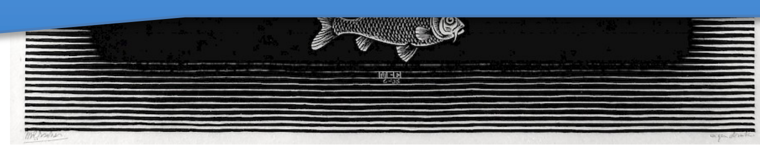
And now for something a little bit different!



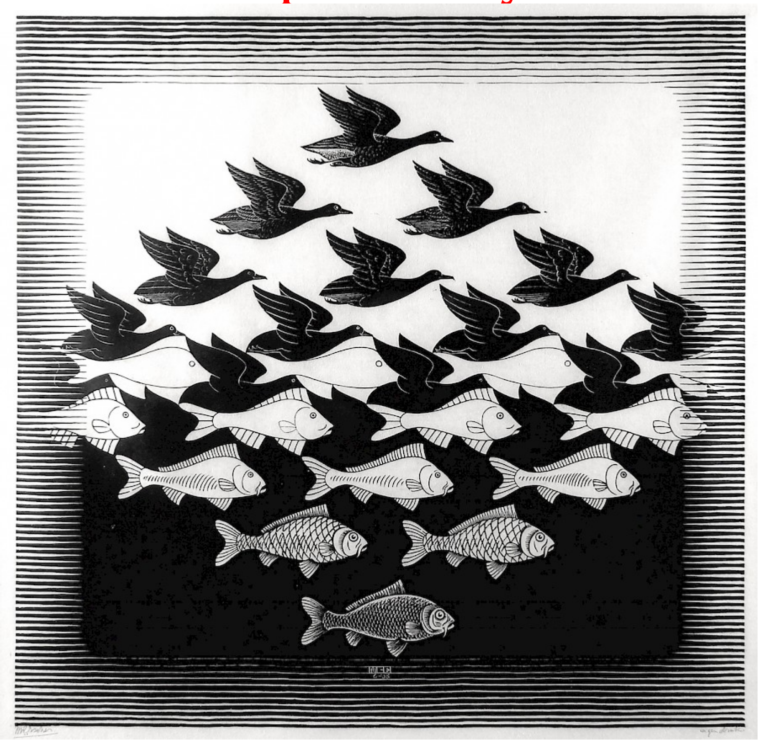
SAN DIEGO STATE UNIVERSITY

Calvin W. Johnson, San Diego State University

his material is based upon work supported by the U.S. Department of rgy, Office of Science, Office of Nuclear Physics, under Award Number DE-FG02-96ER40985”

Progress in ab initio methods/ TRIUMF / Feb 28 2019

The Similarity Renormalization Group seen through the lens of Group Theory



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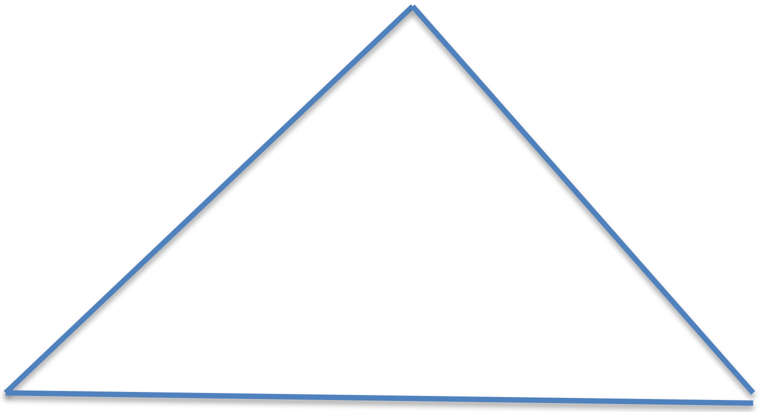
Progress in ab initio methods/ TRIUMF / Feb 28 2019

San Diego State University

This talk has the shape of a triangle:



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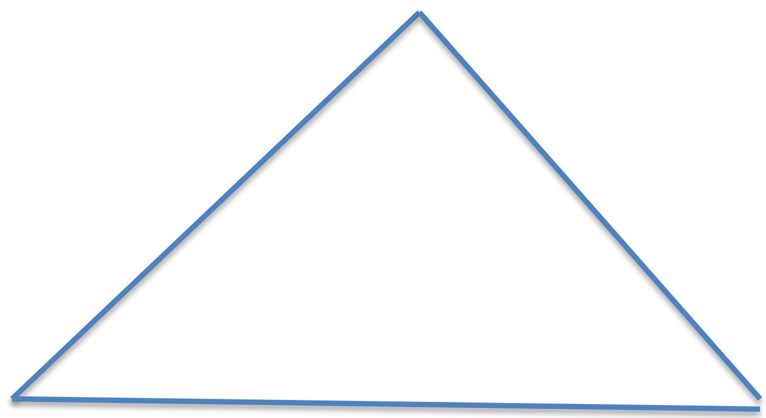
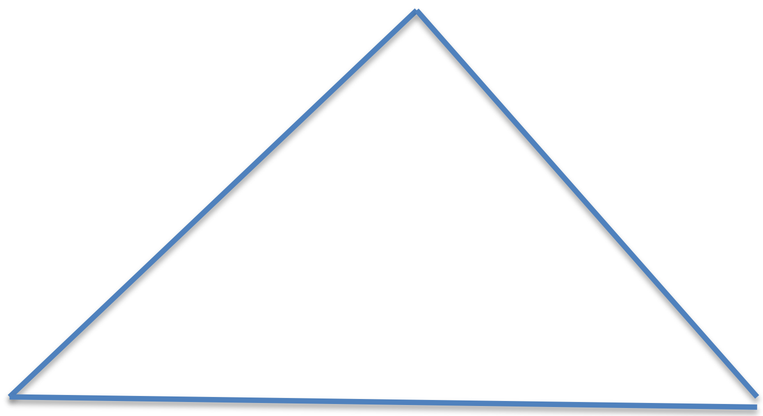


SRG: the similarity renormalization group:
-> *unitary transformations*

San Diego State University

This talk has the shape of a triangle:

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



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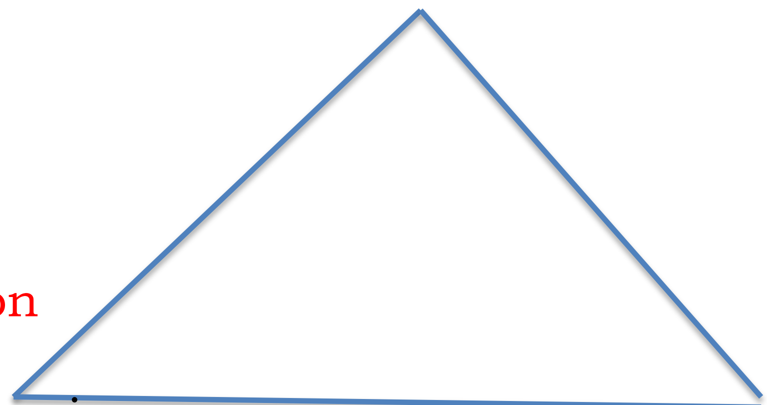

Spectral distribution theory, a metric on the space of Hamiltonians
-> a new way to look at SRG and a new SRG

SRG: the similarity renormalization group:
-> unitary transformations

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

we use the matrix formalism


Maria Mayer

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

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

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

To facilitate calculations, we often "soften" the nuclear interaction using *the similarity renormalization group*

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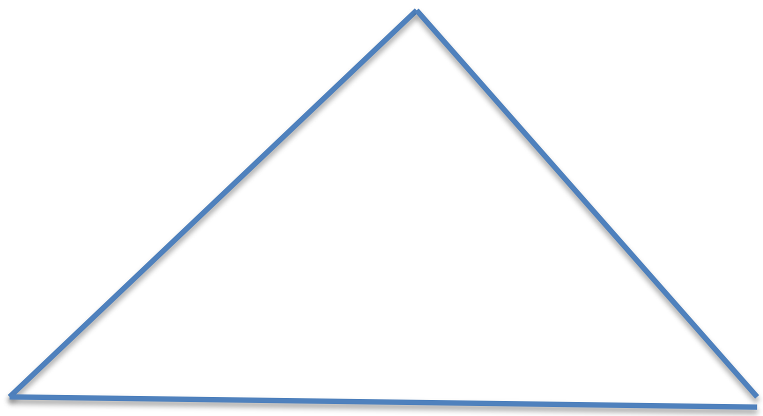

SRG: the similarity renormalization group:
-> *unitary transformations*

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

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

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

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

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SAN DIEGO STATE UNIVERSITY

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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

$H(s) =$

U

$dH($

SRG is applied at the few-body level;
how can we understand the effect
on the many-body wave function?

The nuclear force

η = [G,H]

the *generator* .

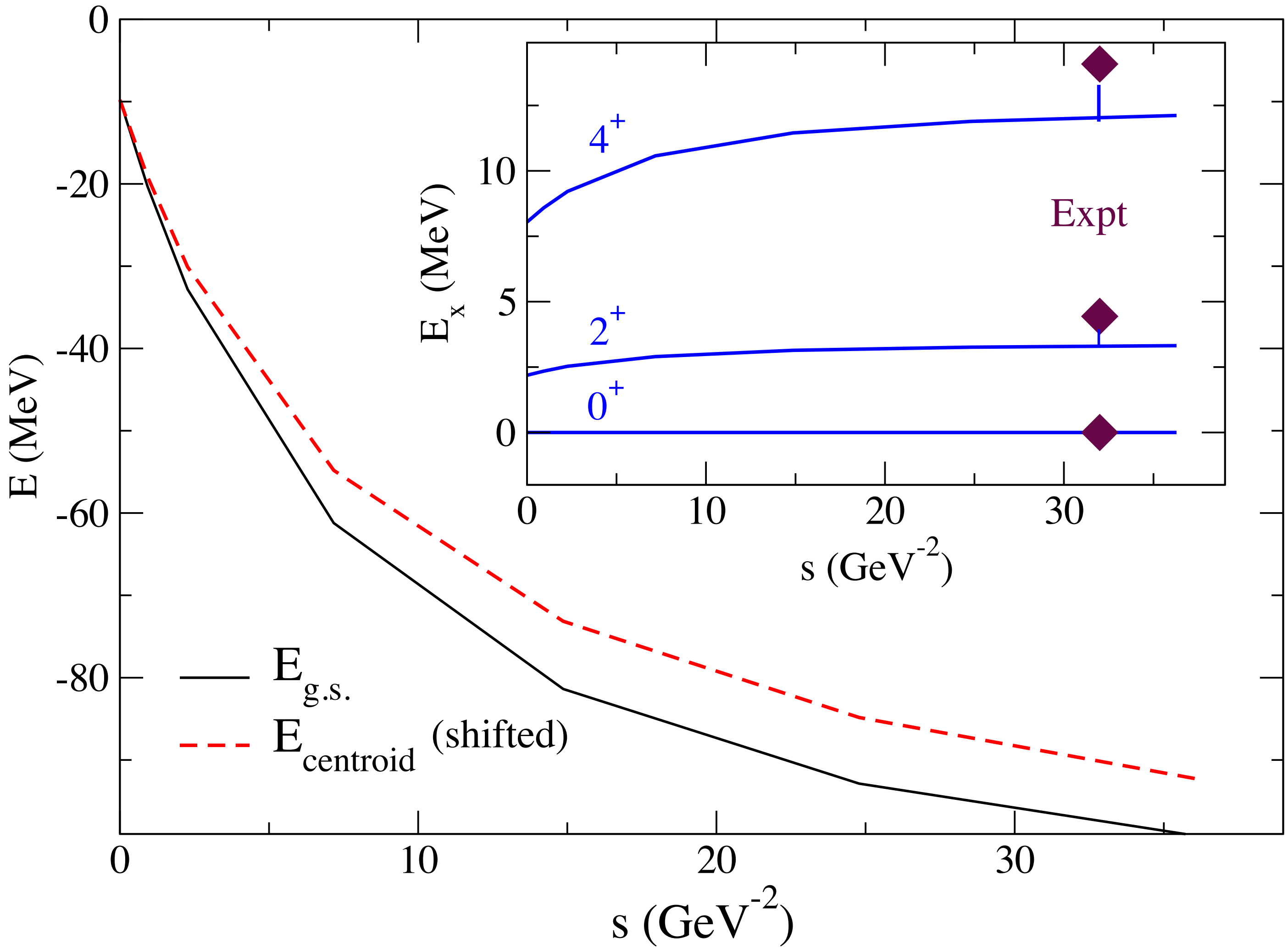
H(s) to be "more like" G.

his soon).

A common choice is the kinetic energy

^{12}C, N_{max} =6 Entem-Machleidt evolved via SRG

CWJ, Phys. Lett. B. **774**, 465 (2017)



^{12}C, $N_{max}=6$

Entem-Machleidt evolved via SRG

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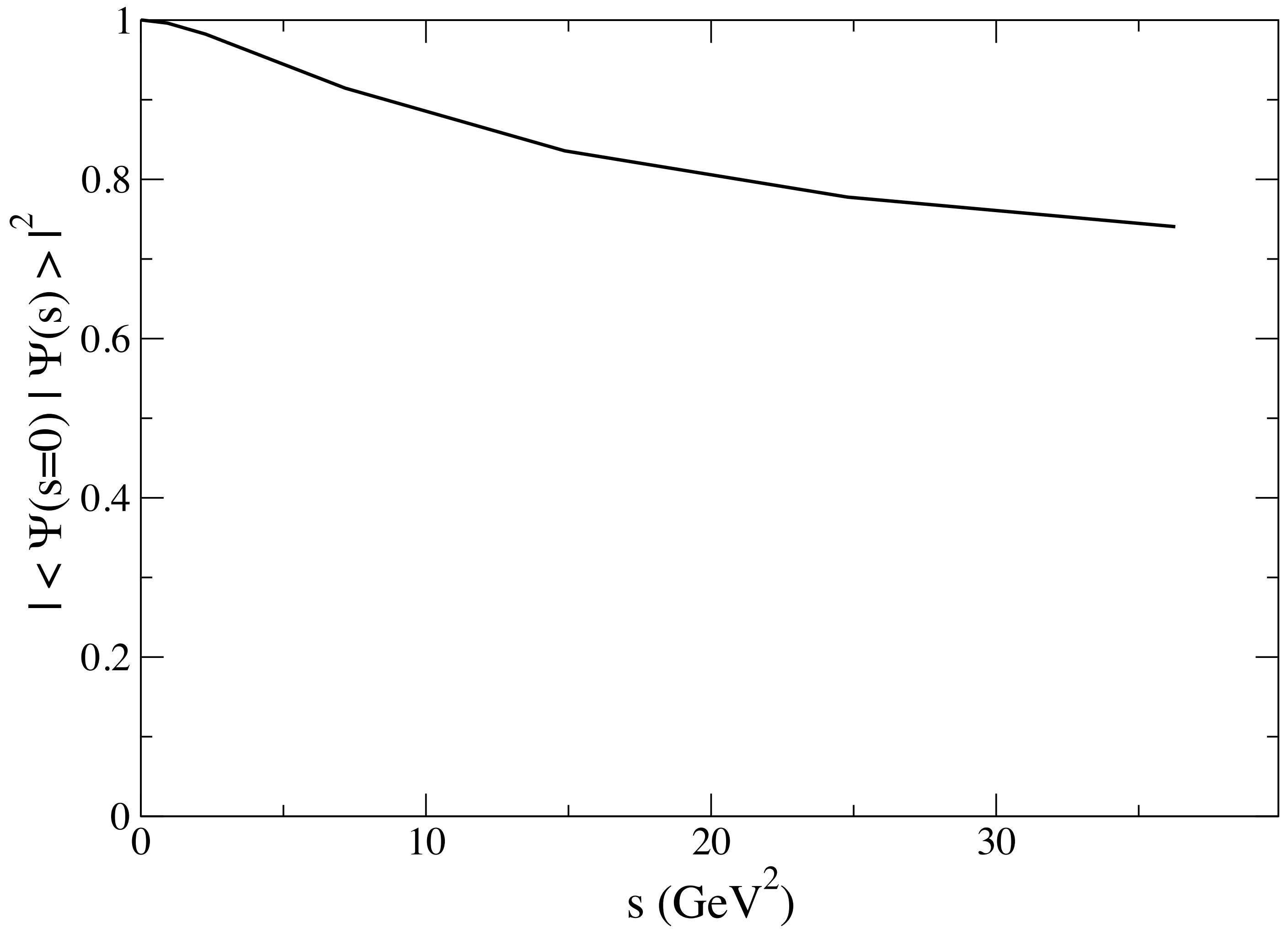

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For example....

