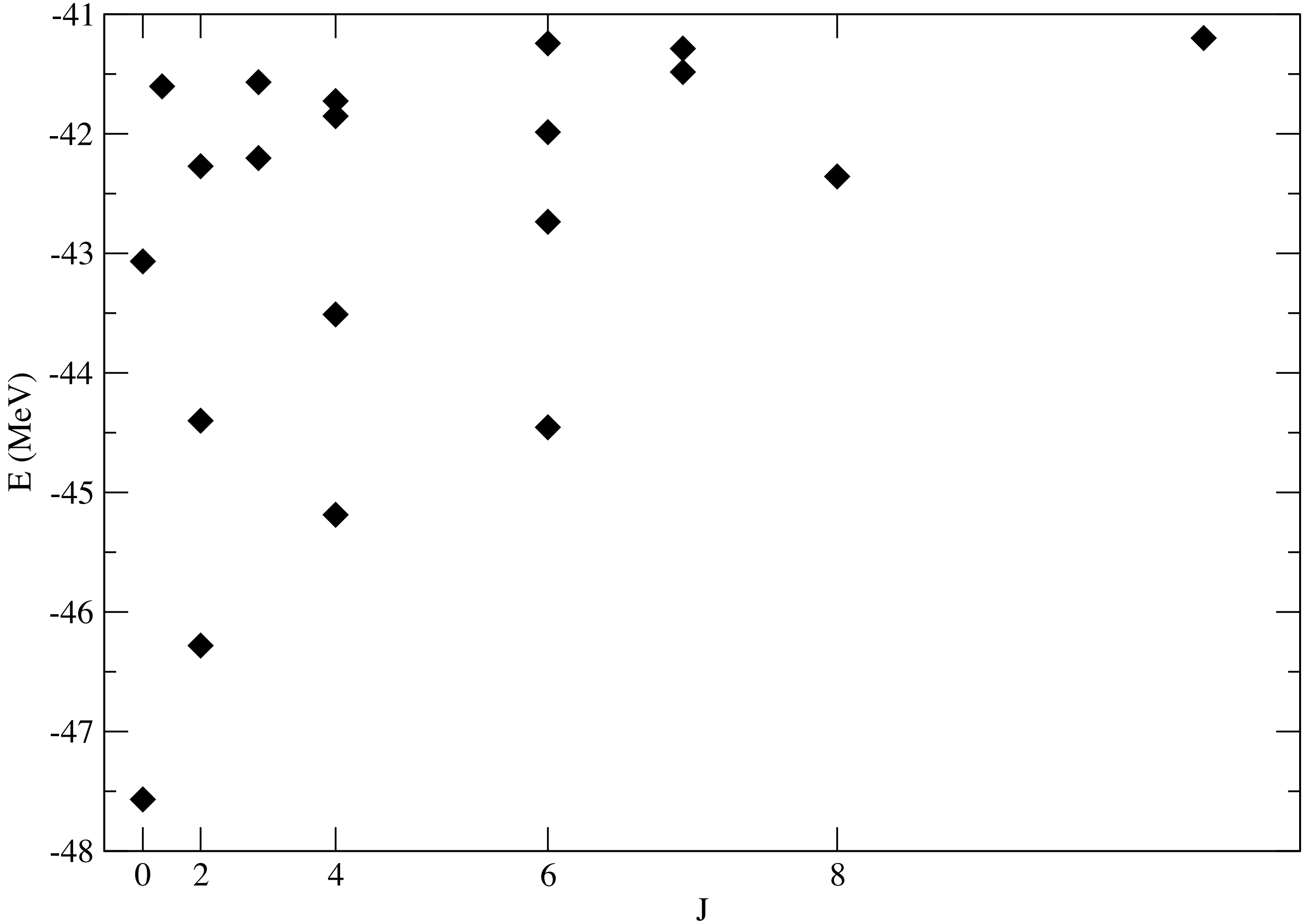
^{28}Ne

USDB interaction

6_1 state

new SRG

SAN DIEGO STATE UNIVERSITY



^{44}Ti

GX1A interaction

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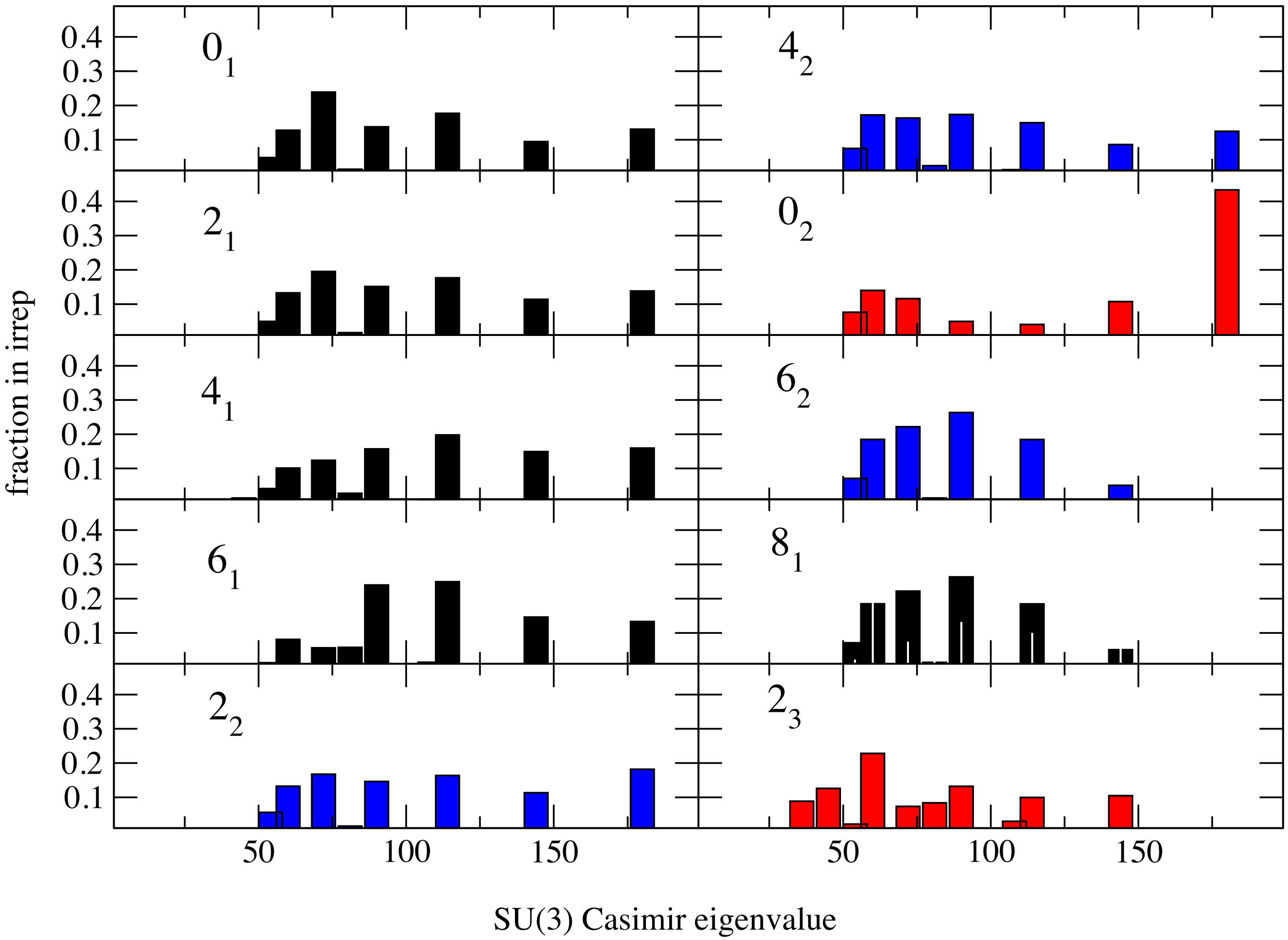
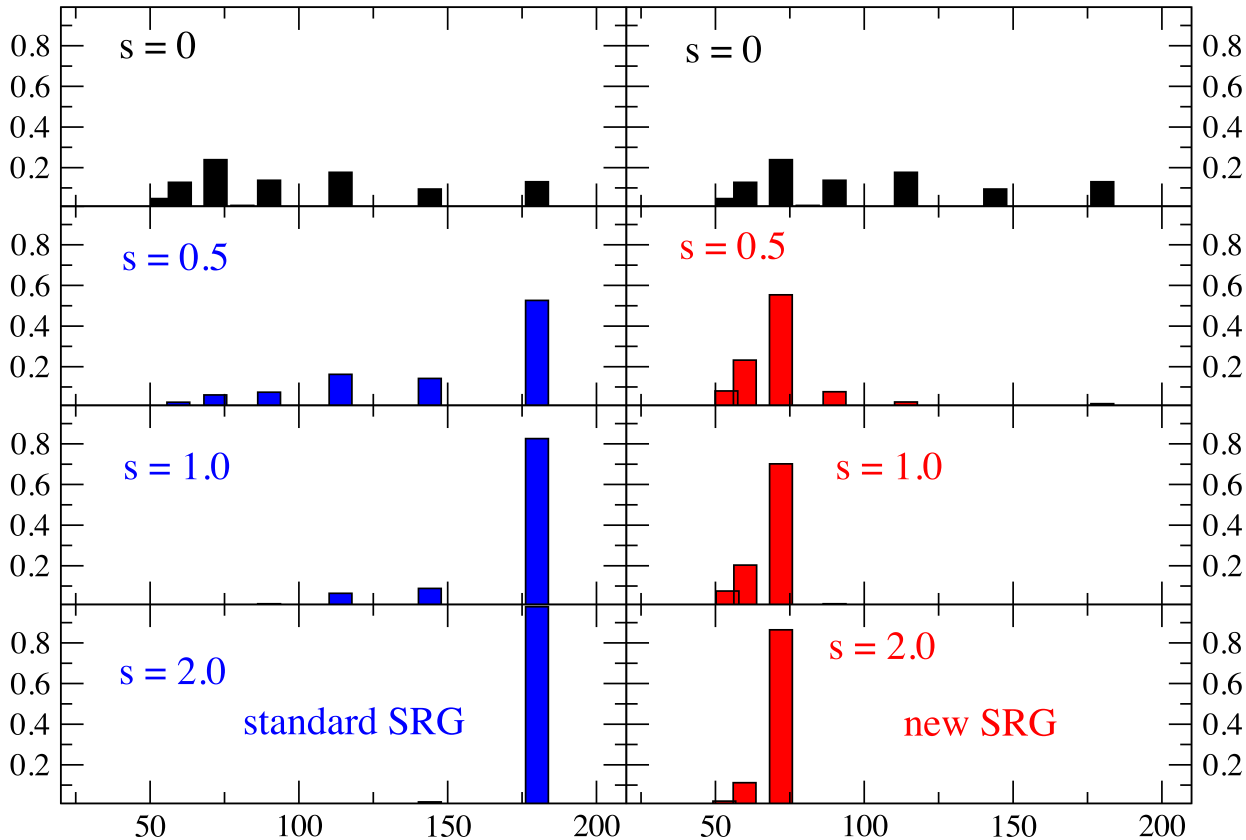


^{44}Ti

GX1A interaction

San Diego State University



^{44}Ti

GX1A interaction

0_1 g.s.