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

we use the matrix formalism

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

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

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

$\hat{\mathbf{H}}$

$c_\alpha|\alpha\rangle$

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

Largest (?) known M-scheme calculation

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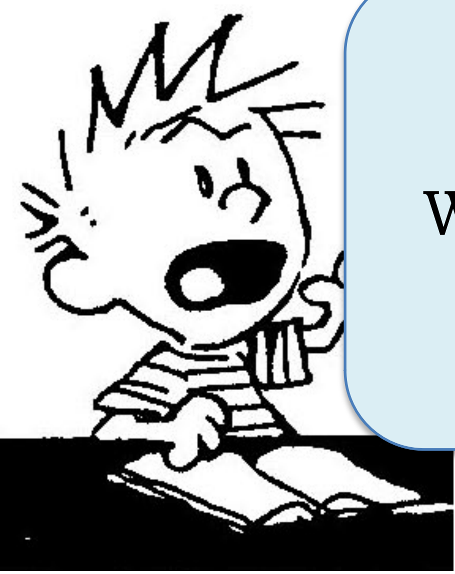
For example

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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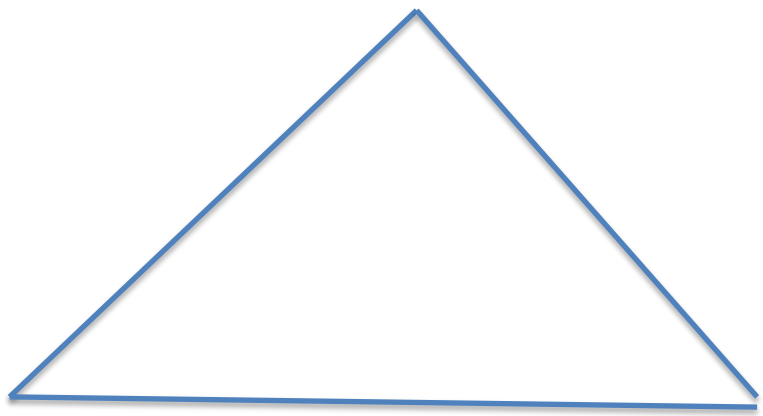
San Diego State University

This talk has its own triangle:

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



SRG: the similarity
renormalization group:
-> *unitary*
transformations

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

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Casimir

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

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*)

SAN DIEGO STATE UNIVERSITY

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*

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

SAN DIEGO STATE UNIVERSITY

Casimir

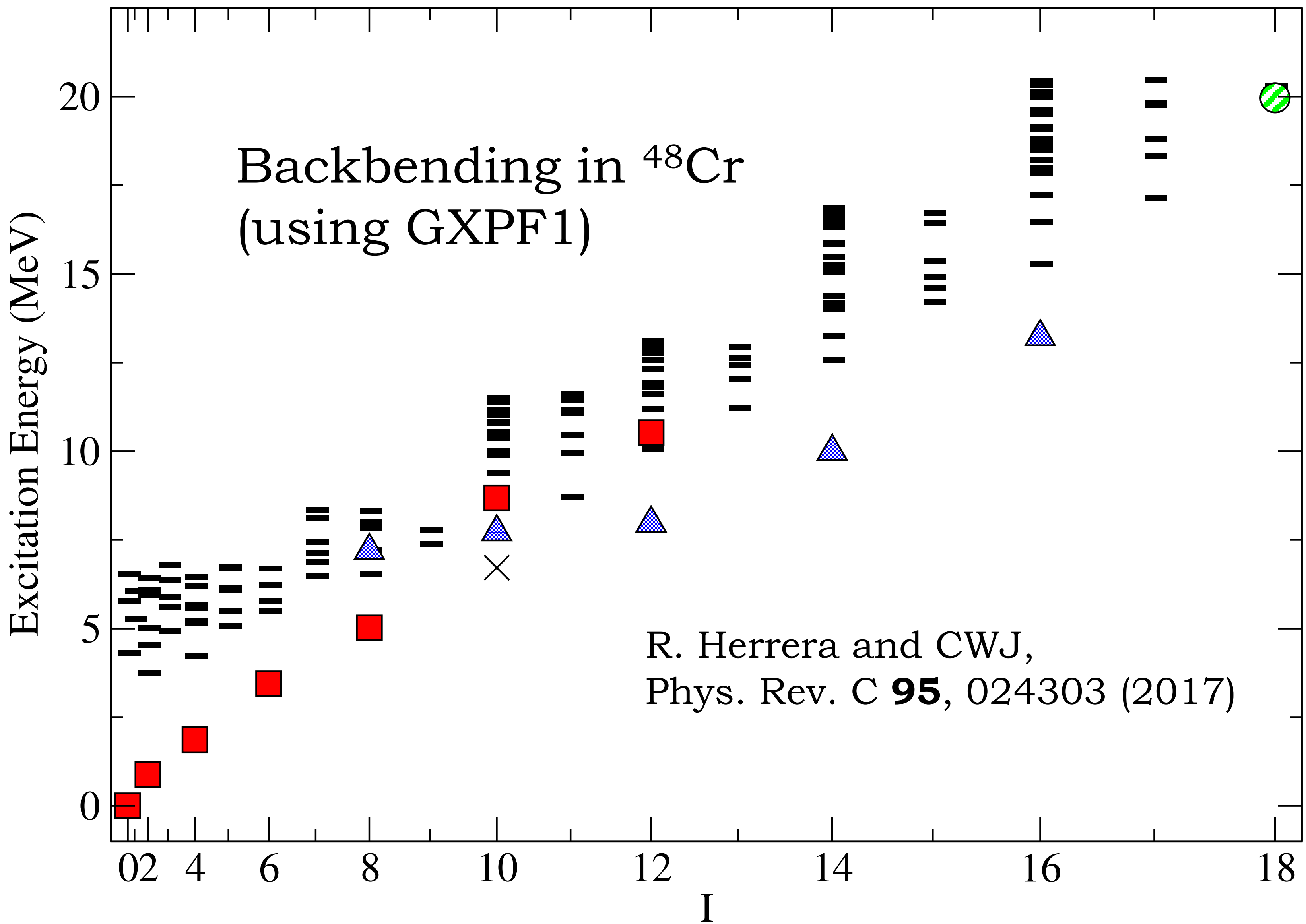
$$\hat{C}\left|z,\alpha\right\rangle = z\left|z,\alpha\right\rangle$$

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

Fo ... ne

the ... *rrep*

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


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)

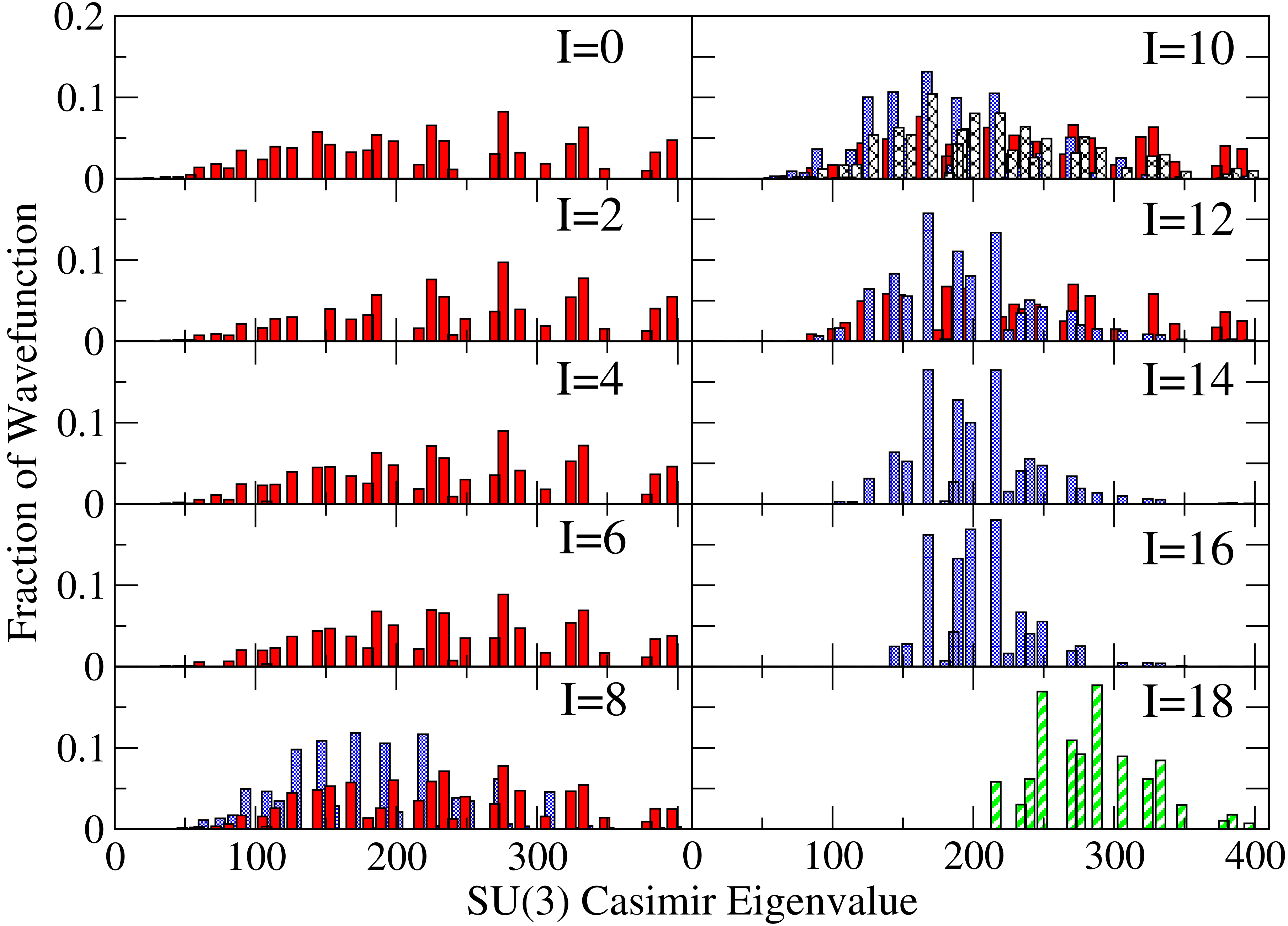
Wave functions computed in interacting shell model* using GXPF1 interaction; then SU(3) 2-body Casimir read in and decomposition done with Lanczos

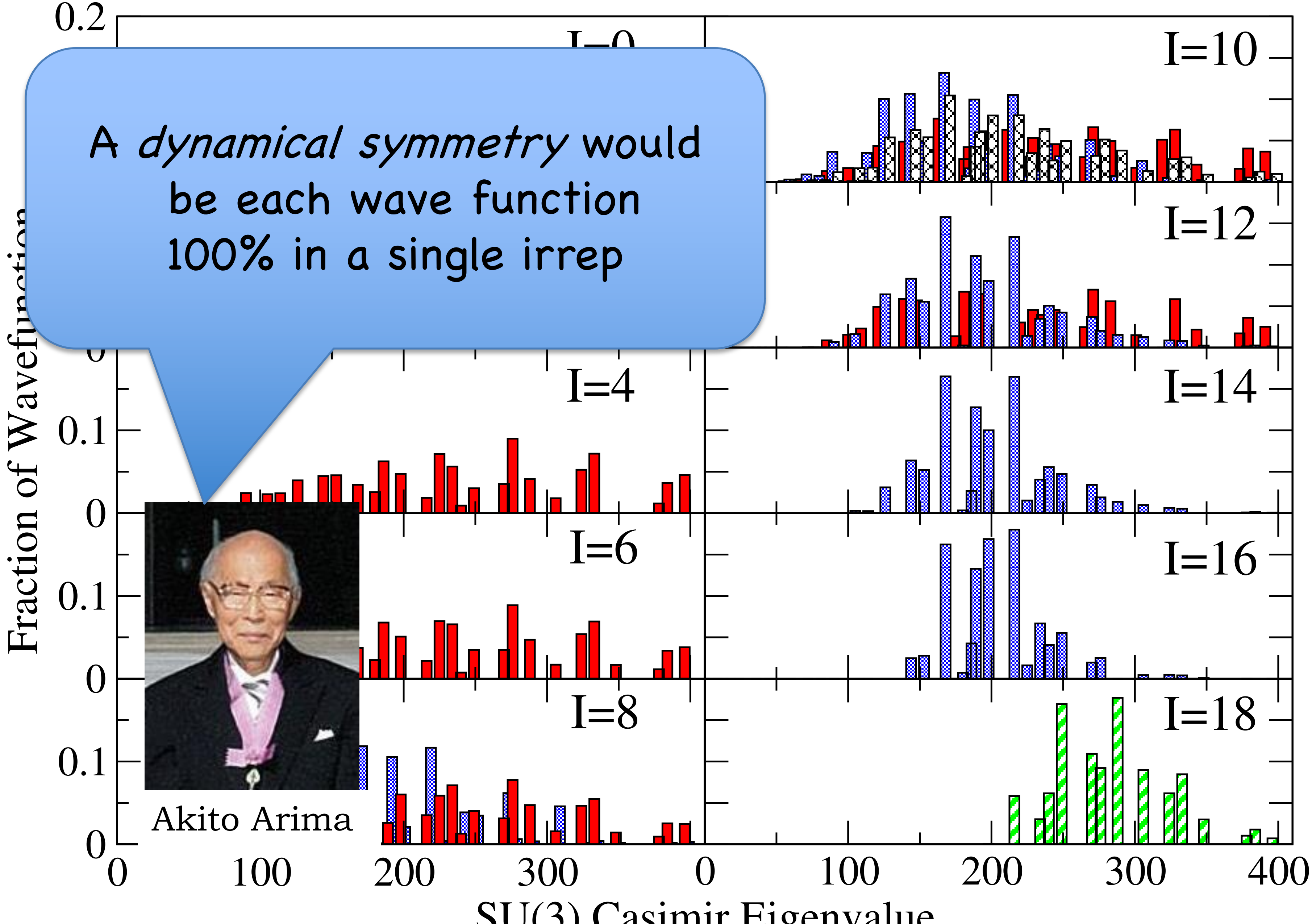
R. Herrera and CWJ,
Phys. Rev. C **95**, 024303 (2017)

*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


Fraction of Wavefunction
SU(3) Casimir Eigenvalue
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


A *dynamical symmetry* would be each wave function 100% in a single irrep
Akito Arima
Fraction of Wavefunction
SU(3) Casimir Eigenvalue
I=0
I=4
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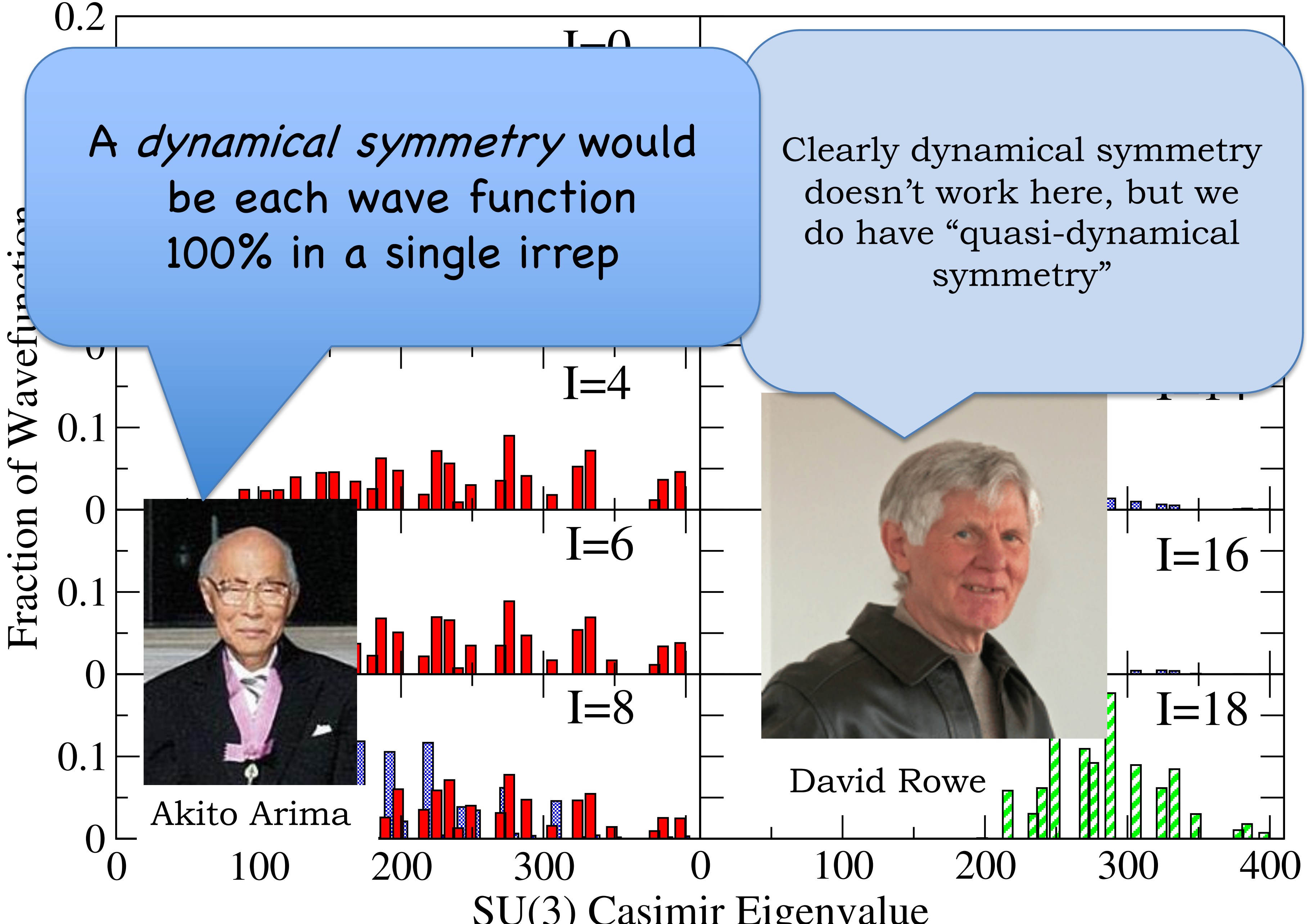
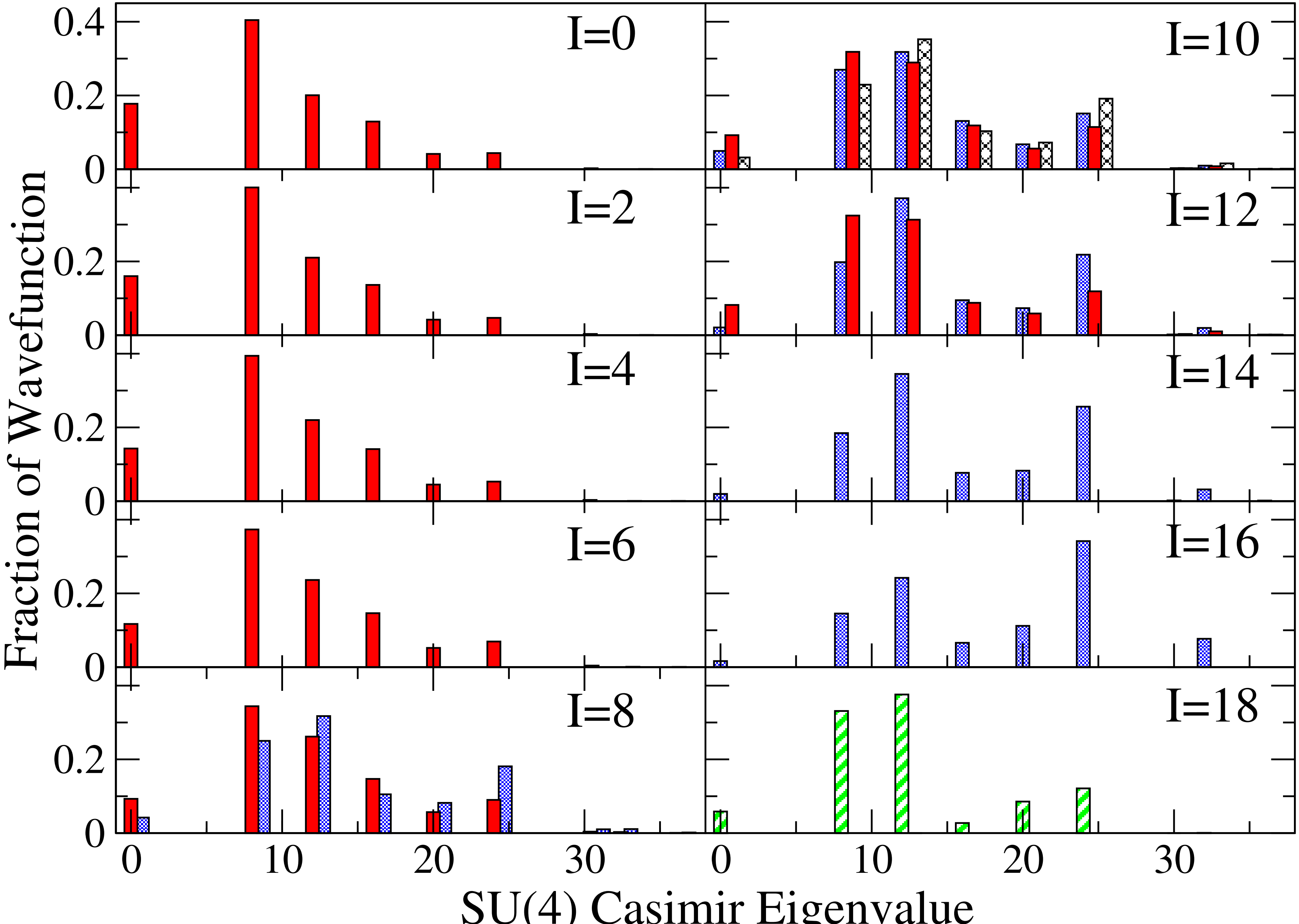

A *dynamical symmetry* would be each wave function 100% in a single irrep
Clearly dynamical symmetry doesn't work here, but we do have "quasi-dynamical symmetry"
Akito Arima
David Rowe
Fraction of Wavefunction
SU(3) Casimir Eigenvalue
I=4
I=6
I=8
I=16
I=18
0.2
0.1
0
0
100
200
300
400

What about other groups?

Eugene Wigner



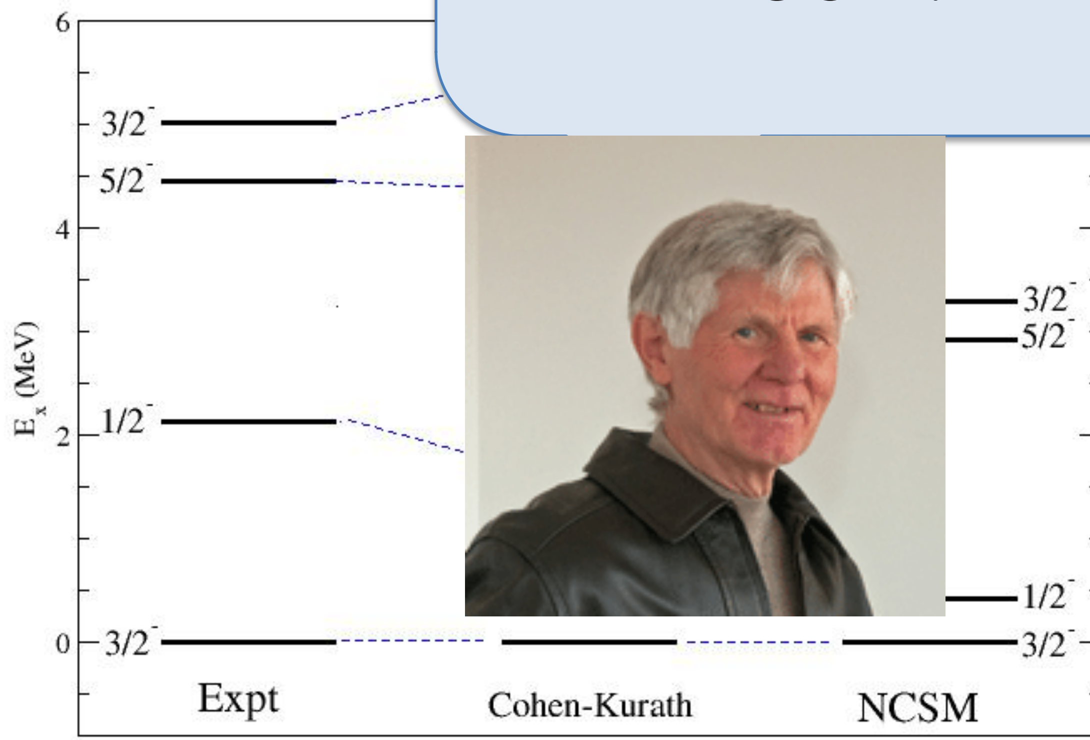
I=0
I=2
I=4
I=6
I=8
I=10
I=12
I=14
I=16
I=18
0.4
0.2
0
Fraction of Wavefunction
0
10
20
30
SU(4) Casimir Eigenvalue

^{11}B

Phenomenological Cohen-Kurath *m*-scheme dim

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

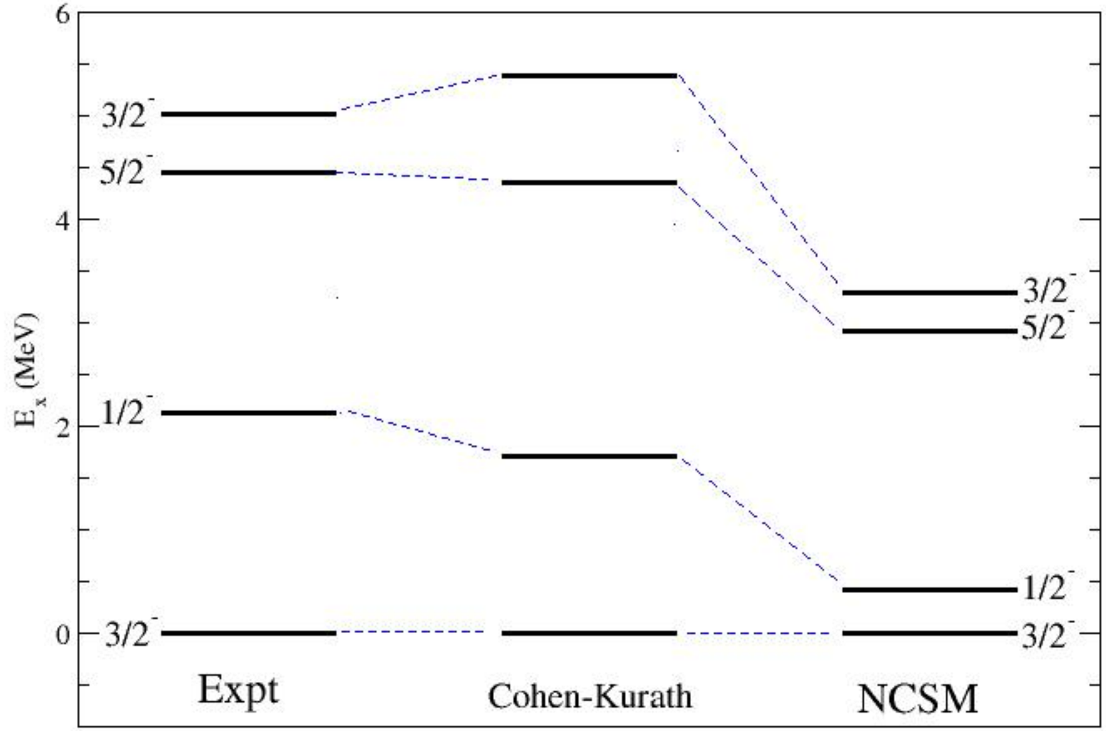
What about
in the
NCSM?