Increasing evolution

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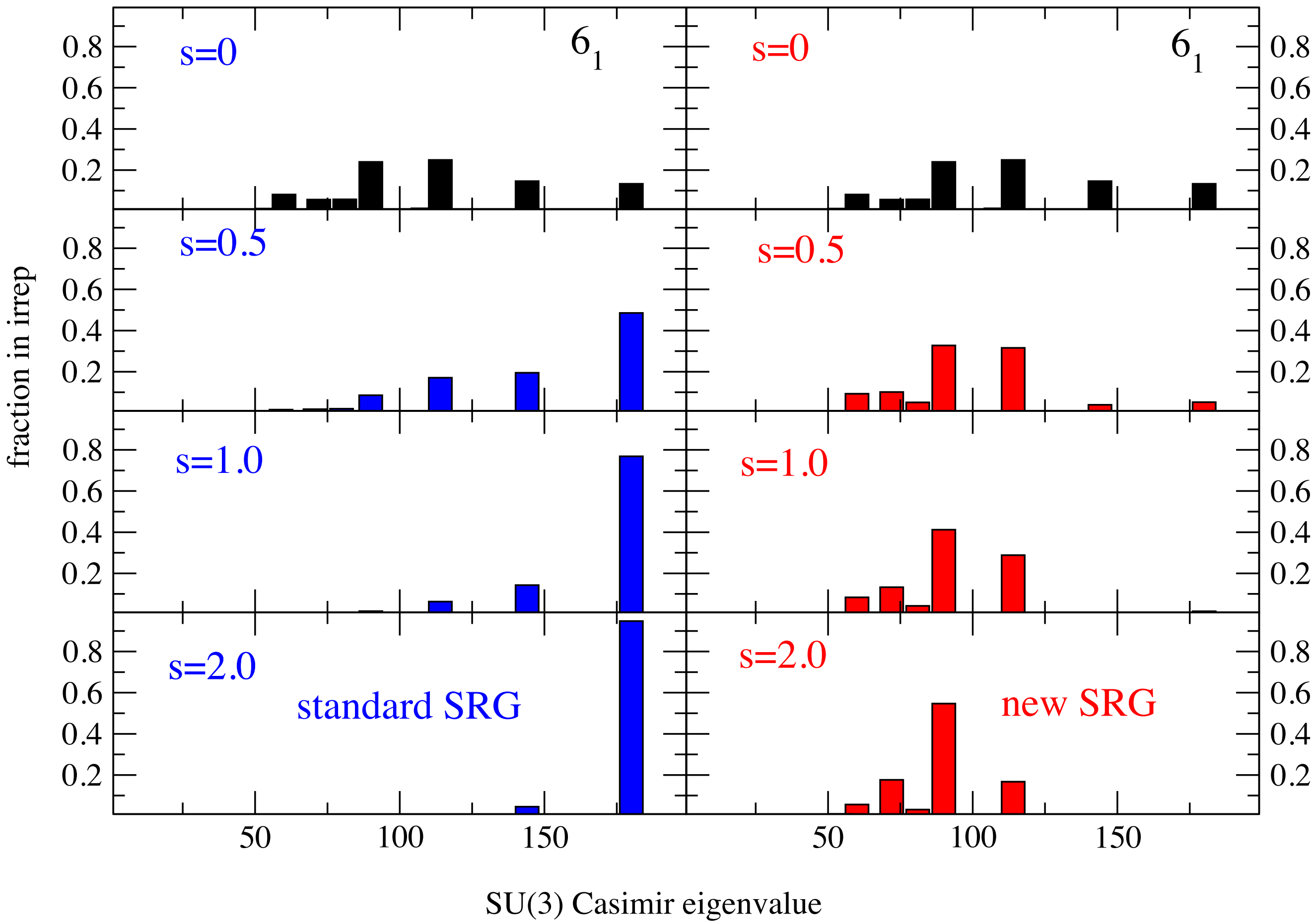


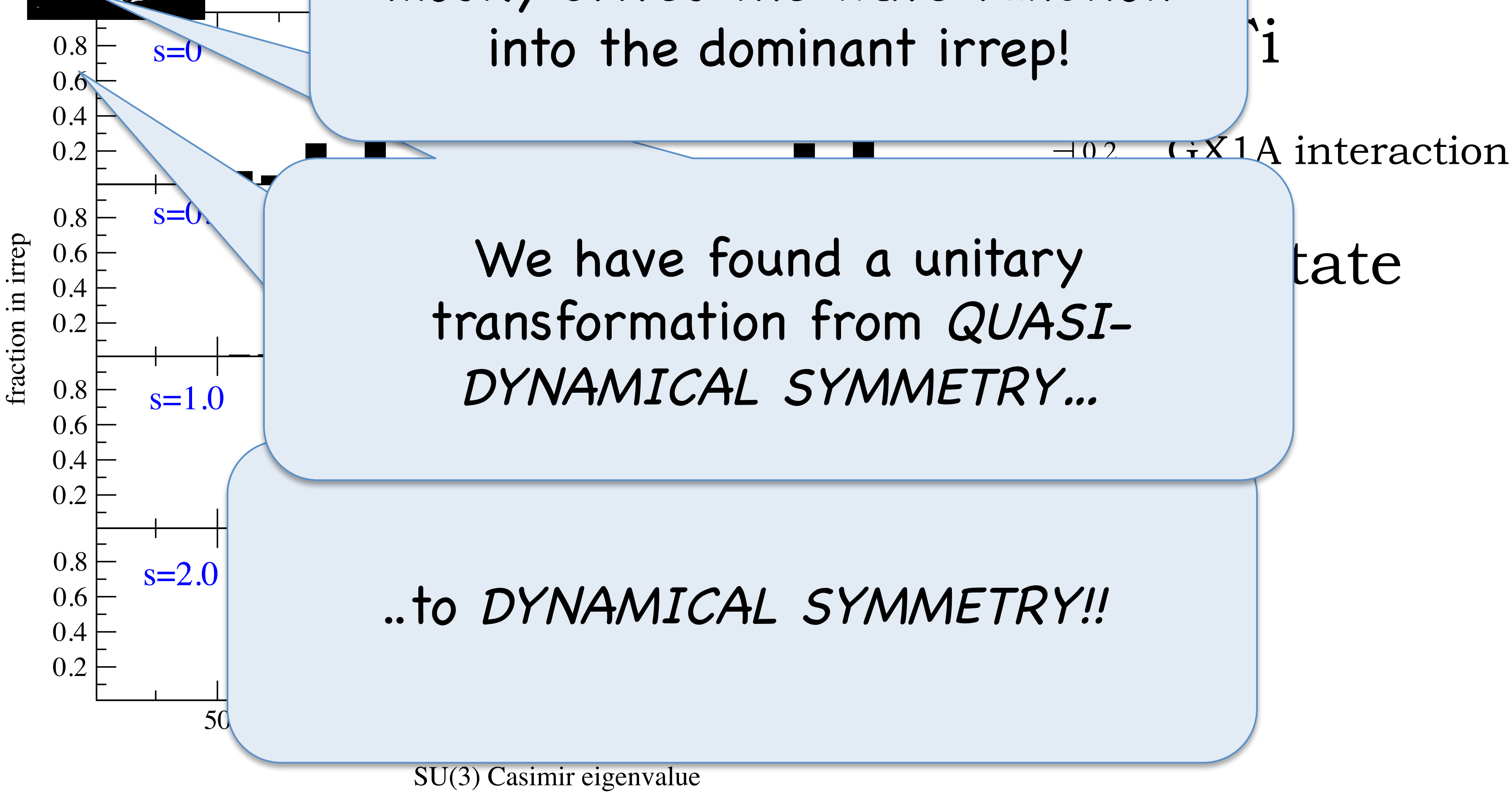
^{44}Ti

GX1A interaction

6_1 state

Increasing evolution

In other words, this 'new SRG' mostly drives the wave function into the dominant irrep!



We have found a unitary transformation from *QUASI-DYNAMICAL SYMMETRY*…

..to *DYNAMICAL SYMMETRY!!*

Summary:

*Group theory allows us to peer into the structure of complicated wave functions

* *Dynamical symmetry* (dominance by a single irrep) is rare, but *quasi-dynamical symmetry* is ubiquitous.

- We can construct a unitary transformation from *quasi-dynamical symmetry* to *dynamical symmetry*, using the similarity renormalization group (SRG).

- Standard SRG pushes wave functions towards irreps with extremal Casimir eigenvalues, but I can formulate a new SRG that fixes this problem!

Future work:

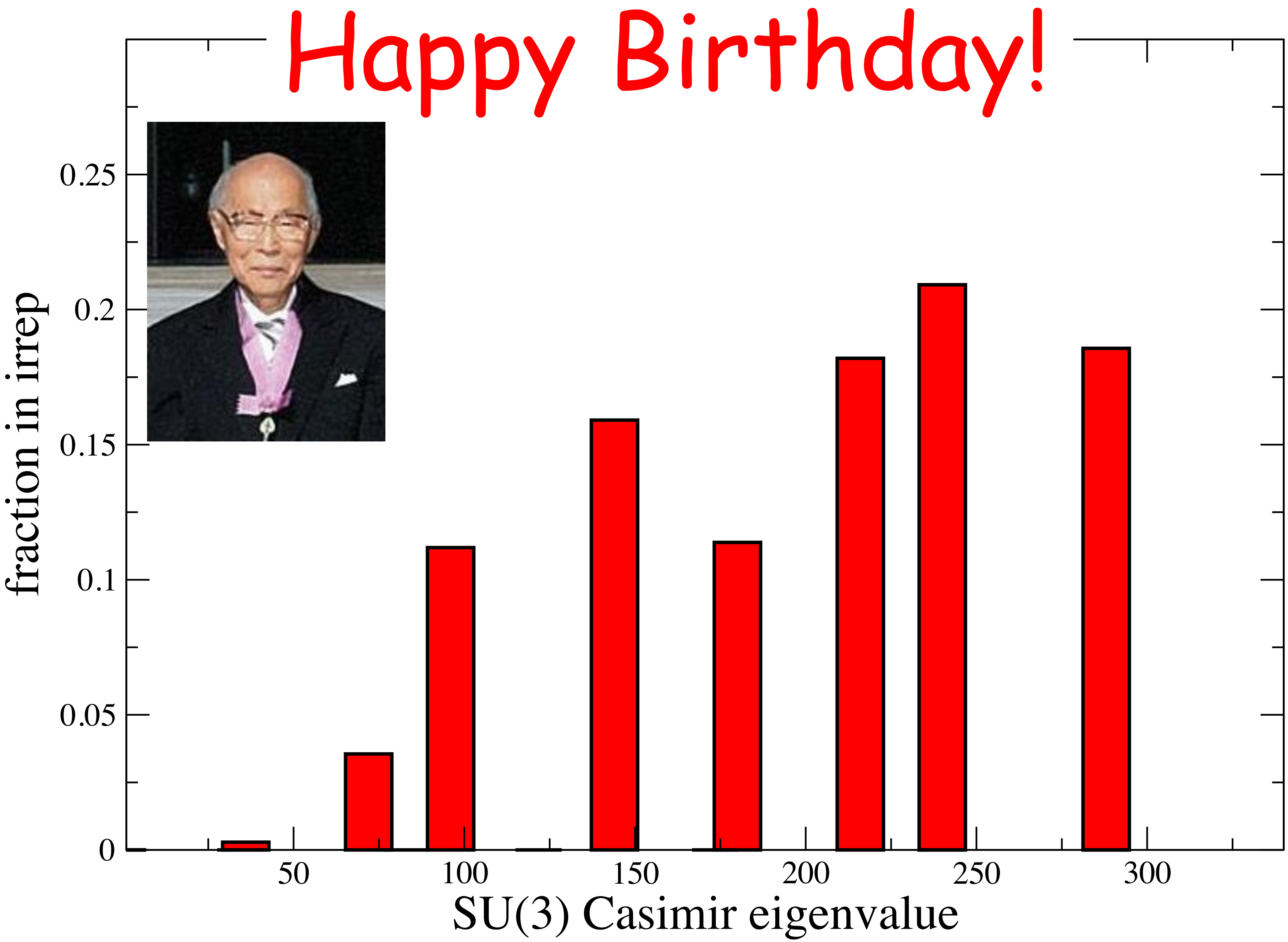
- Transitions! How do B(E2)s change?

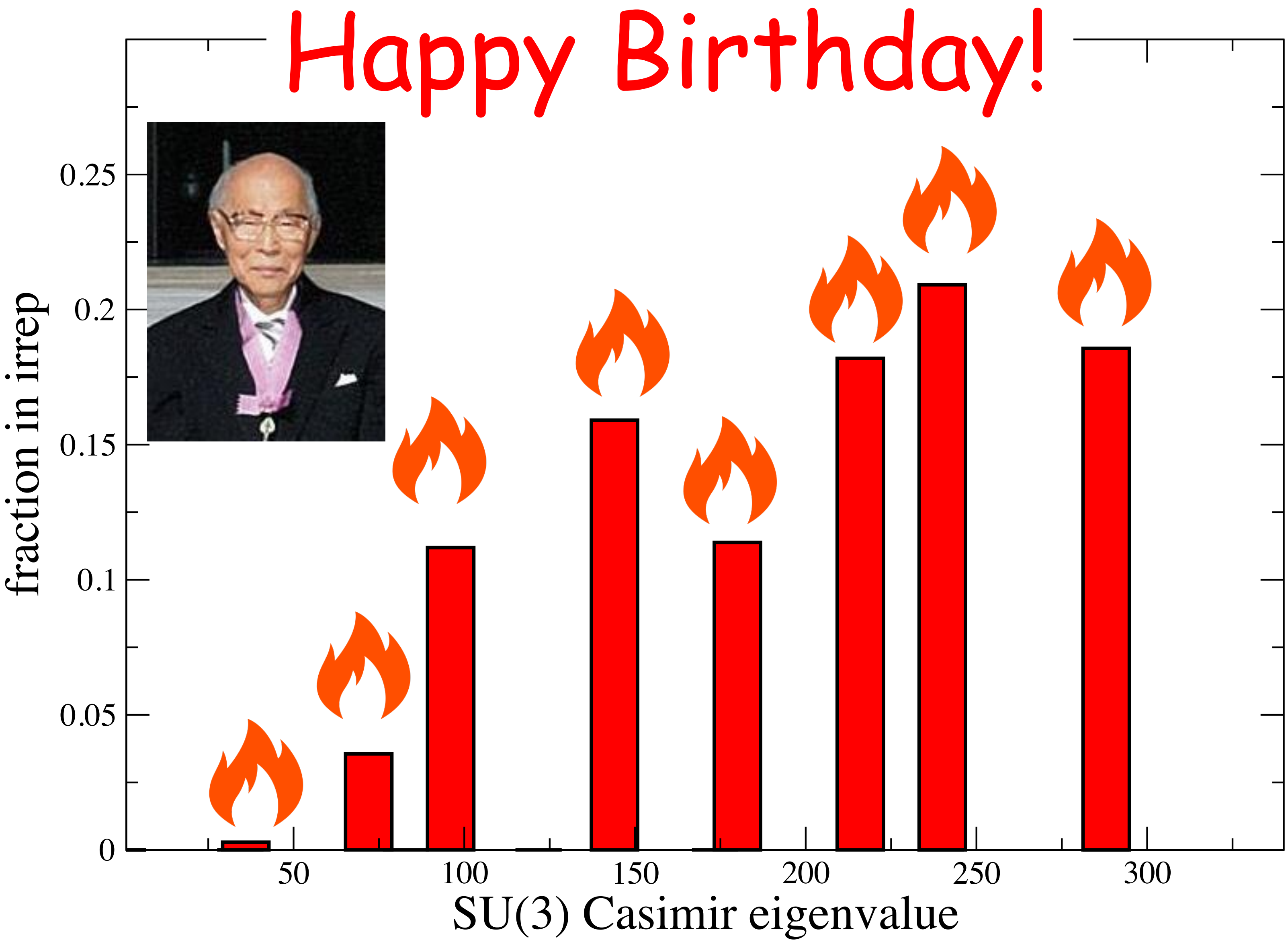
- Use ”new” SRG in both momentum space (original application of SRG in nuclear structure) and truncated shells (“in-medium SRG”).

Can this be an **improved SRG** for nuclear structure?

- What about random interactions?

Thank you!


Happy Birthday!
fraction in irrep
0.25
0.2
0.15
0.1
0.05
0
50
100
150
200
250
300
SU(3) Casimir eigenvalue


Happy Birthday!
fraction in irrep
0
0.05
0.1
0.15
0.2
0.25
50
100
150
200
250
300
SU(3) Casimir eigenvalue

Additional slides

for curious people

Derivation of SRG, old and new

Standard SRG: want to **increase** tr (H(s)G)

so choose evolution that maximizes derivative

$$d/ds\ tr(H(s)G) = tr\ (dH(s)/ds\ G) = tr\ ([\eta,H(s)]G)$$

This derivative can be rewritten as

tr (h [G,H]) using cyclic property of traces

The derivative is maximal when

h is proportional to [G,H]

hence $d/ds\ H(s) = [\eta,H] = [[G,H],H]$

"New" SRG: want to **decrease** tr $[H(s),G]^2$

so choose evolution that maximizes derivative

$$-d/ds\, tr([H(s),G]^2) = -2\, tr([dH/ds, G][H,G]) = -2\, tr([[\eta,H],G][H,G])$$

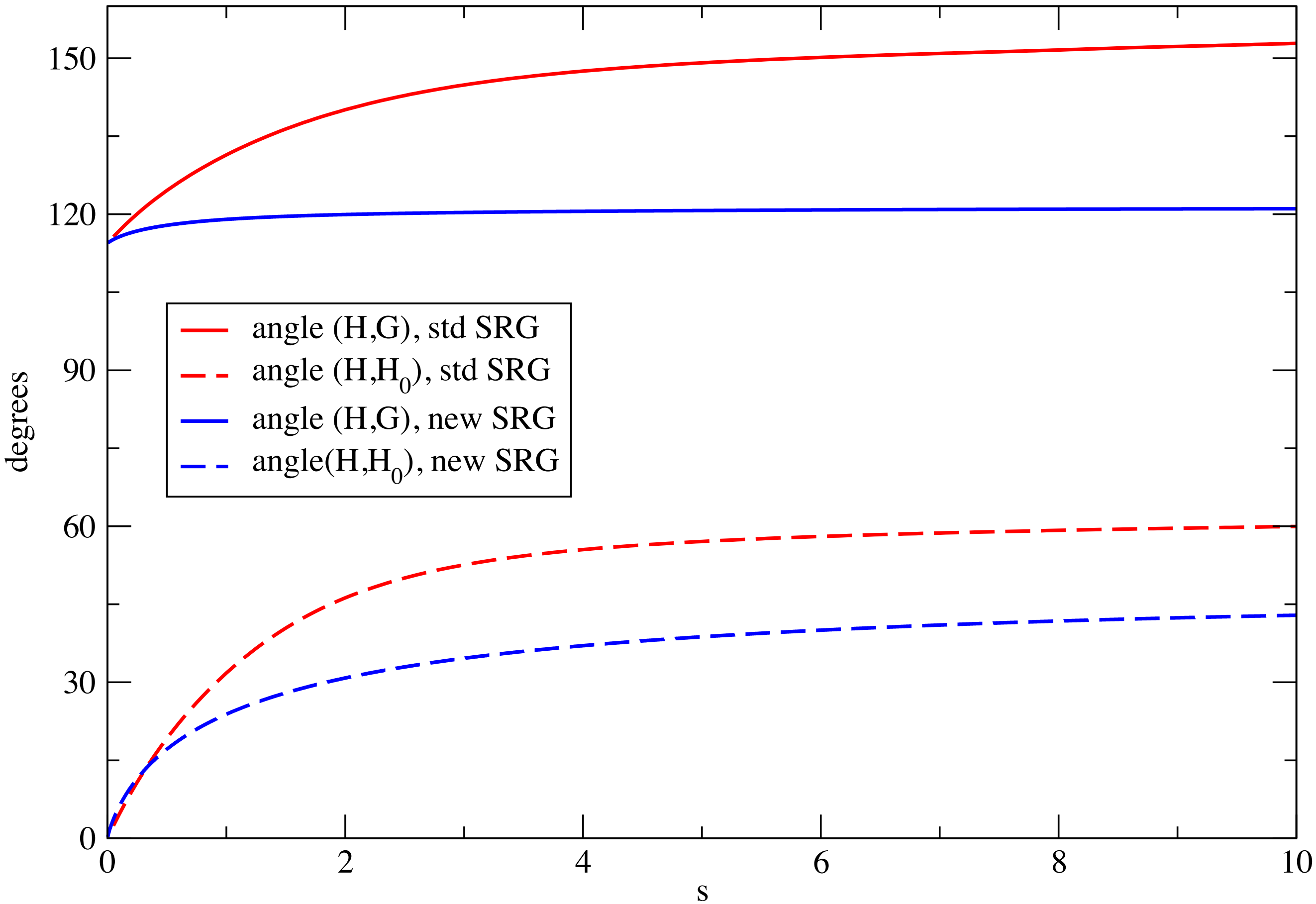
This derivative can be rewritten as

-tr (h [[[H,G],G],H])

The derivative is maximal when

h is proportional to [[[G,H],G],H]