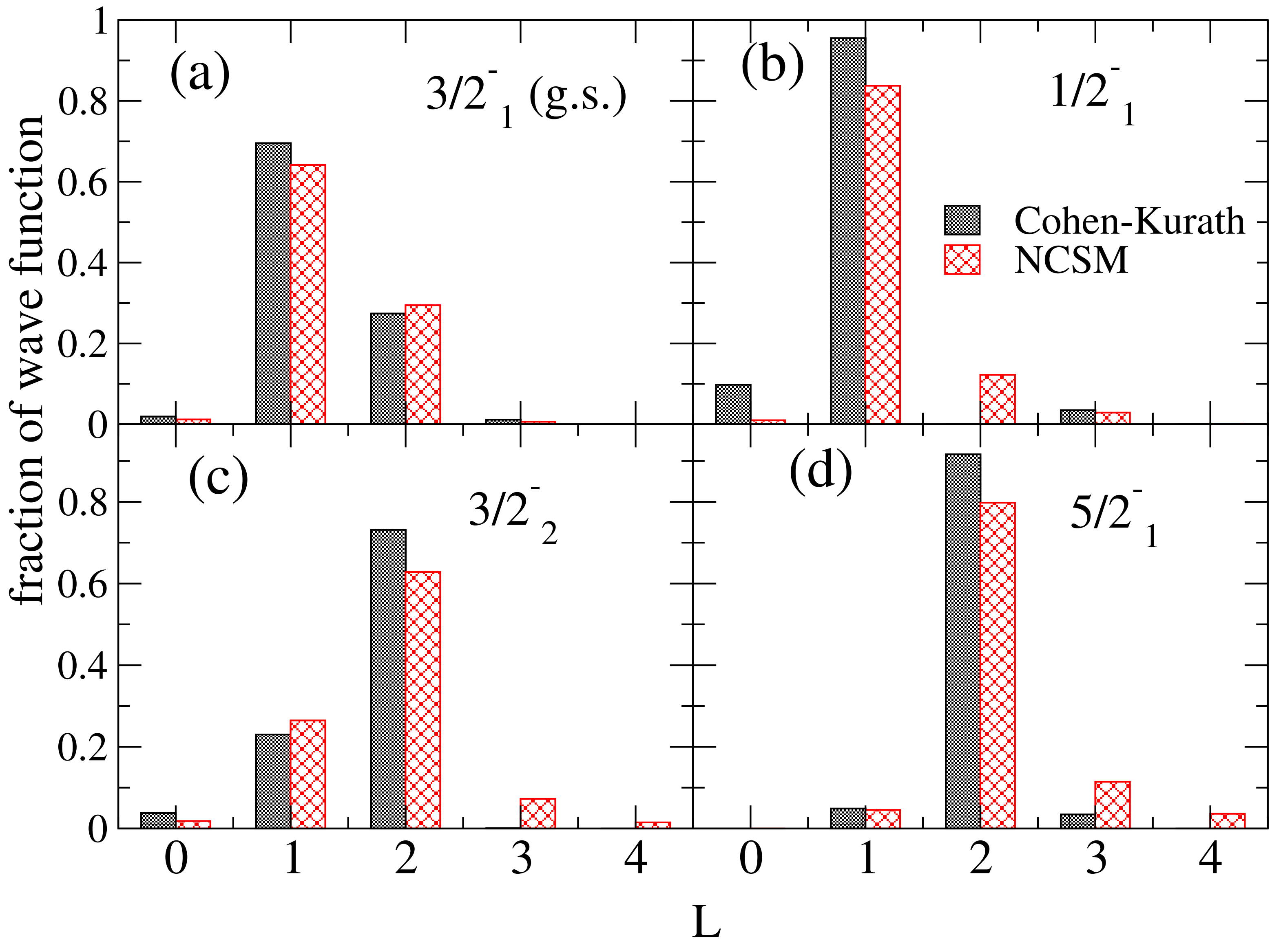


^{11}B

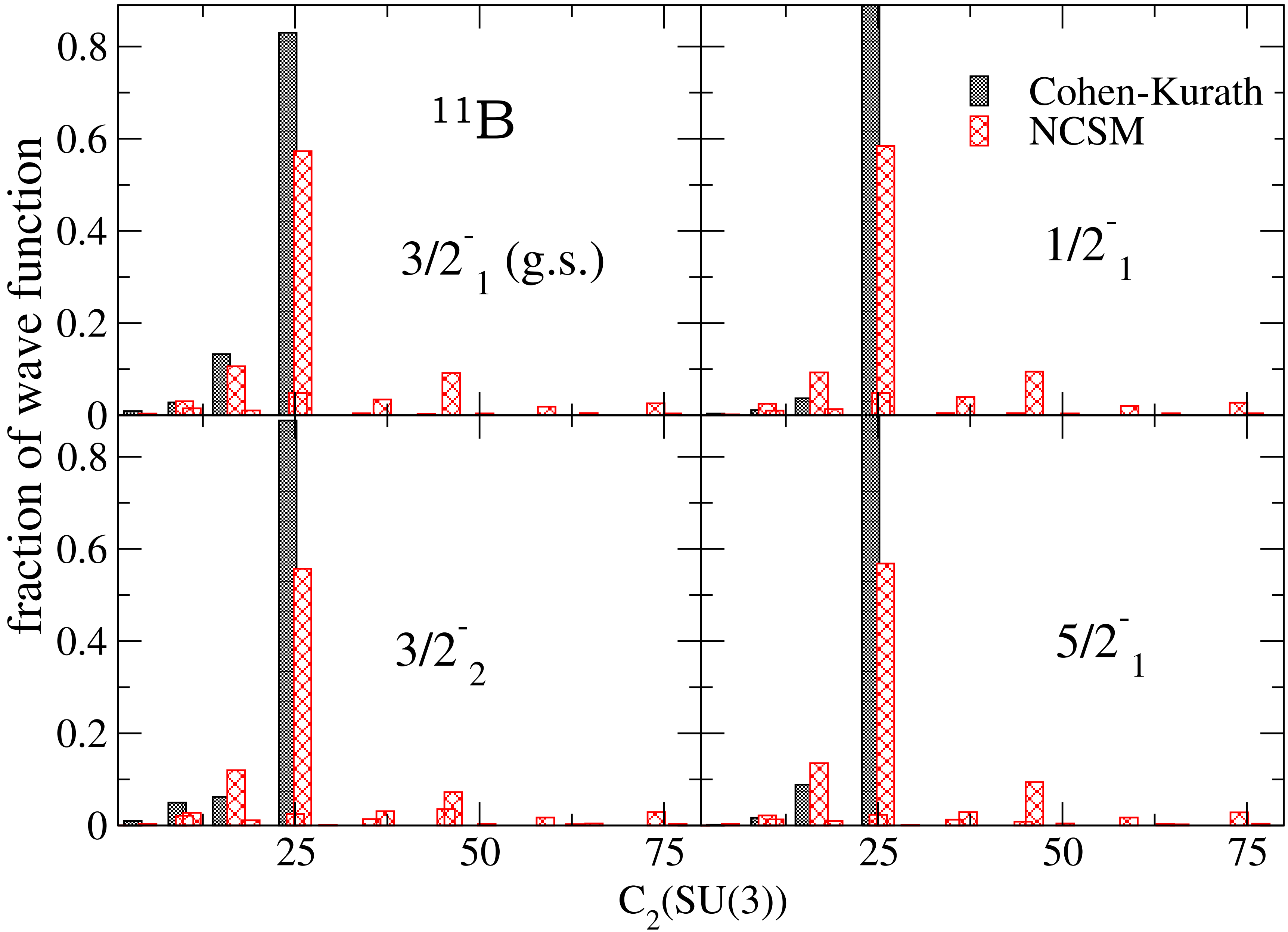
Phenomenological Cohen-Kurath *m*-scheme dimension: 62

NCSM: N3LO chiral 2-body force SRG evolved to λ = 2.0 fm^{-1}, N_{max} = 6, ħω=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
0.2
0.4
0.6
0.8
^{11}B
$3/2^-_1$ (g.s.)
$1/2^-_1$
$3/2^-_2$
$5/2^-_1$
Cohen-Kurath
NCSM
25
50
75
$C_2(SU(3))$

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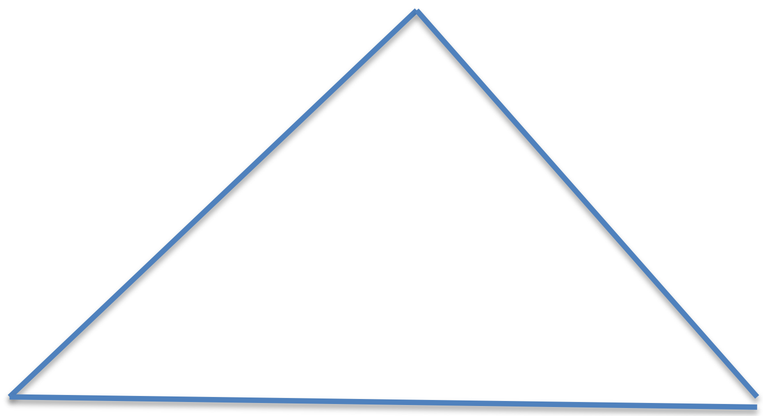
Is there some way to turn a *quasi*-dynamical symmetry into a *dynamical* symmetry? Like a unitary transformation?

SAN DIEGO STATE UNIVERSITY

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)?*

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



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

San Diego State University

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

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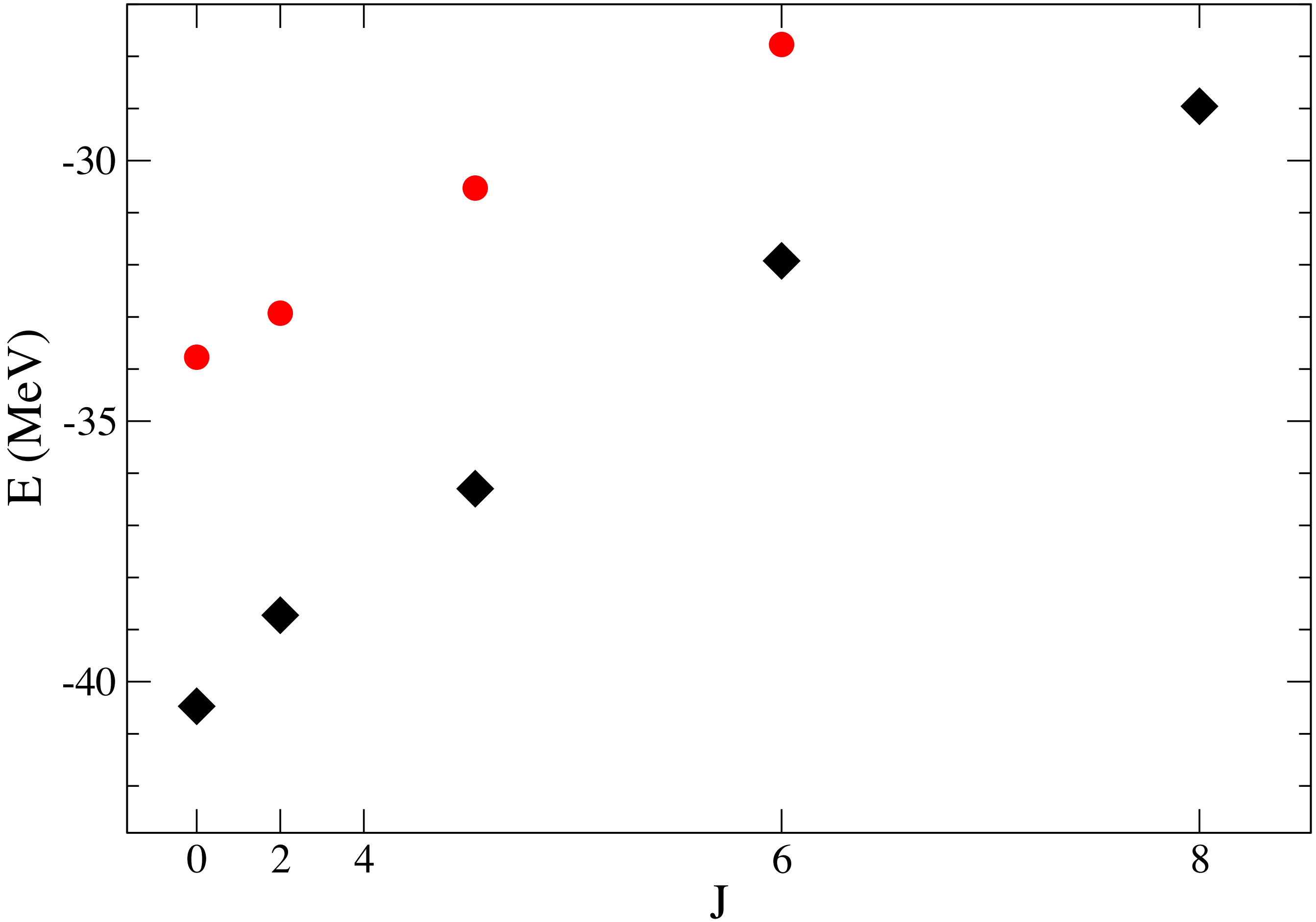
(More on this soon).

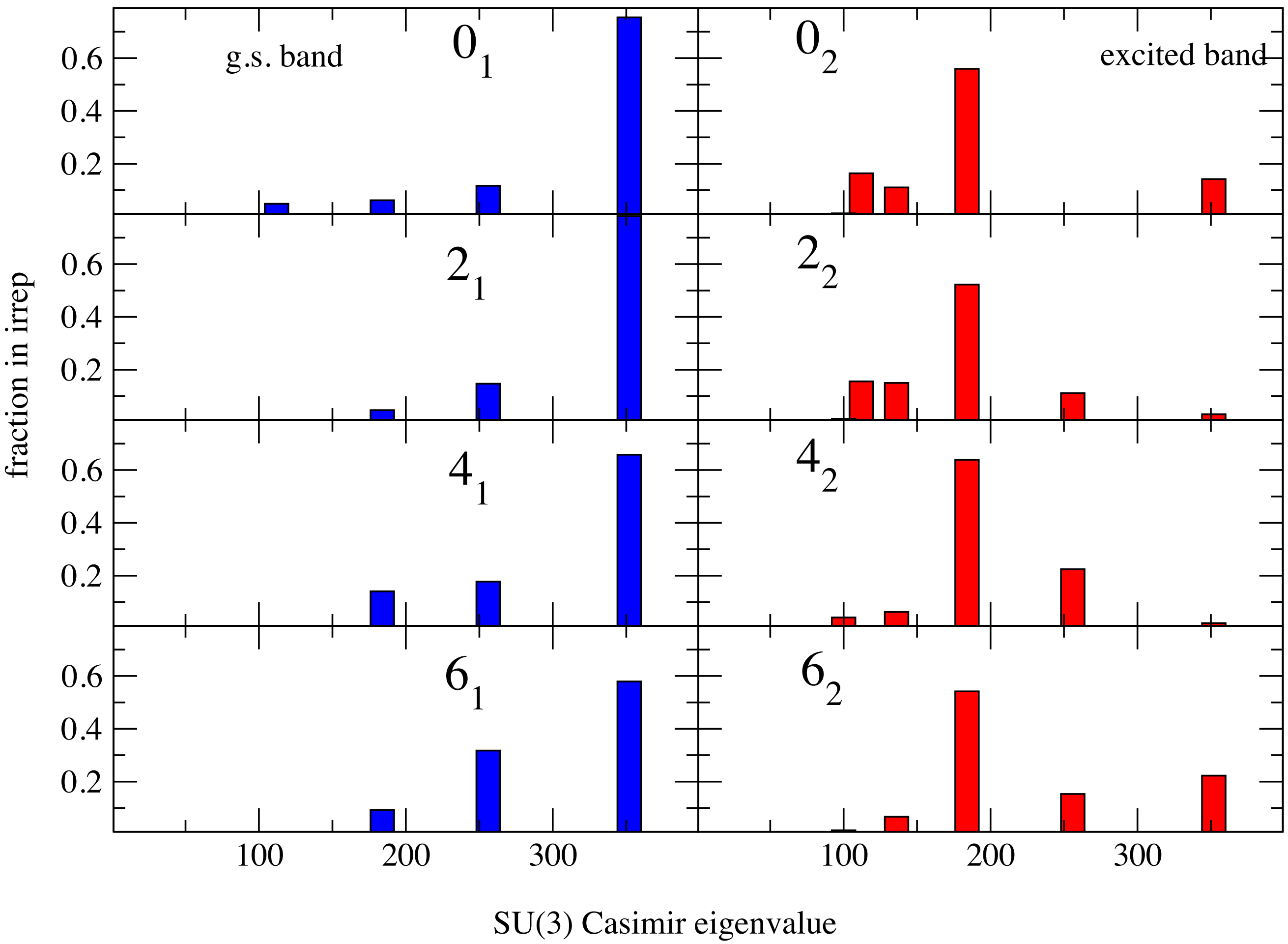
The *similarity renormalization group (SRG)* is widely used in *ab initio* calculations to transform and soften the nuclear force