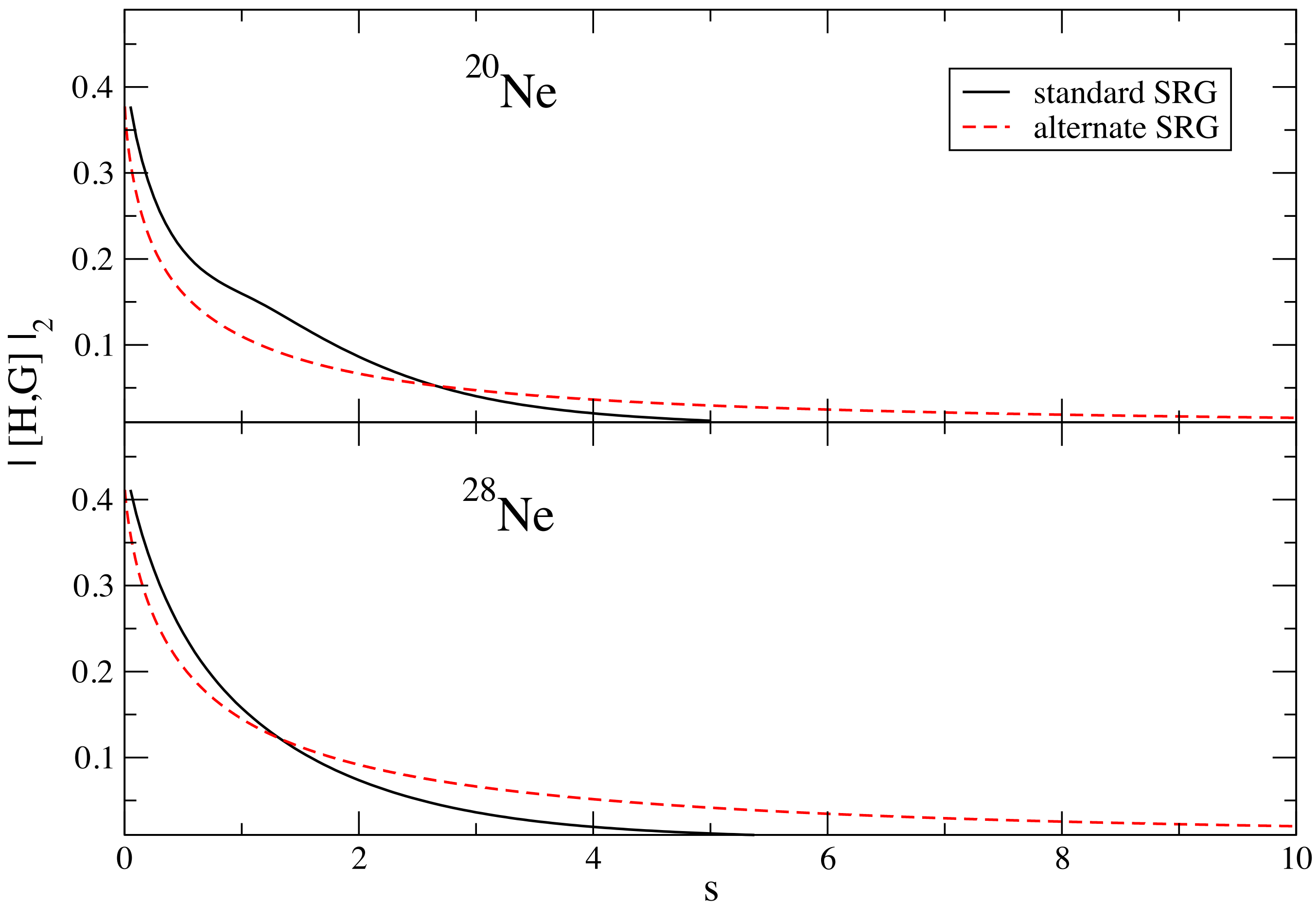
hence $d/ds\, H(s) = [\eta,H] = [[[[G,H],G],H],H]$



^{28}Ne

USDB interaction

G = SU(3)
2-body Casimir



^{20,28}Ne

USDB interaction

G = SU(3)
2-body Casimir

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Some technical details

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*

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

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How are those decompositions calculated?

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

For some wavefunction $|\Psi\rangle$, 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

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

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

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

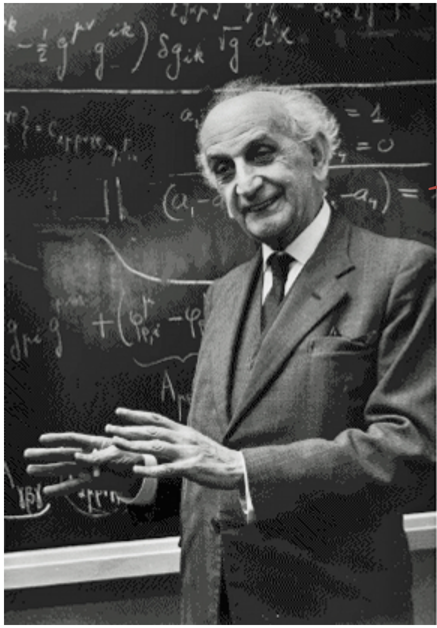
Casi

This can be done very efficiently using the Lanczos algorithm (see, e.g., CWJ, PRC **91**, 034313 (2015)

F
th

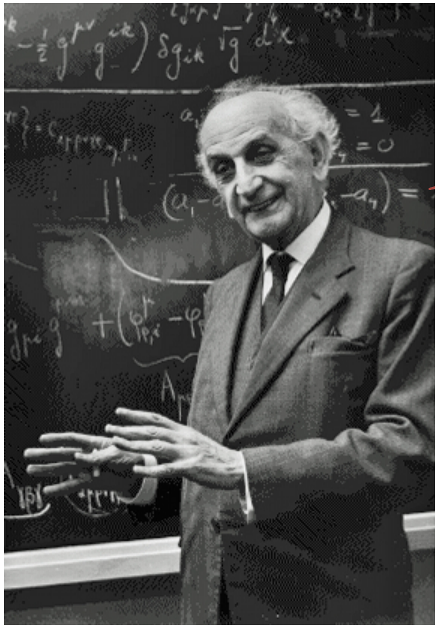
$$F(z) = \sum_{\alpha} \left| \left\langle z, \alpha \middle| \Psi \right\rangle \right|^2$$

ries



There is another way

(Cornelius Lanczos)



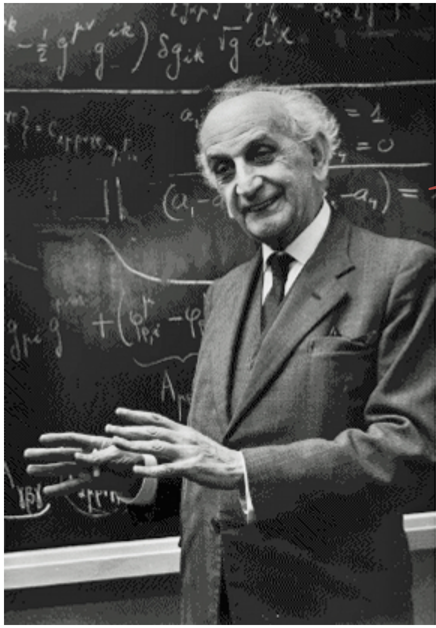
(Cornelius Lanczos)

ies

The Lanczos Algorithm!

ries

There is another way



(Cornelius Lanczos)

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

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

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

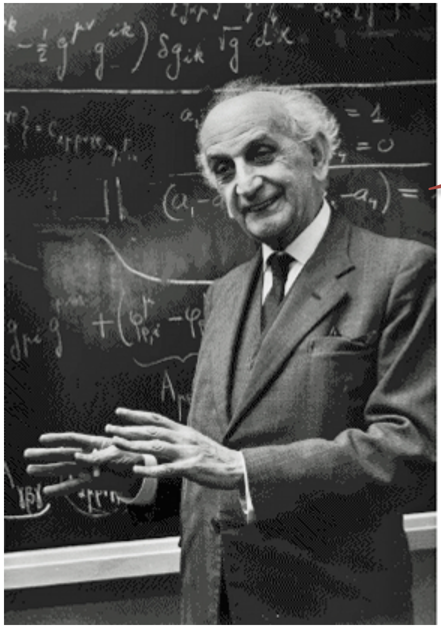
$$\mathbf{A}\vec{v}_4 = \beta_3\vec{v}_3 + \alpha_4\vec{v}_4 + \beta_4\vec{v}_5$$

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”: $|\psi\rangle = c_1 |v_1\rangle + c_2 |v_2\rangle + c_3 |v_3\rangle + \ldots$

ries

There is another way



(Cornelius Lanczos)

Eigenvectors are expressed as a linear combination of the “Lanczos vectors”:

$$|\psi> = c_1 \, |v_1> + c_2 \, |v_2> + c_3 \, |v_3> + \ldots$$

It is easy to read off the overlap of an eigenstate with the “pivot” :

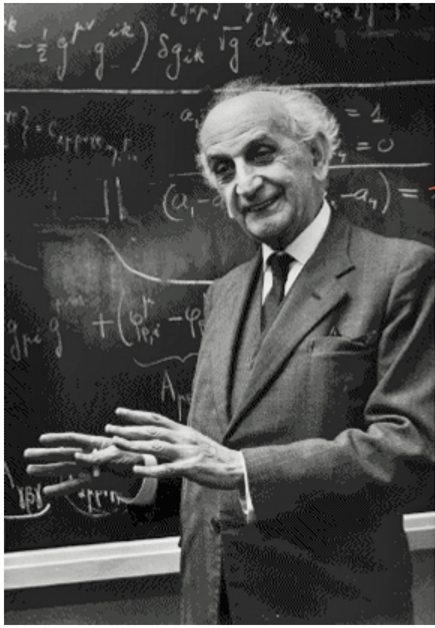
$$|< v_1 \, |\psi >|^2 = c_1^{\,2}$$

Furthermore, the only eigenvectors (of **A**) that are contained in the Krylov space are those with nonzero overlap with the pivot $|v_1>$.

If **A** is say $\mathbf{L}^2$ then we can efficiently expand any state $|v_1>$ into its components with good L.

ies

There is another way



(Cornelius Lanczos)

This trick has been applied before

Computing strength functions

Caurier, Poves, and Zuker, Phys. Lett. B252, 13 (1990);
PRL **74**, 1517 (1995)
Caurier *et al*, PRC **59**, 2033 (1999)
Haxton, Nollett, and Zurek, PRC **72**, 065501 (2005)

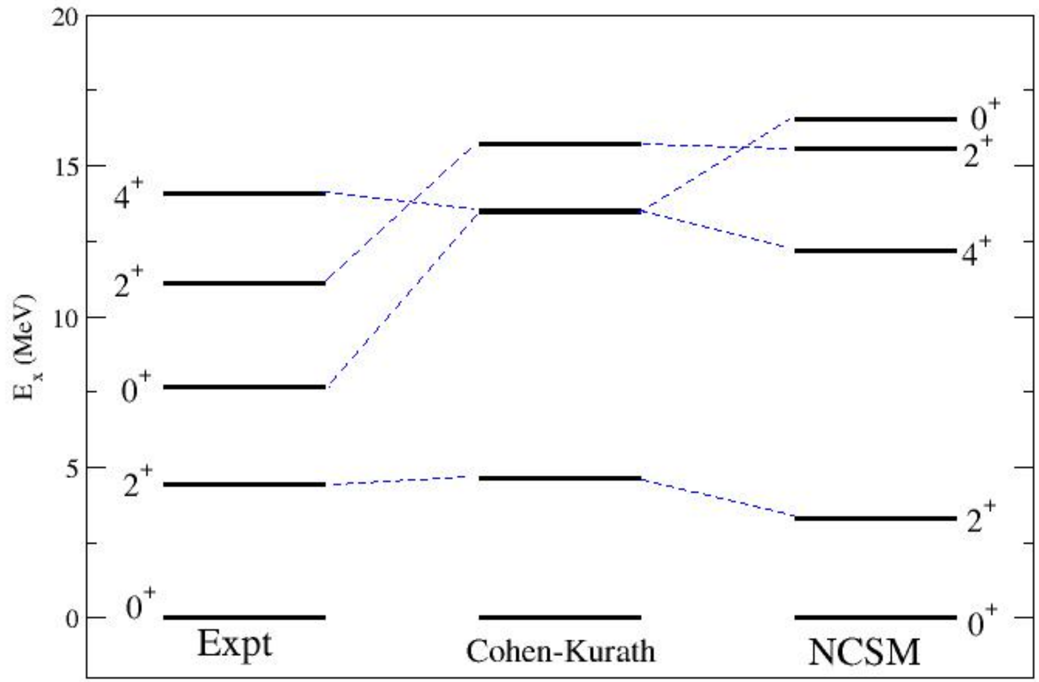
Decomposition of wavefunction into SU(3) components, looking at effect of spin-orbit force:
V. Gueorguiev, J. P Draayer, and C. W. J., PRC **63,** 014318 (2000).

Present calculations carried out using BIGSTICK shell-model code:
Johnson, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761 (2013).

^{12}C

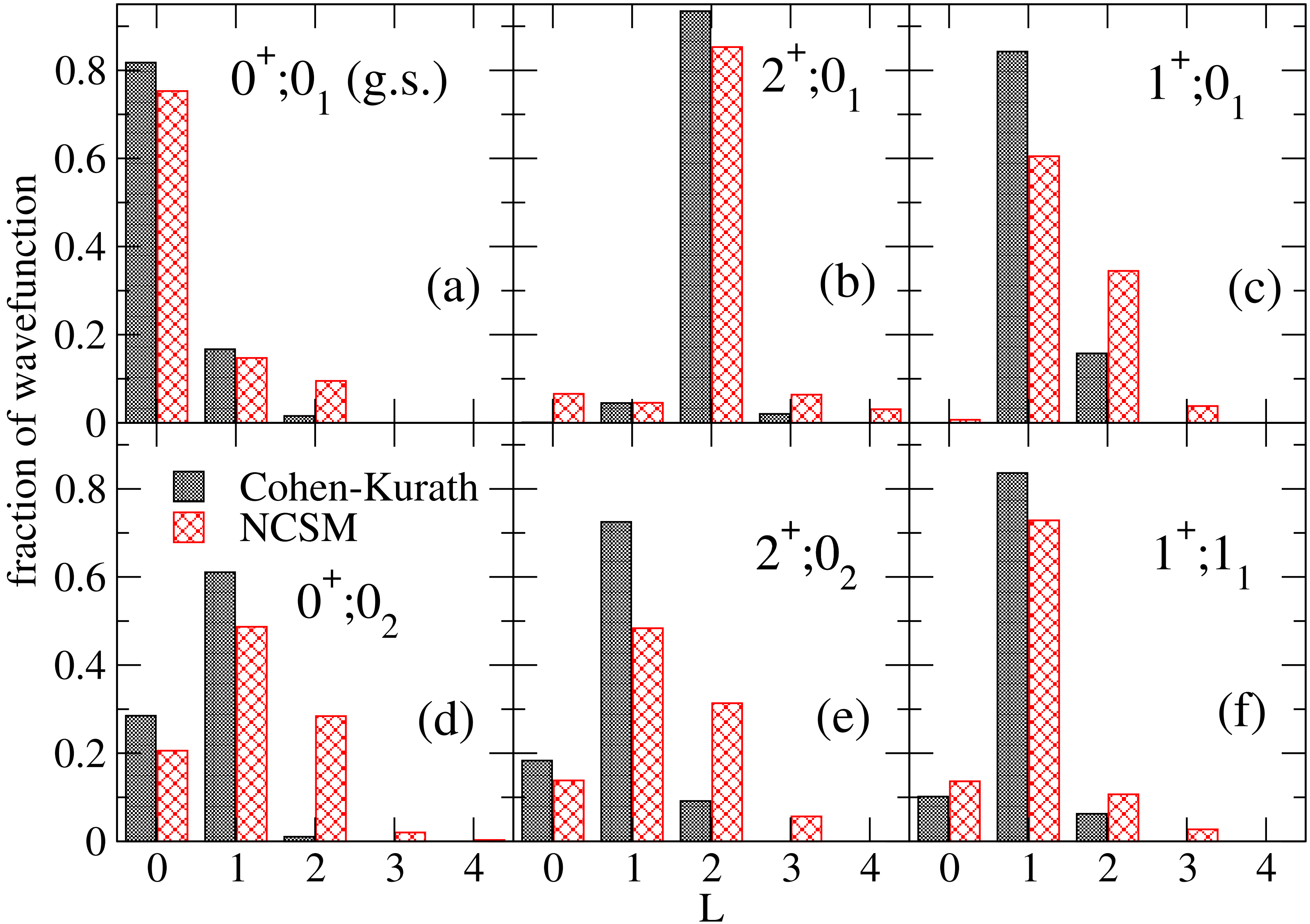
Phenomenological Cohen-Kurath force (1965) in 0*p* shell
m-scheme dimension: 51

NCSM: N3LO chiral 2-body force SRG evolved* to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 35 million



(Calculations carried out using BIGSTICK shell-model code: Johnson, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761 (2013).)

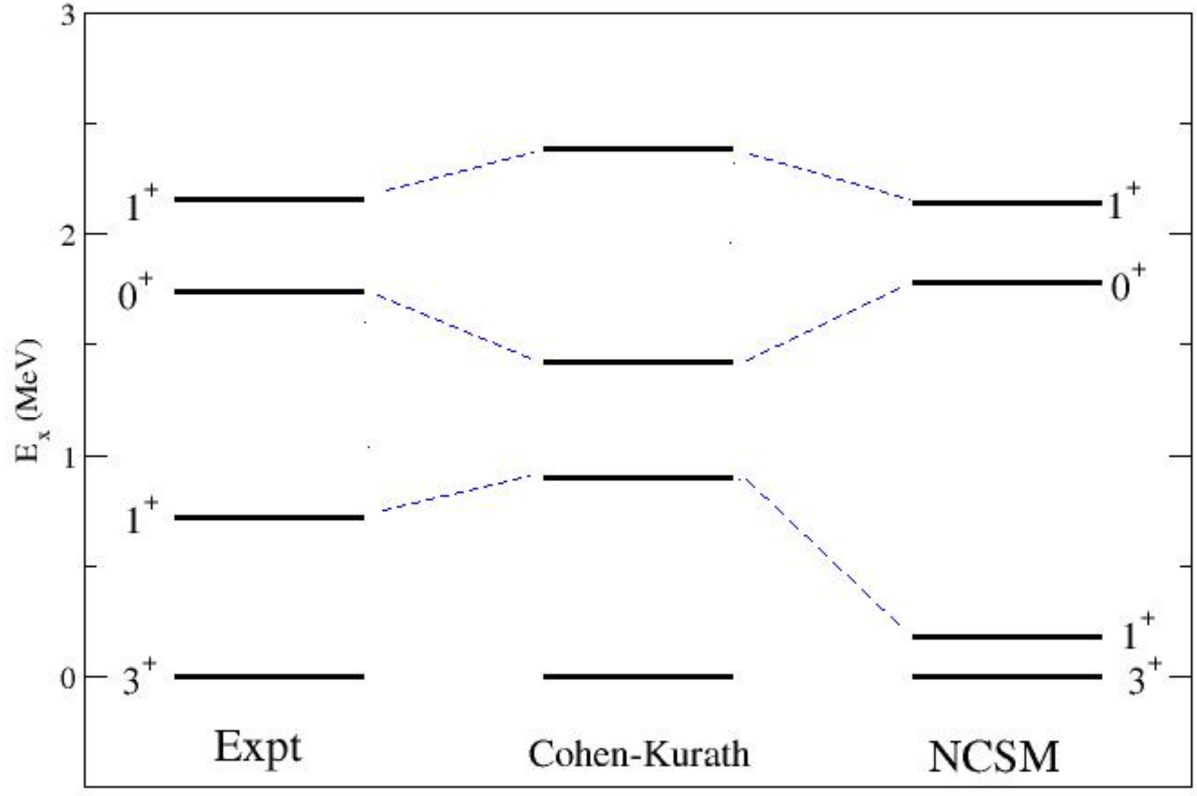
*code courtesy of P. Navratil, any mistakes in using it are mine!