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



^{20}Ne

USDB interaction



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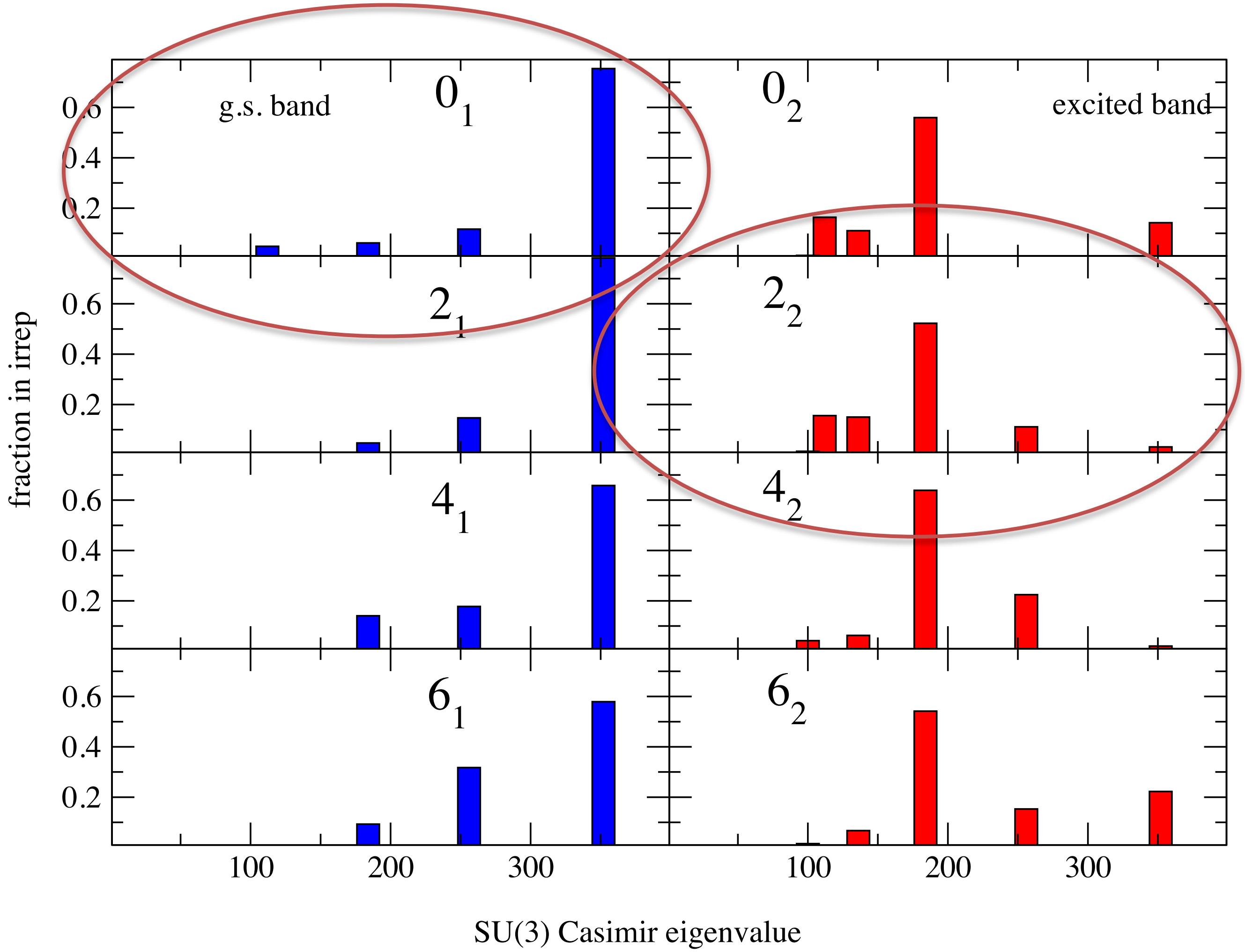
USDB interaction

San Diego State University



^{20}Ne

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

Now I will apply SRG

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

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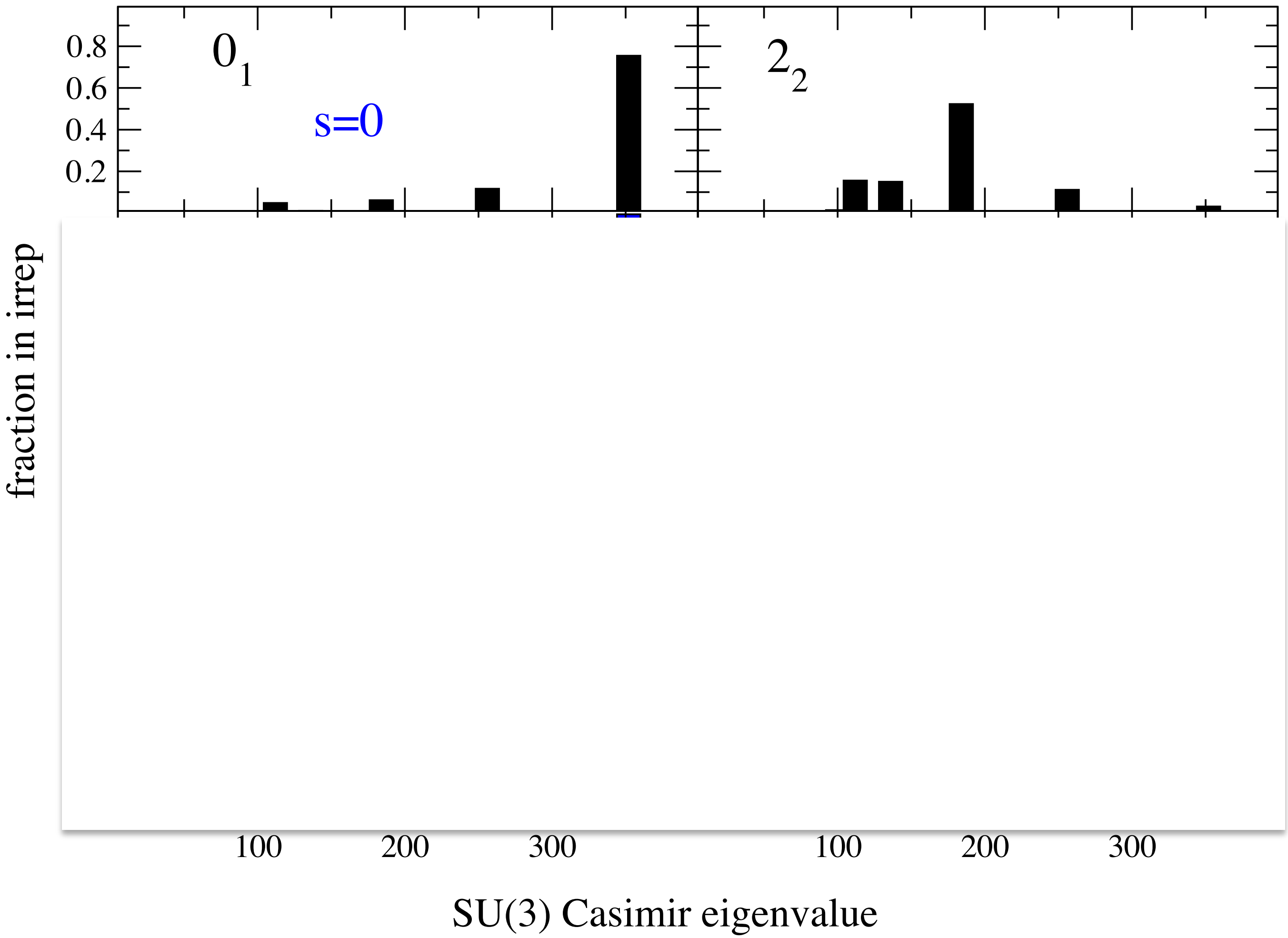

^{20}Ne

USDB interaction

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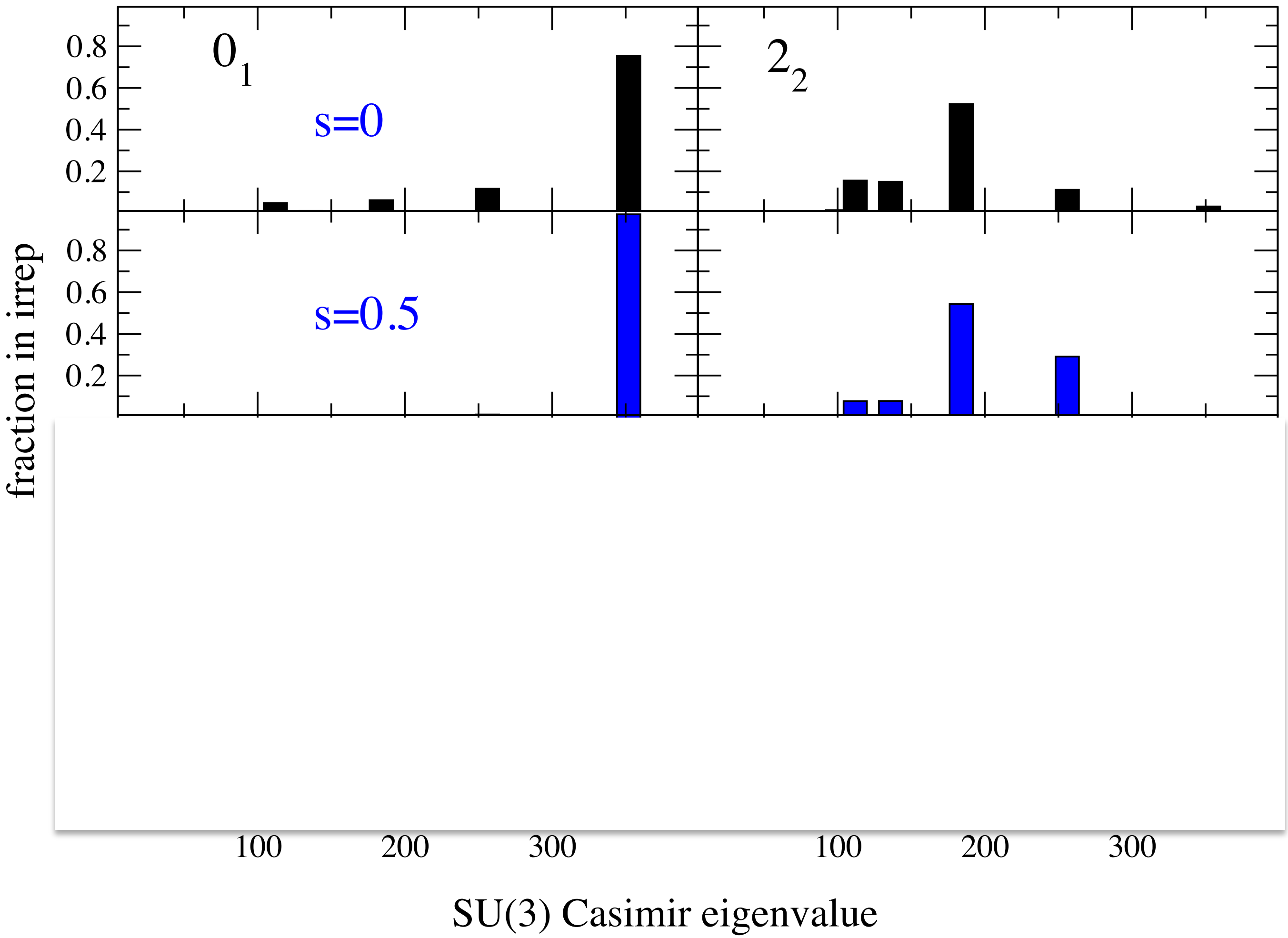