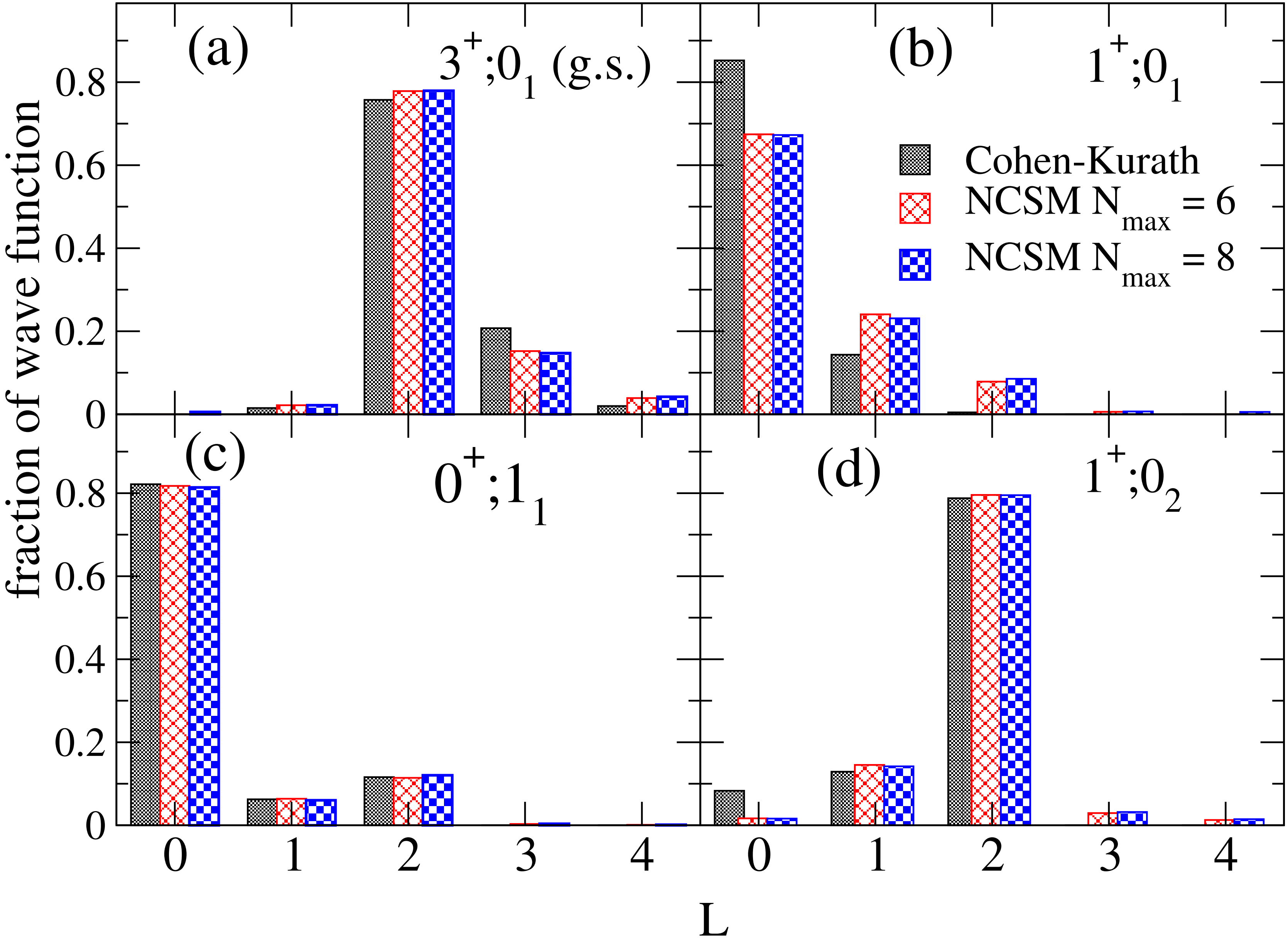

fraction of wavefunction
0.8
0.6
0.4
0.2
0
$0^+;0_1$ (g.s.)
(a)
$2^+;0_1$
(b)
$1^+;0_1$
(c)
Cohen-Kurath
NCSM
$0^+;0_2$
(d)
$2^+;0_2$
(e)
$1^+;1_1$
(f)
0 1 2 3 4
L

^{10}B

Phenomenological Cohen-Kurath *m*-scheme dimension: 84

NCSM: N3LO chiral 2-body force SRG evolved to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 12 million

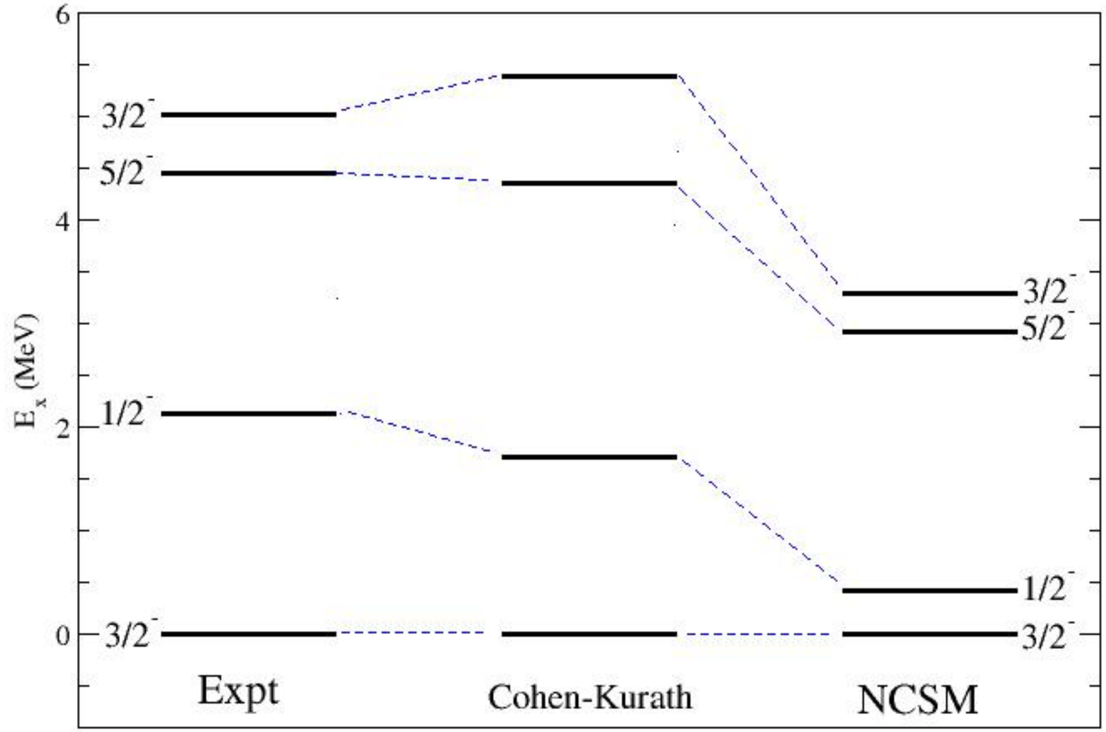


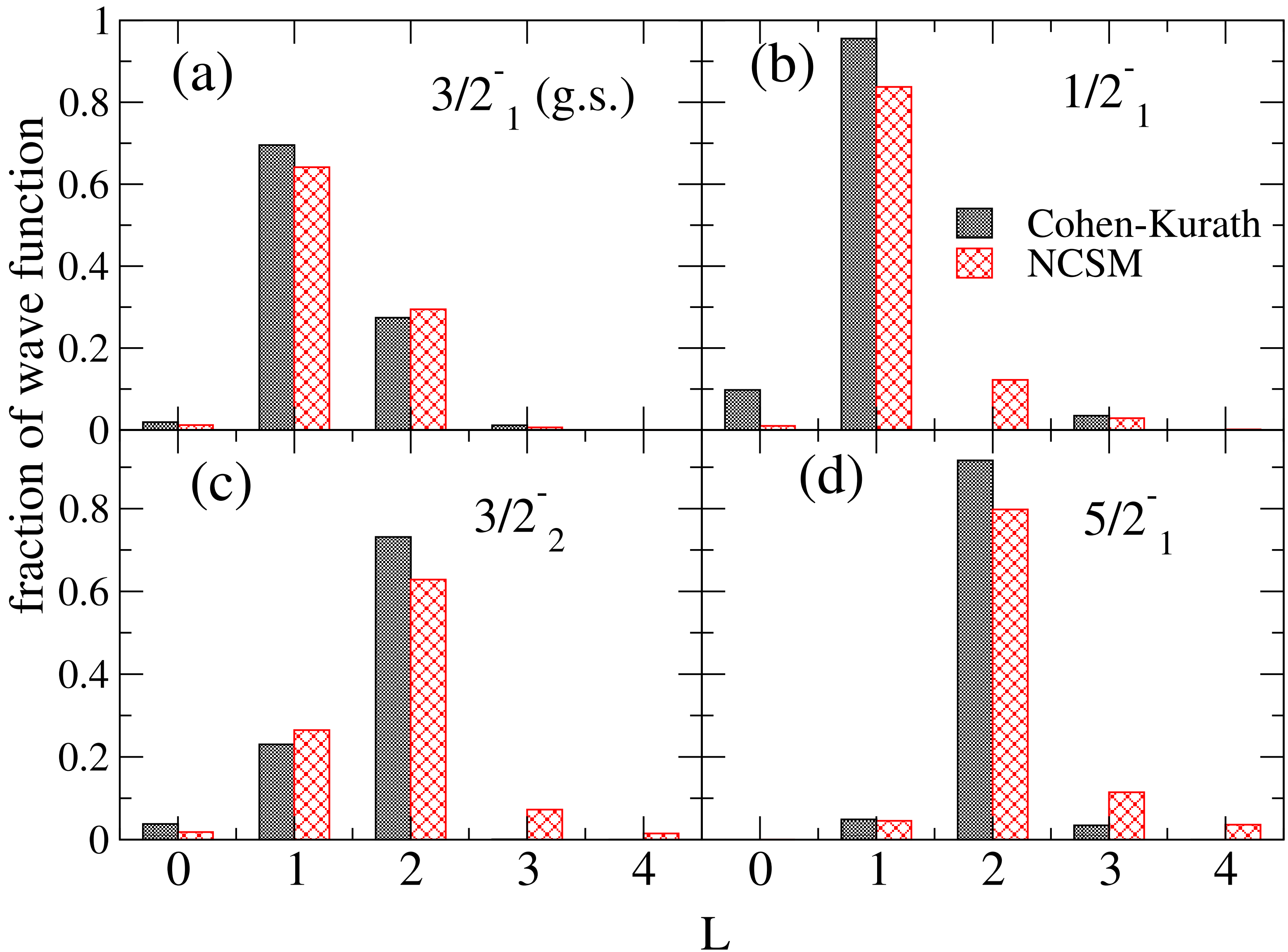

(a)
3+;01 (g.s.)
(b)
1+;01
Cohen-Kurath
NCSM Nmax = 6
NCSM Nmax = 8
(c)
0+;11
(d)
1+;02
fraction of wave function
0
0.2
0.4
0.6
0.8
0
1
2
3
4
L

^{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

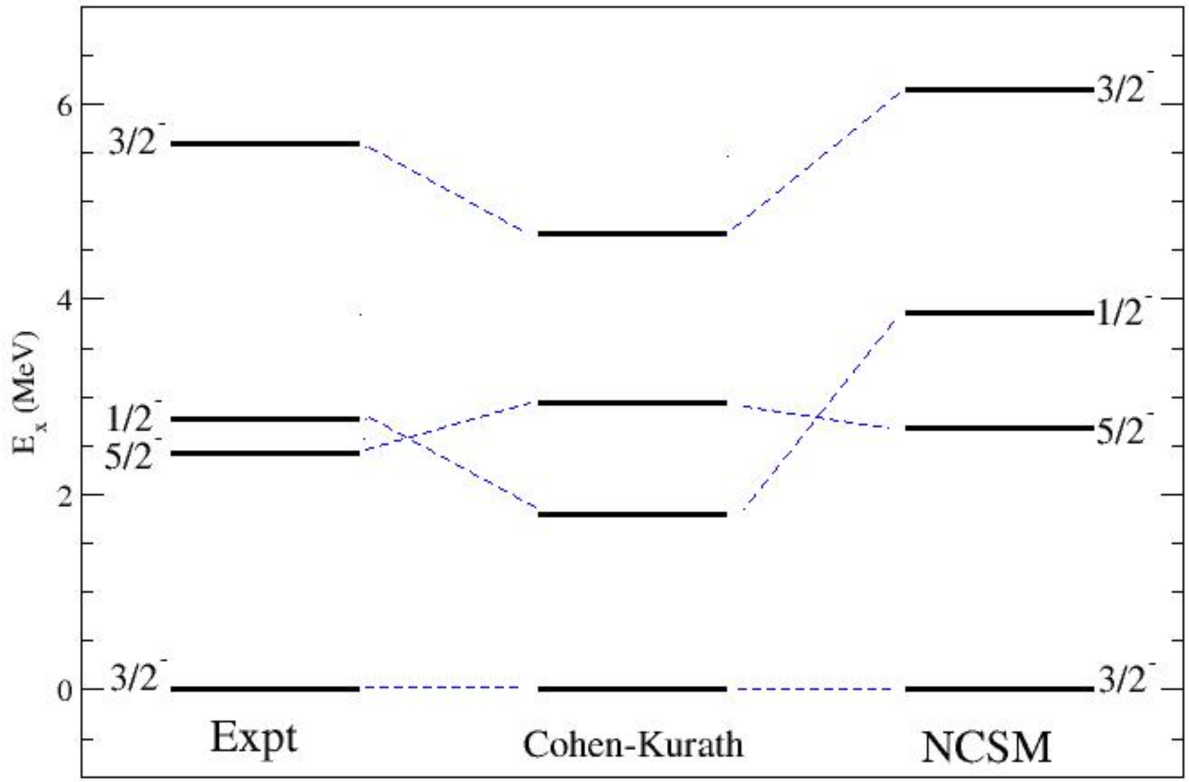


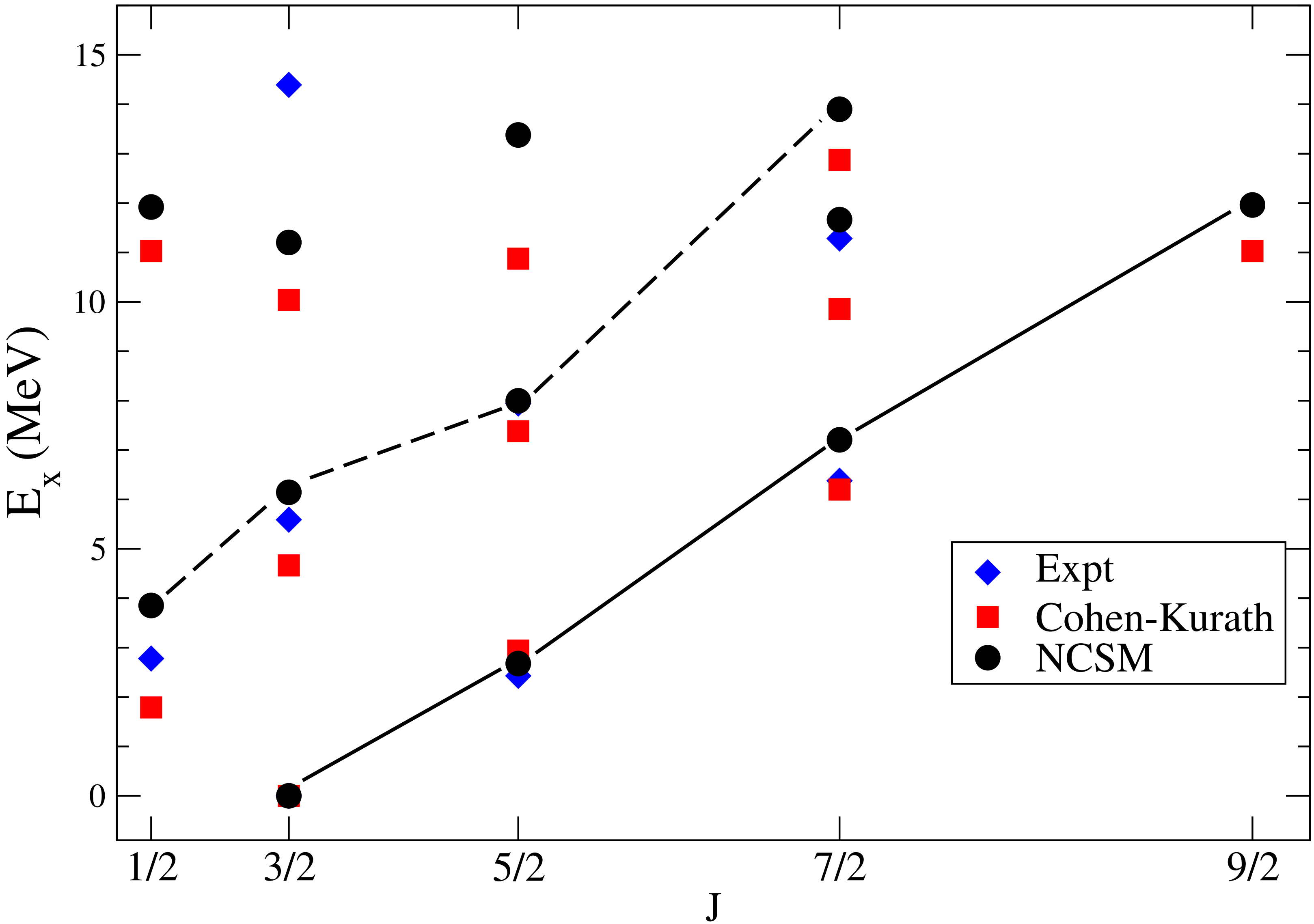

fraction of wave function
L
(a)
3/2$^-_1$ (g.s.)
(b)
1/2$^-_1$
(c)
3/2$^-_2$
(d)
5/2$^-_1$
Cohen-Kurath
NCSM
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4

^{9}Be

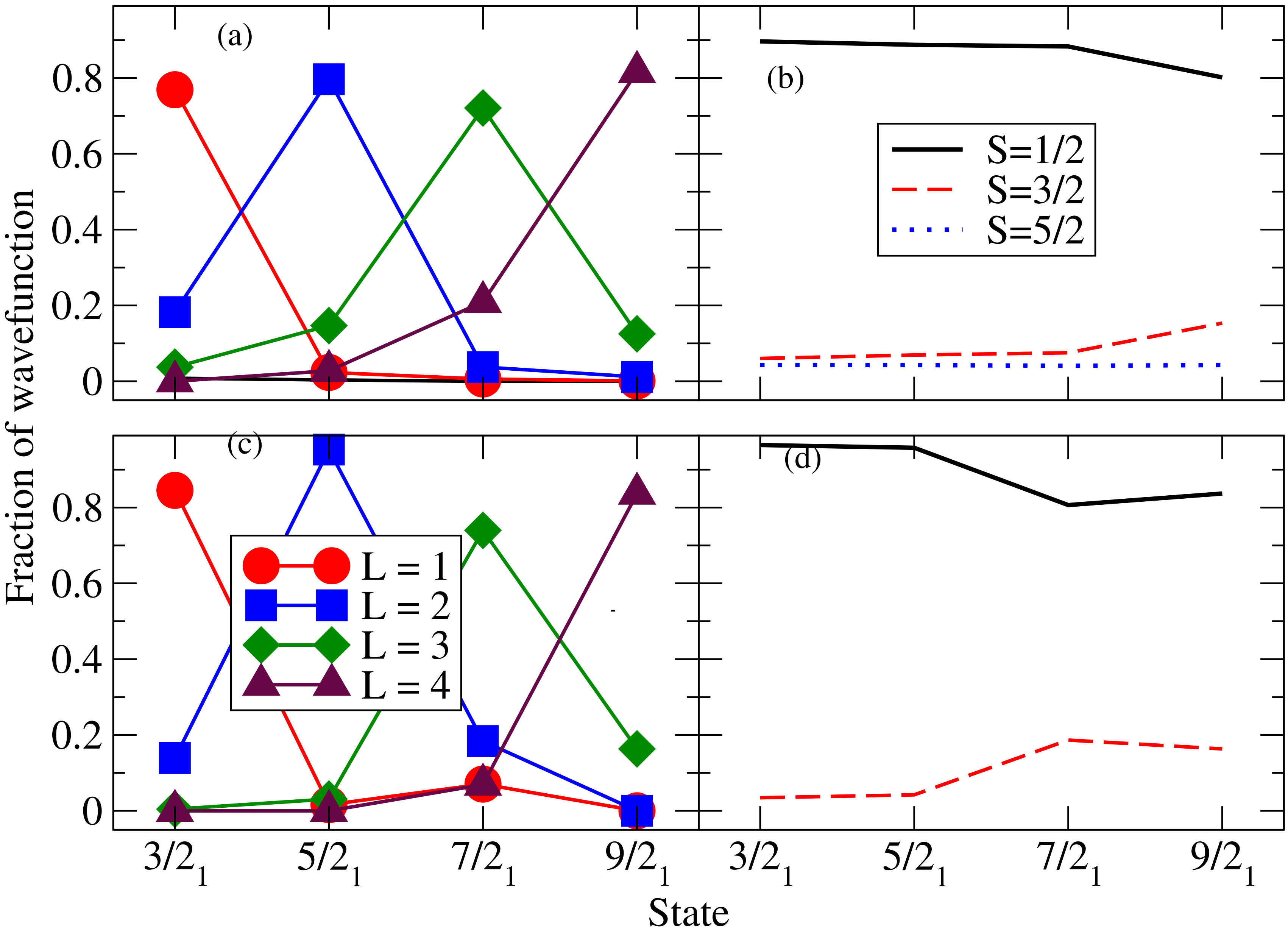
Phenomenological Cohen-Kurath *m*-scheme dimension: 62