^{20}Ne

USDB interaction

Increasing evolution

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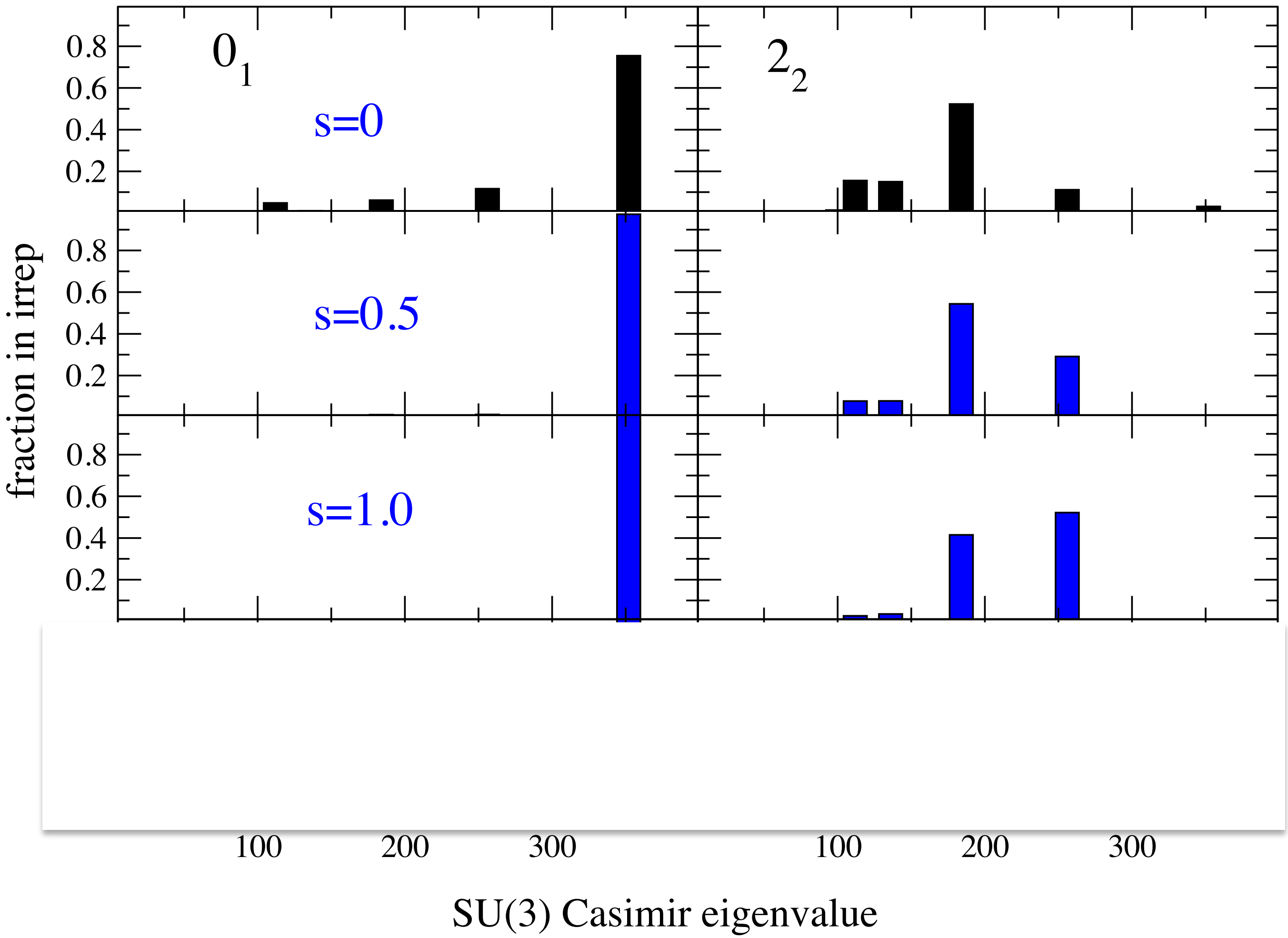
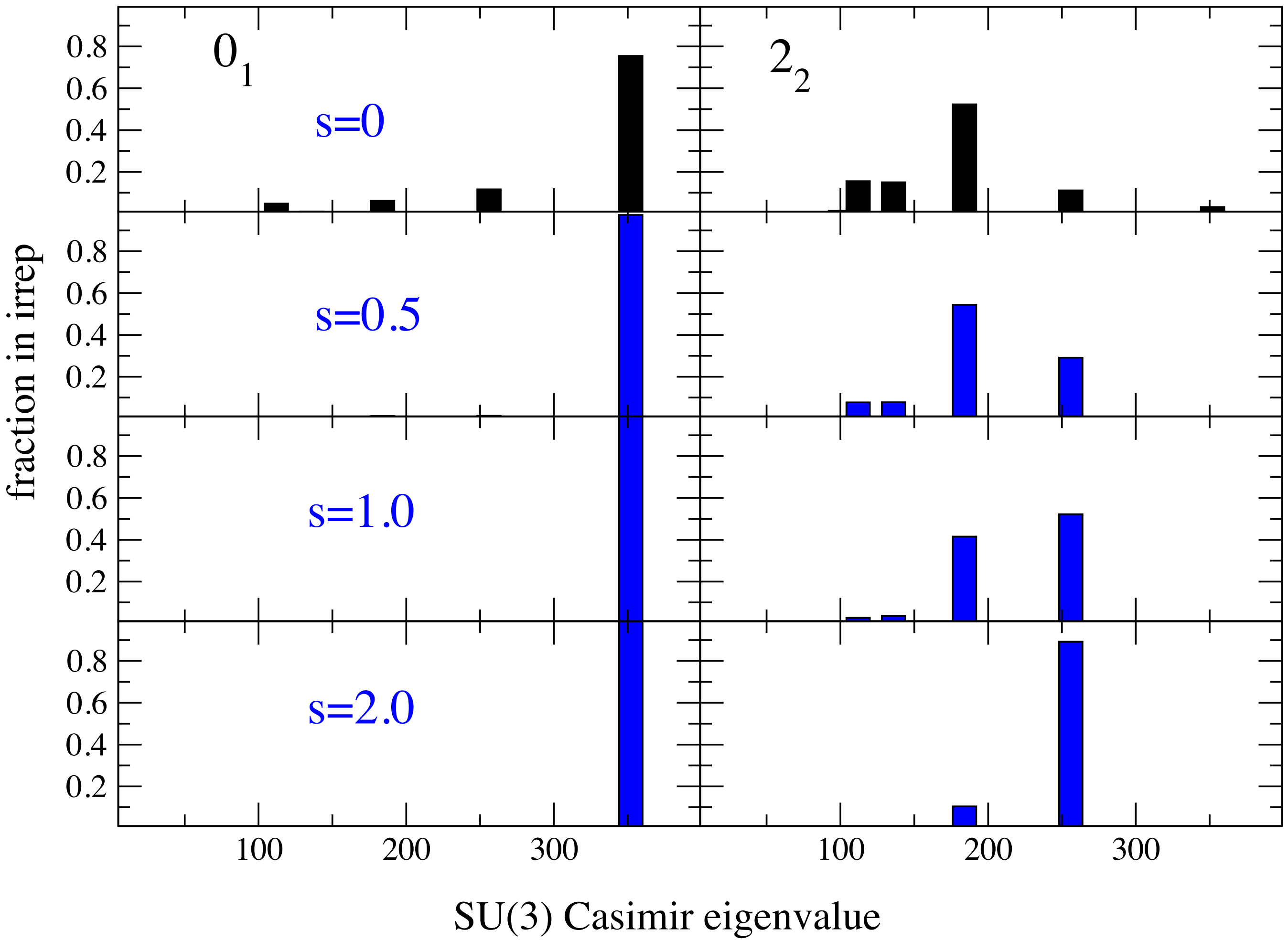


^{20}Ne

USDB interaction

Increasing evolution

San Diego State University

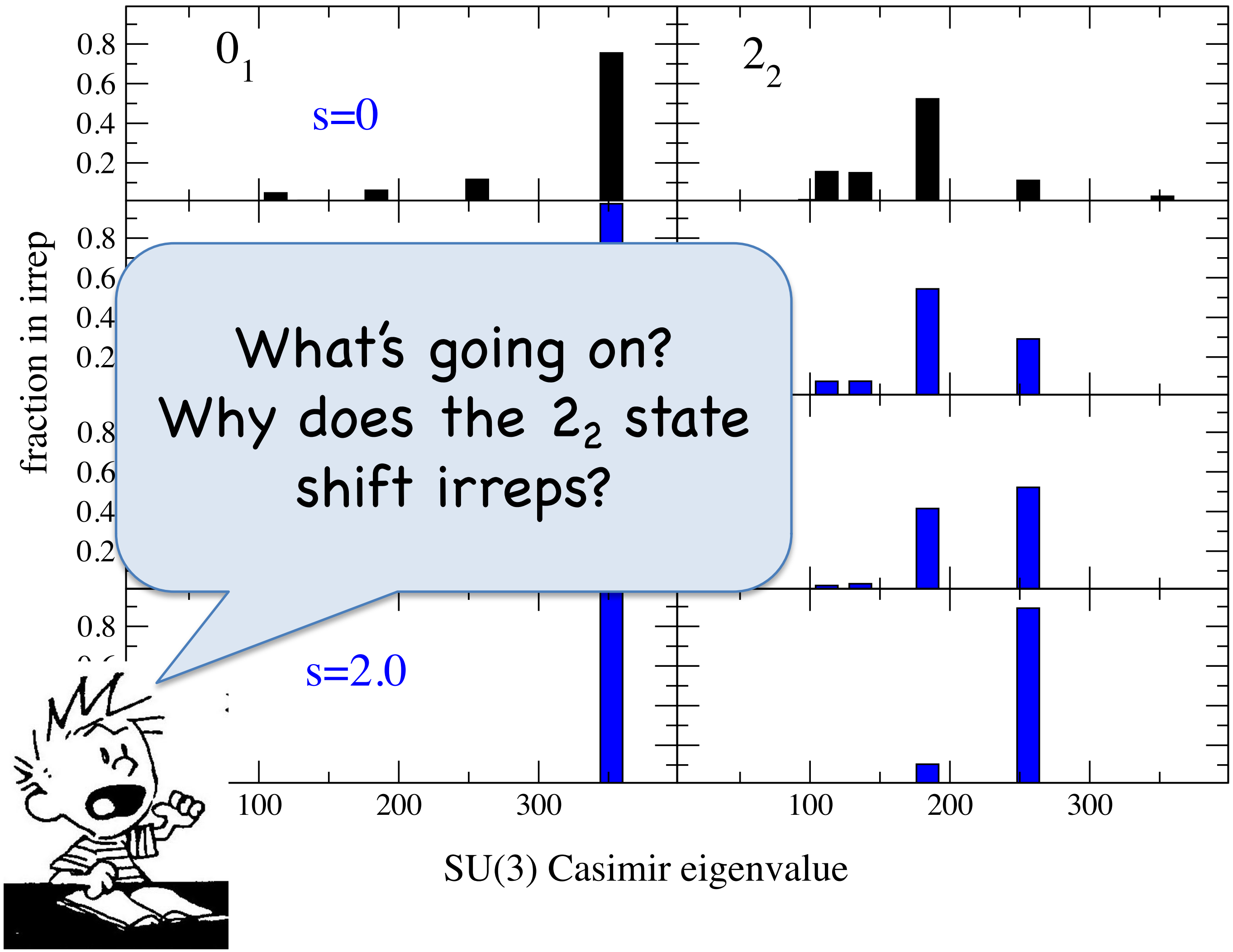


^{20}Ne

USDB interaction

Increasing evolution

SAN DIEGO STATE UNIVERSITY



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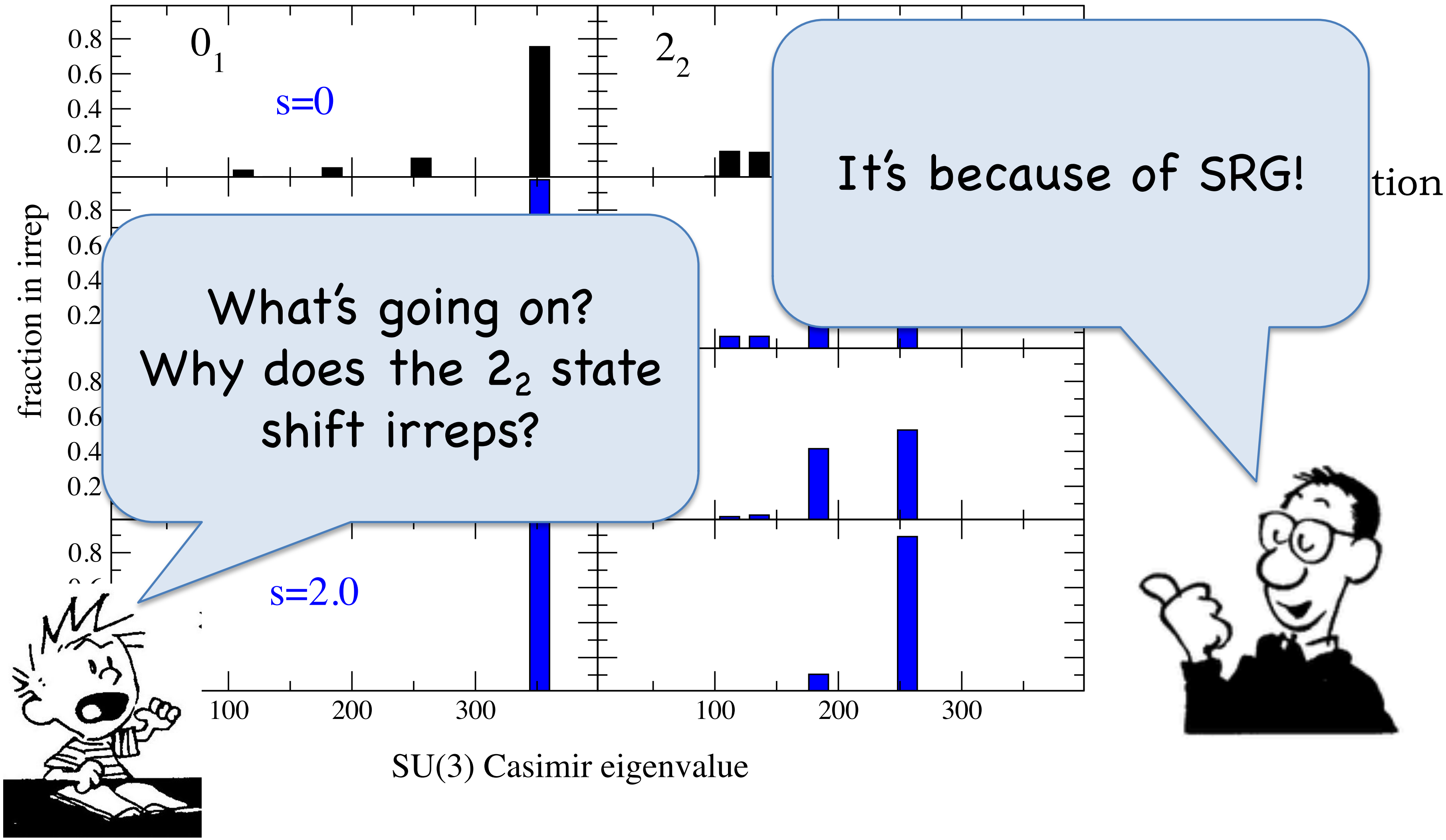
USDB interaction

Increasing evolution

SAN DIEGO STATE UNIVERSITY



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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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One can re-derive SRG using *spectral distribution theory* (French, Ratcliffe, Wong, Draayer, many others)

Define an *inner product* on matrices/Hamiltonian using traces:

$$(A,B) = \mathrm{tr}\ AB^*$$

*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)

SAN DIEGO STATE UNIVERSITY

Suppose we want to transform H(s)

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

so as to increase

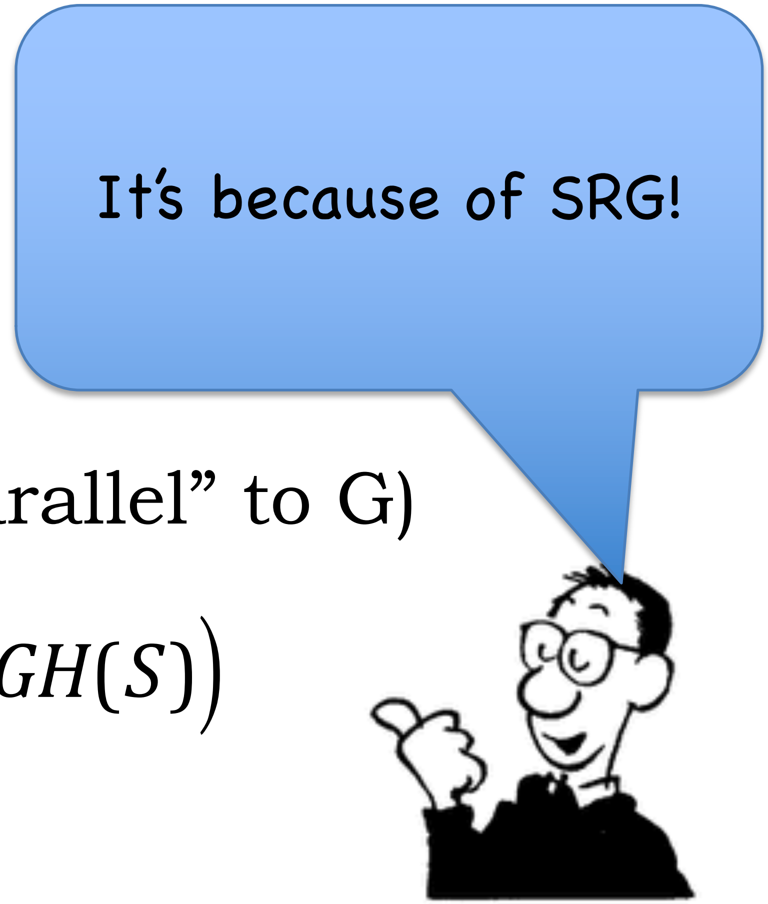
tr (H(s) G)

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

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

leads to standard SRG

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



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

so choose evolution that maximizes derivative

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

This derivative can be rewritten as

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

The derivative is **maximal** when

η is proportional to [G,H]

hence $\frac{d}{ds}H(s) = [\eta, H] = [[G,H],H]$

Suppose we want to transform H(s)