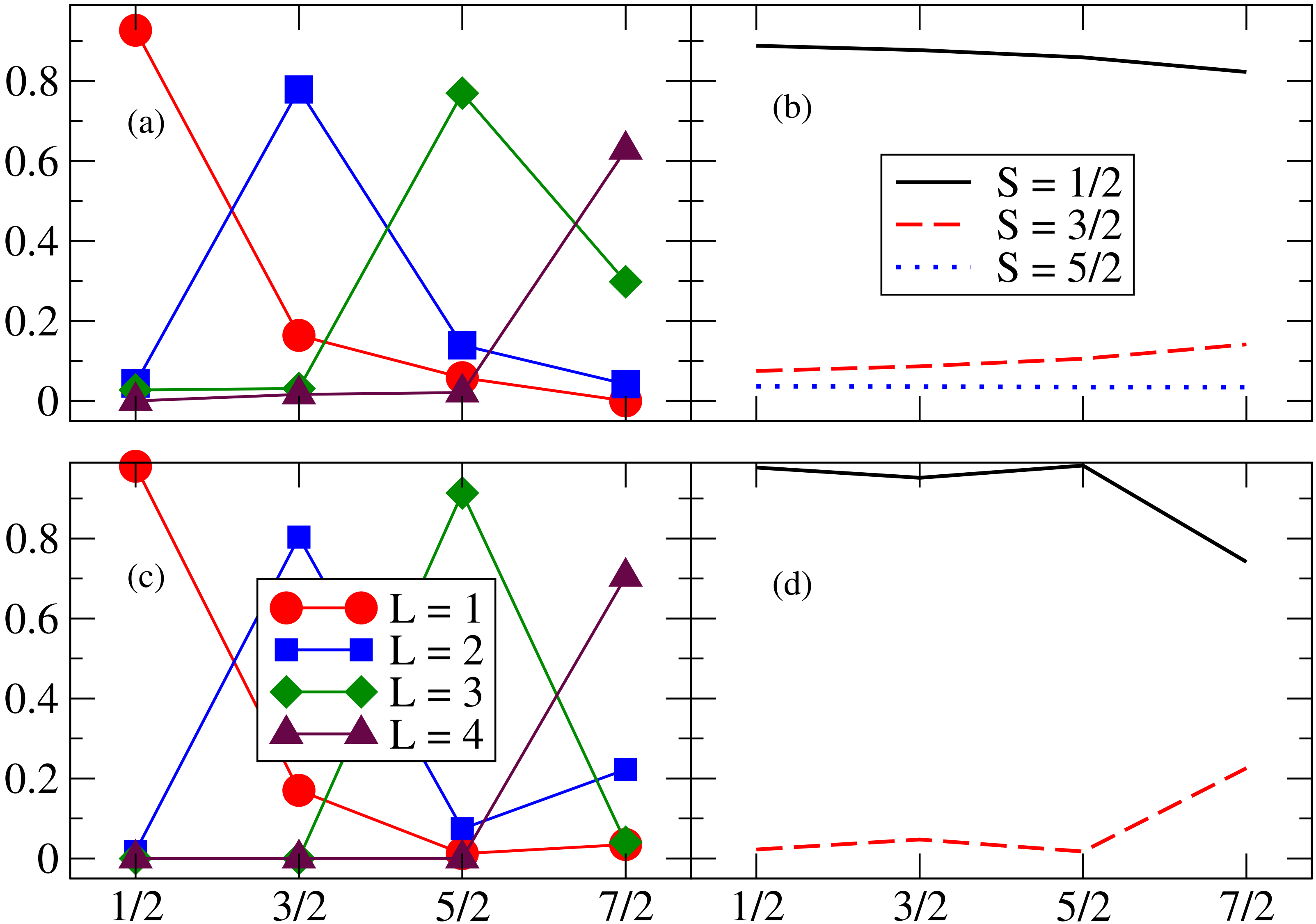
NCSM: N3LO chiral 2-body force SRG evolved to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 5.2 million

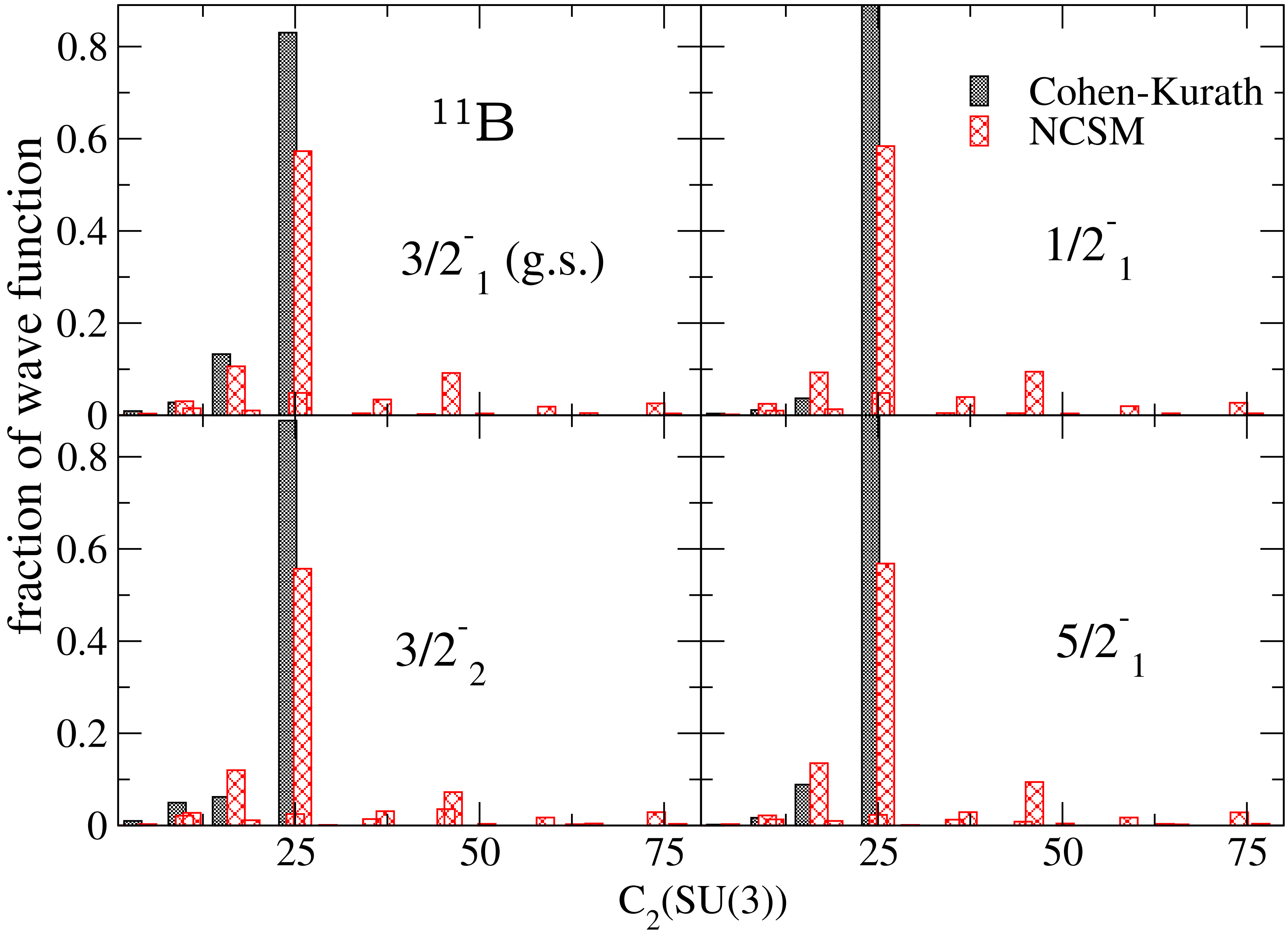




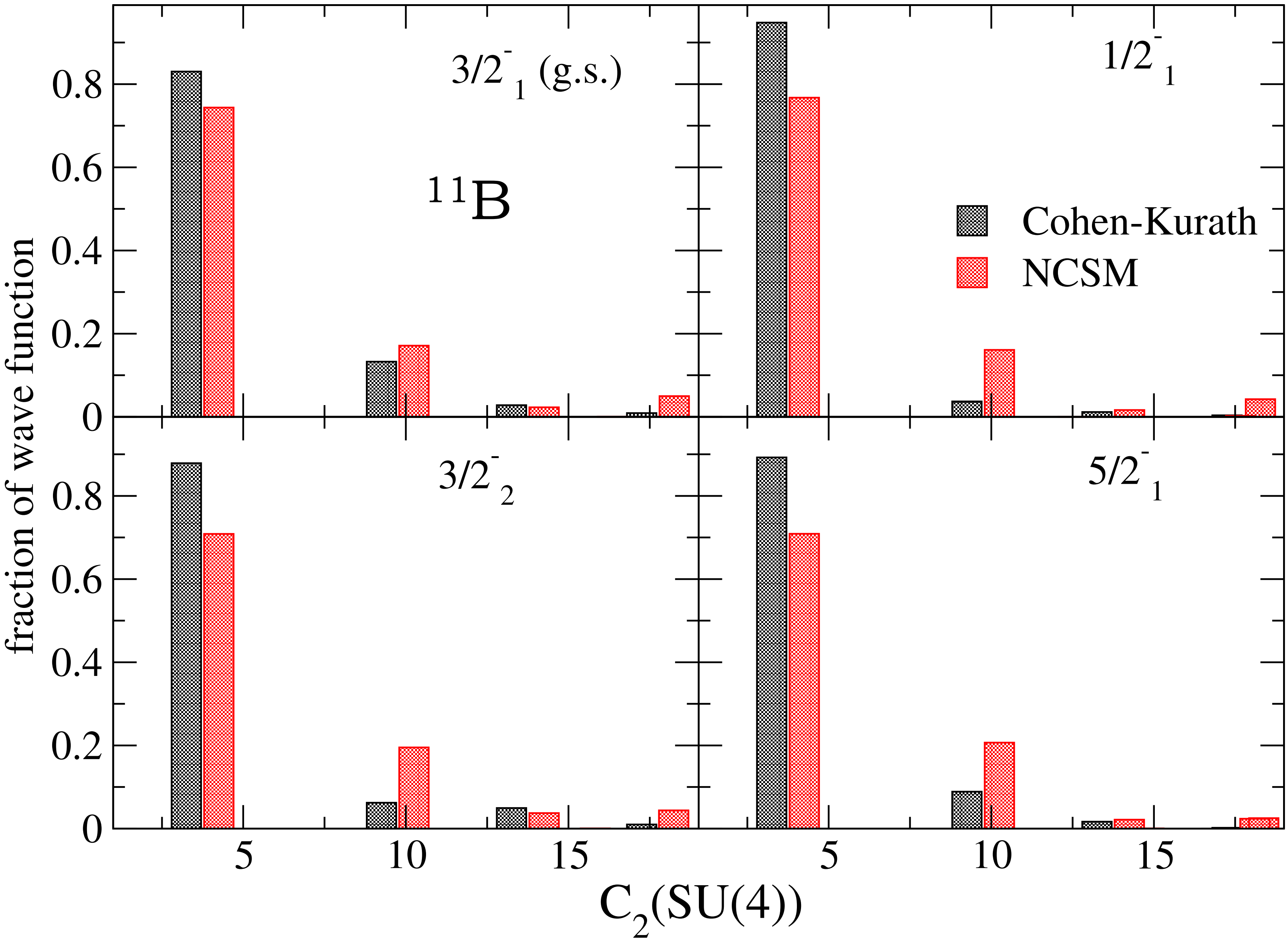
15
10
5
0
E_x (MeV)
1/2
3/2
5/2
7/2
9/2
J
Expt
Cohen-Kurath
NCSM


(a)
(b)
(c)
(d)
S=1/2
S=3/2
S=5/2
L = 1
L = 2
L = 3
L = 4
0
0.2
0.4
0.6
0.8
Fraction of wavefunction
3/2$_1$
5/2$_1$
7/2$_1$
9/2$_1$
State


0.8
0.6
0.4
0.2
0
(a)
(b)
S = 1/2
S = 3/2
S = 5/2
(c)
(d)
L = 1
L = 2
L = 3
L = 4
1/2
3/2
5/2
7/2



0.8
0.6
0.4
0.2
0
fraction of wave function
^{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))


3/2⁻₁ (g.s.)
1/2⁻₁
^{11}B
Cohen-Kurath
NCSM
3/2⁻₂
5/2⁻₁
fraction of wave function
0
0.2
0.4
0.6
0.8
5
10
15
C$_2$(SU(4))