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

so as to increase

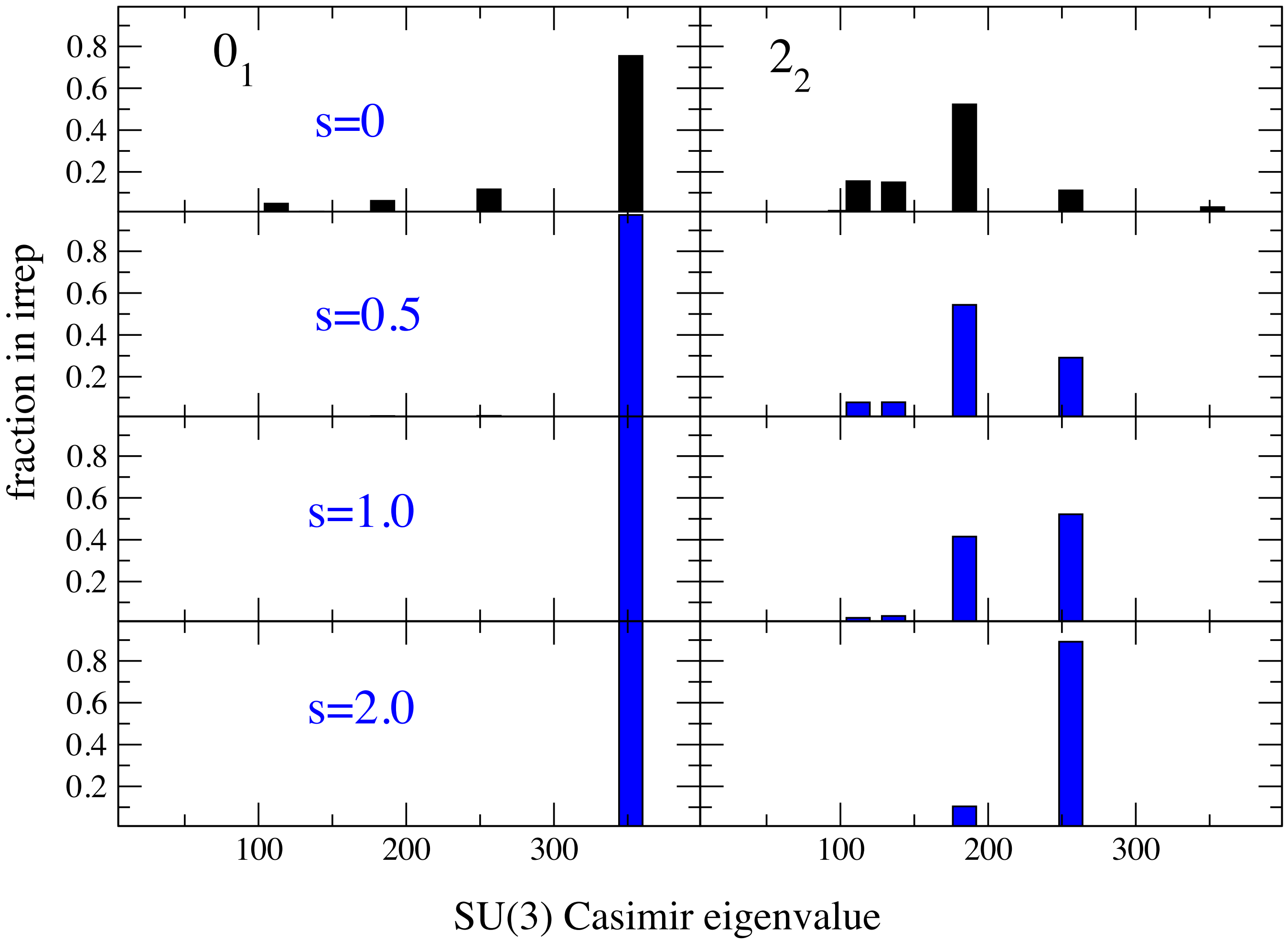
tr (H(s) G)

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

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

leads to standard SRG

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



^{20}Ne

USDB interaction

Increasing evolution

SAN DIEGO STATE UNIVERSITY

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:

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

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

so choose evolution that maximizes derivative

$$-\frac{d}{ds}tr([H(s),G]^2\ ) = -2\ tr\left(\left[\frac{dH}{ds},G\right][H,G]\right) = -2tr([[\eta,H],G][H,G])$$

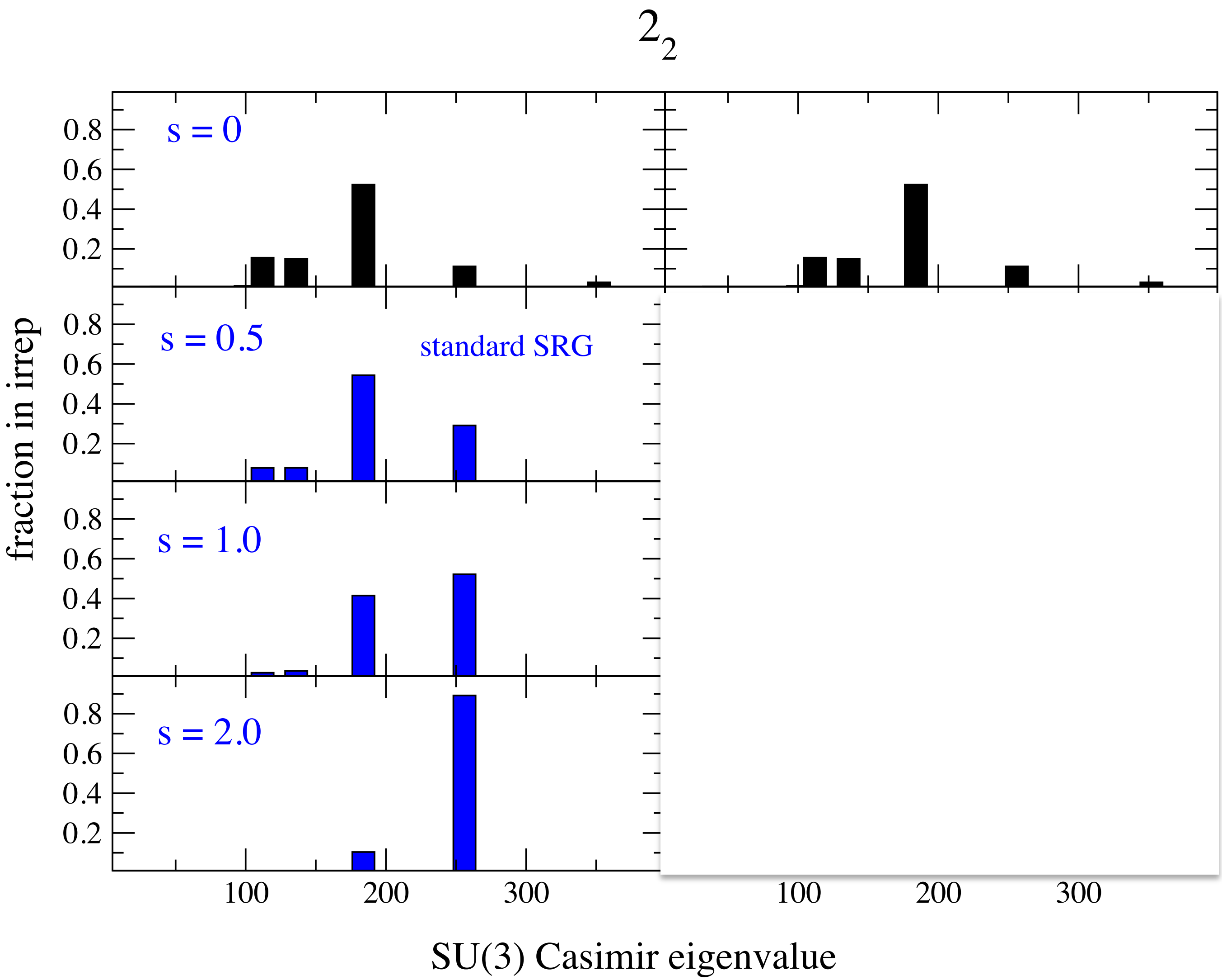
This derivative can be rewritten as

-tr (η [[[H,G],G],H])

The derivative is maximal when

η is proportional to [[[G,H],G],H]

hence $$\frac{d}{ds}H(s) = [\eta,H] = [[[[G,H],G],H],H]$$



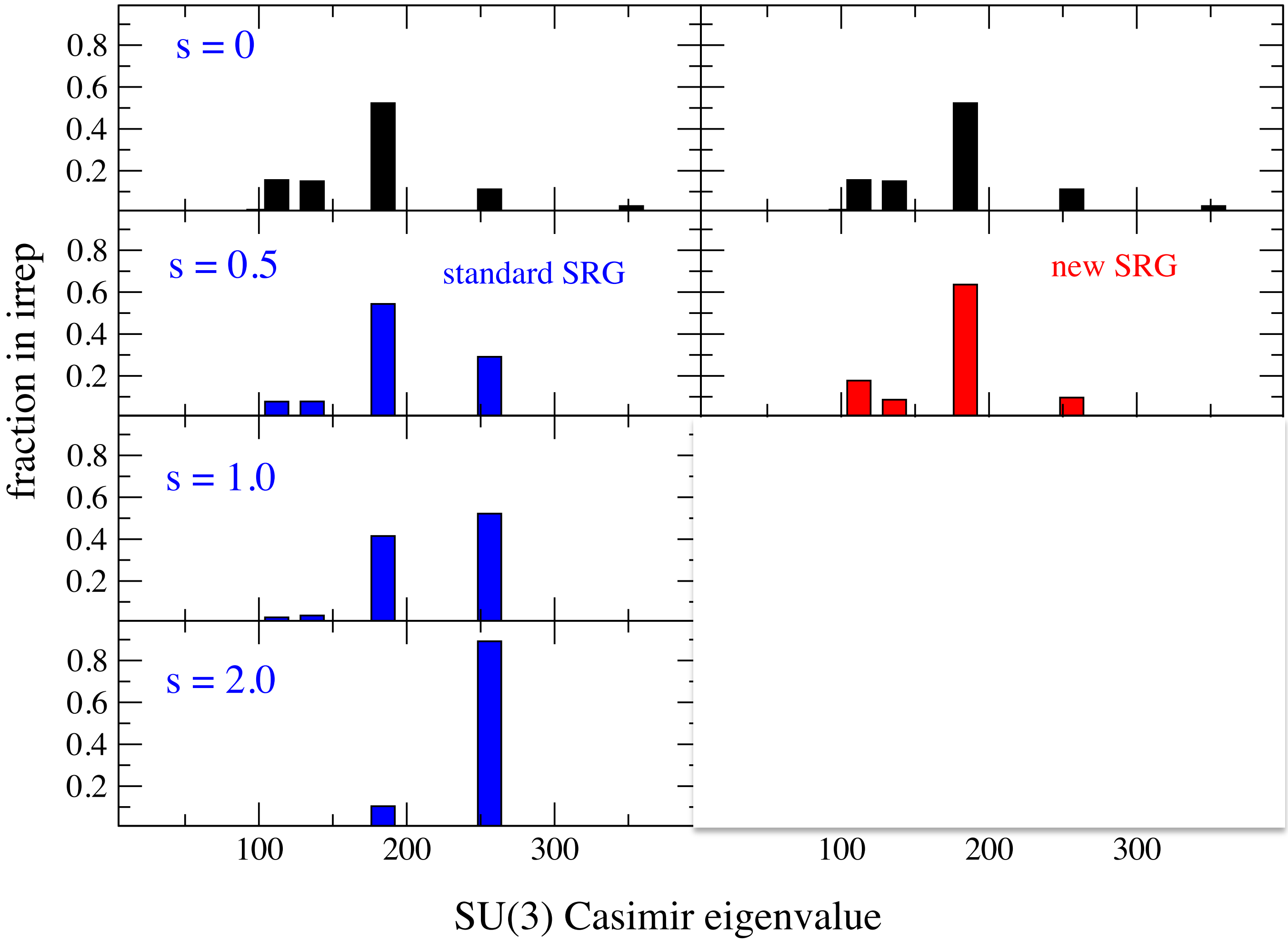
^{20}Ne

USDB interaction

Increasing evolution

San Diego State University

2_2



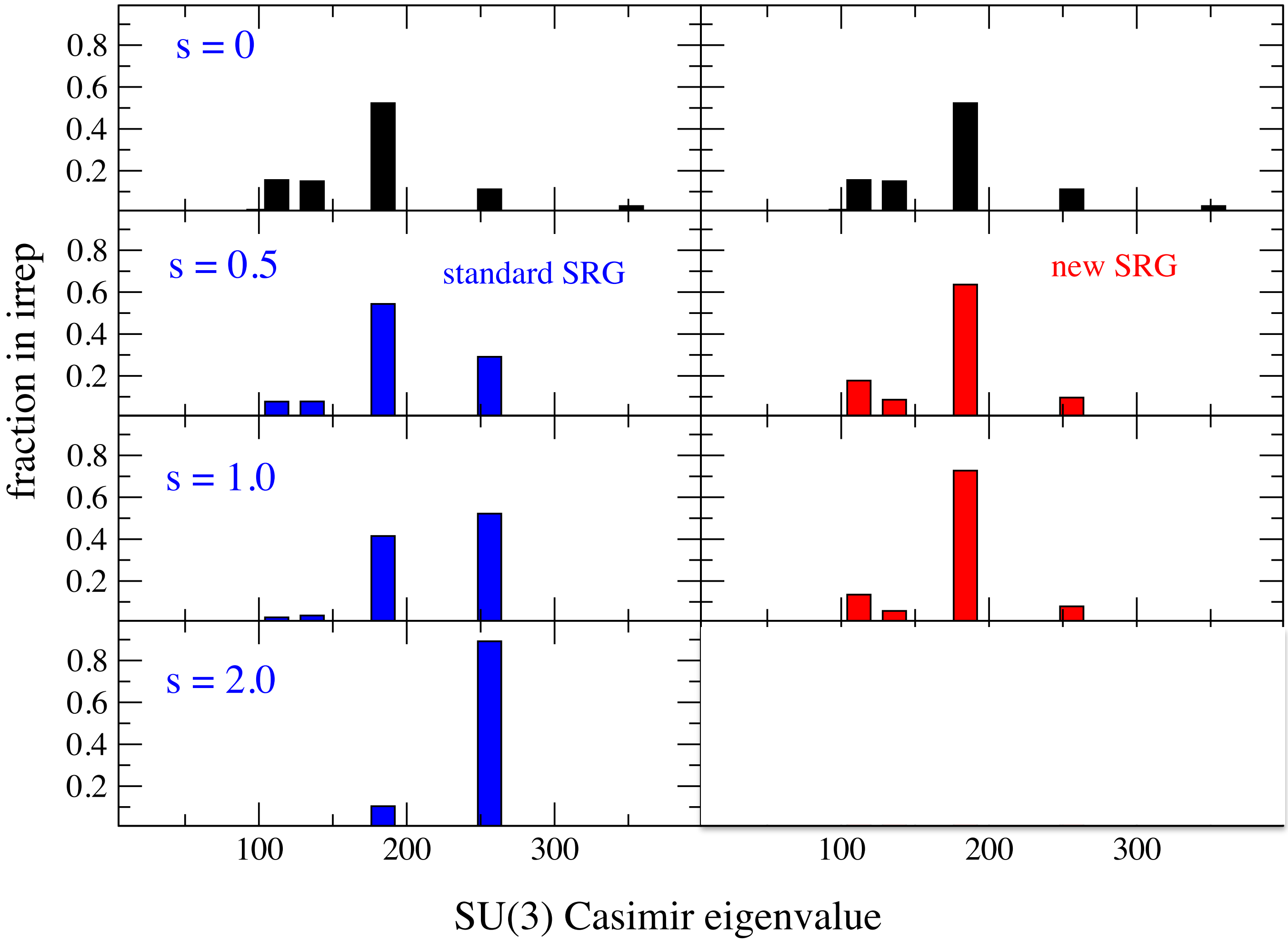
^{20}Ne

USDB interaction

Increasing evolution

SAN DIEGO STATE UNIVERSITY

2_2



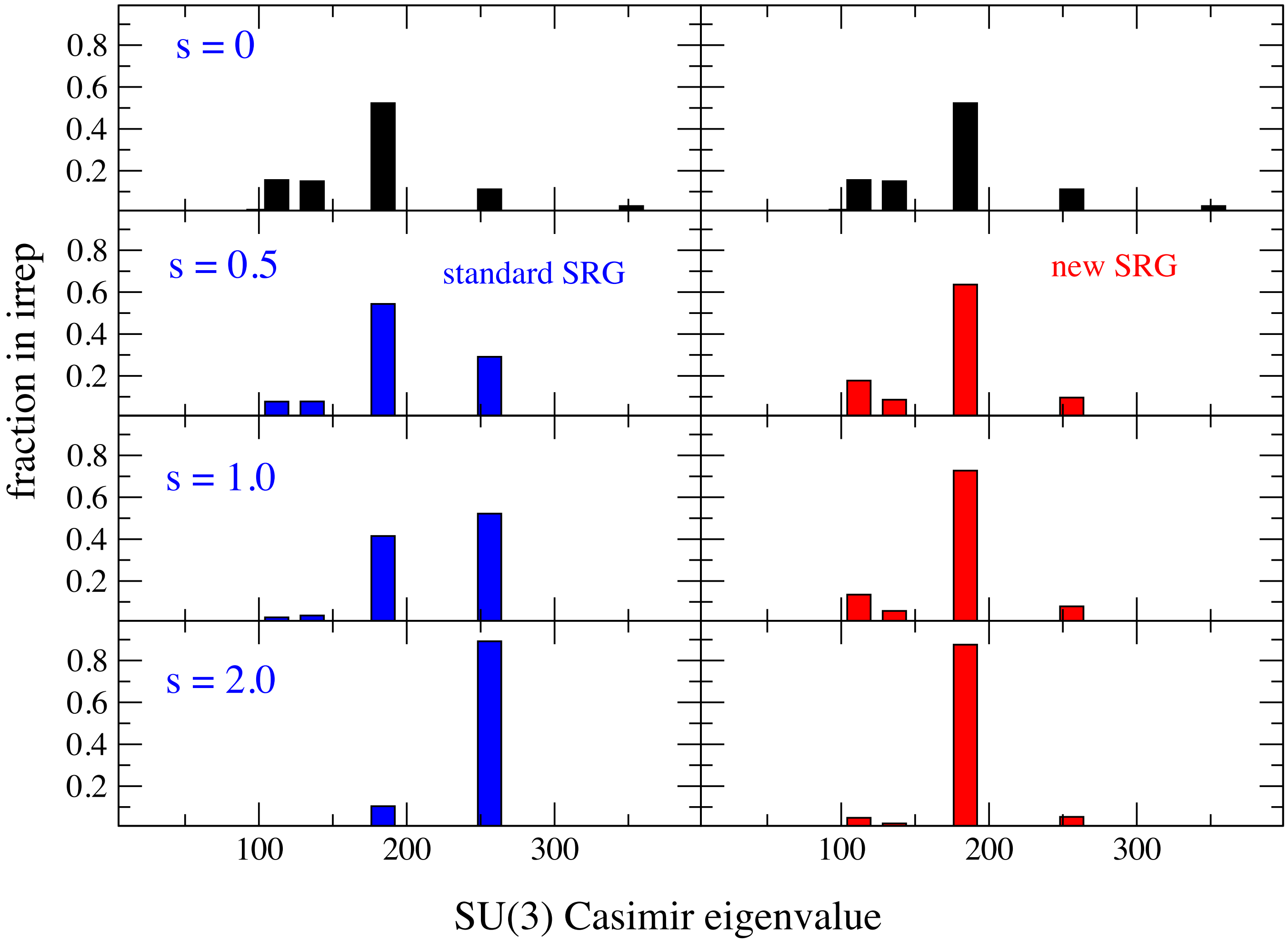
^{20}Ne

USDB interaction

Increasing evolution

San Diego State University

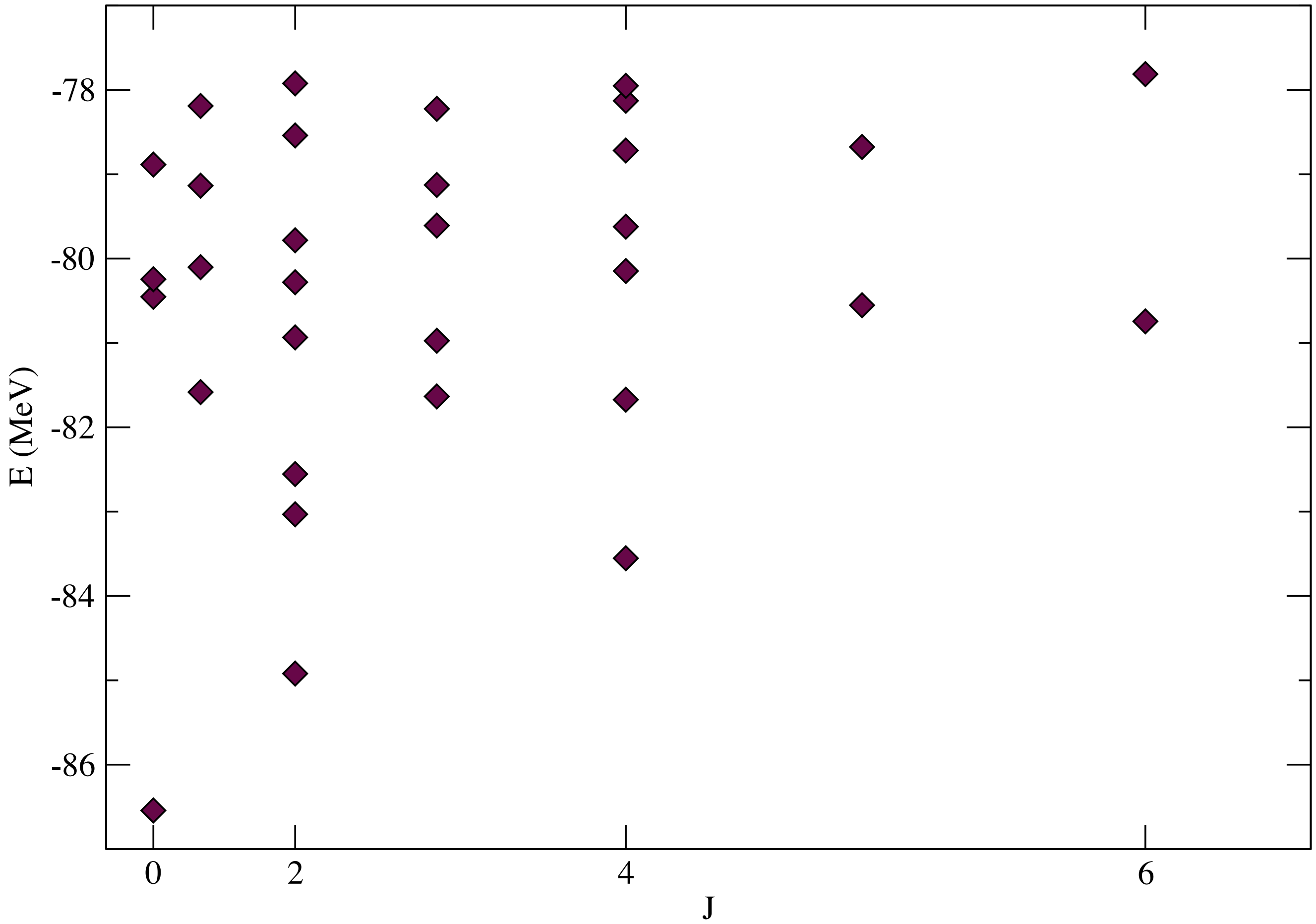
2_2



^{20}Ne

USDB interaction

Increasing evolution



^{28}Ne

USDB interaction

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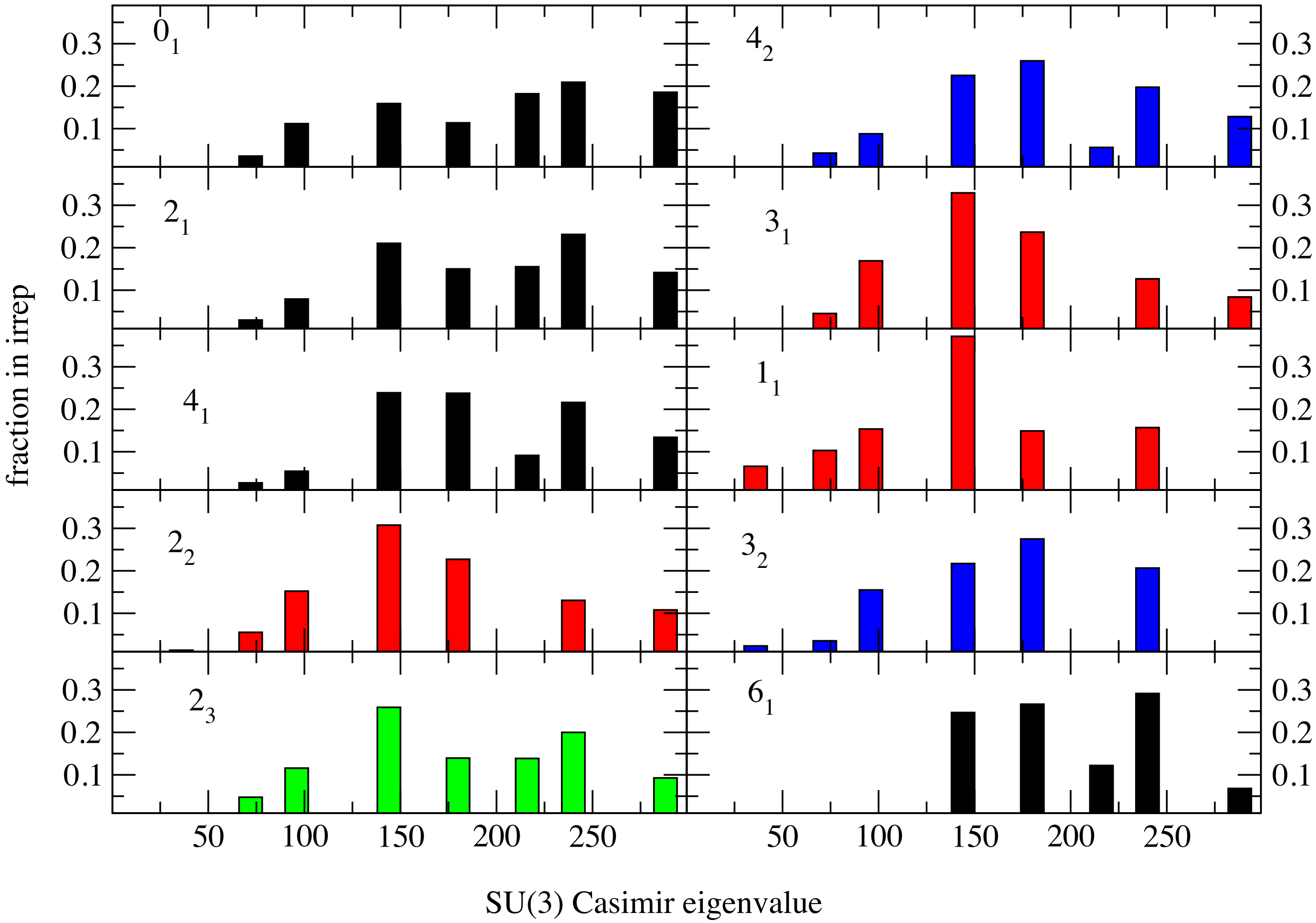
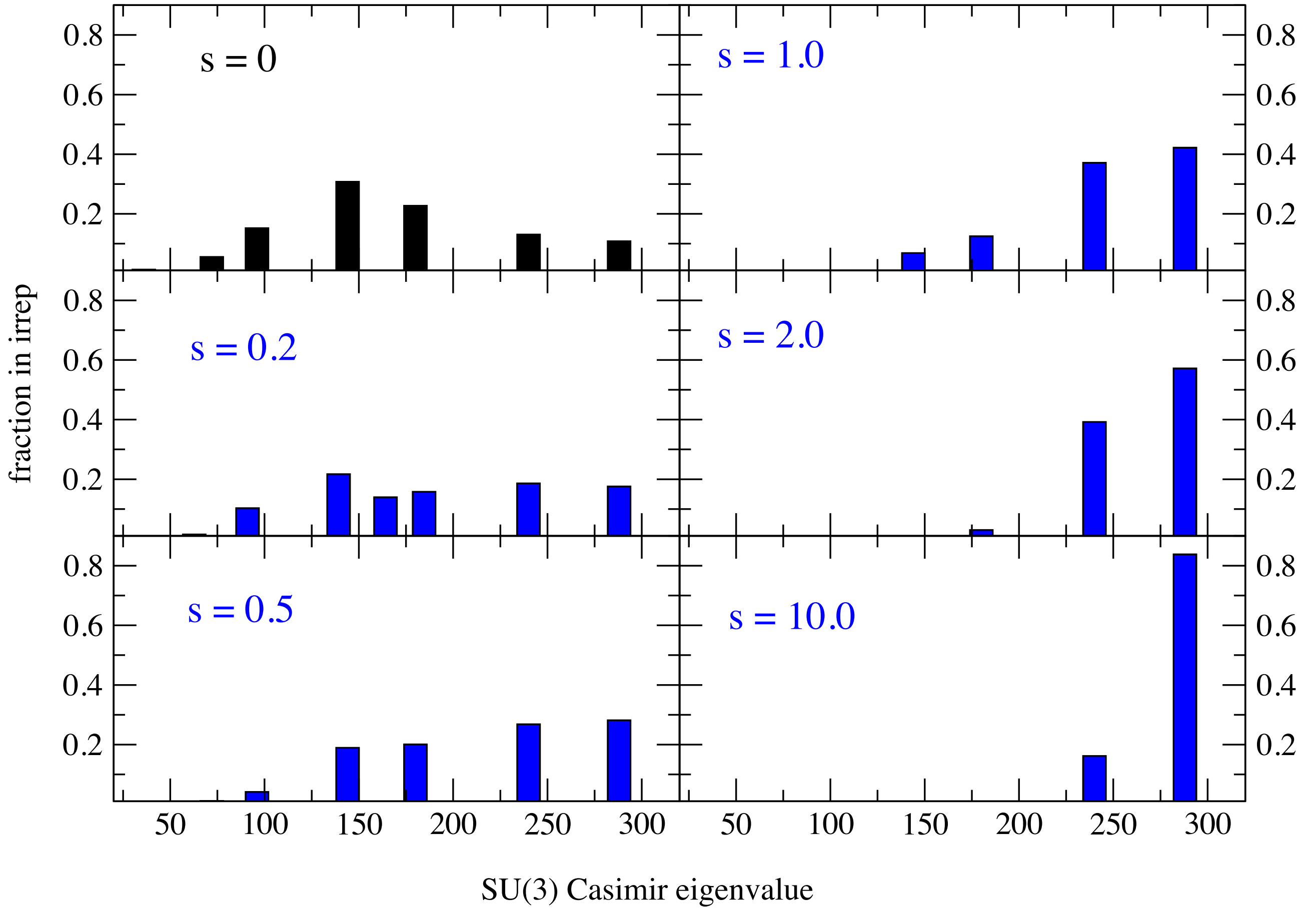


^{28}Ne

USDB interaction

SAN DIEGO STATE UNIVERSITY

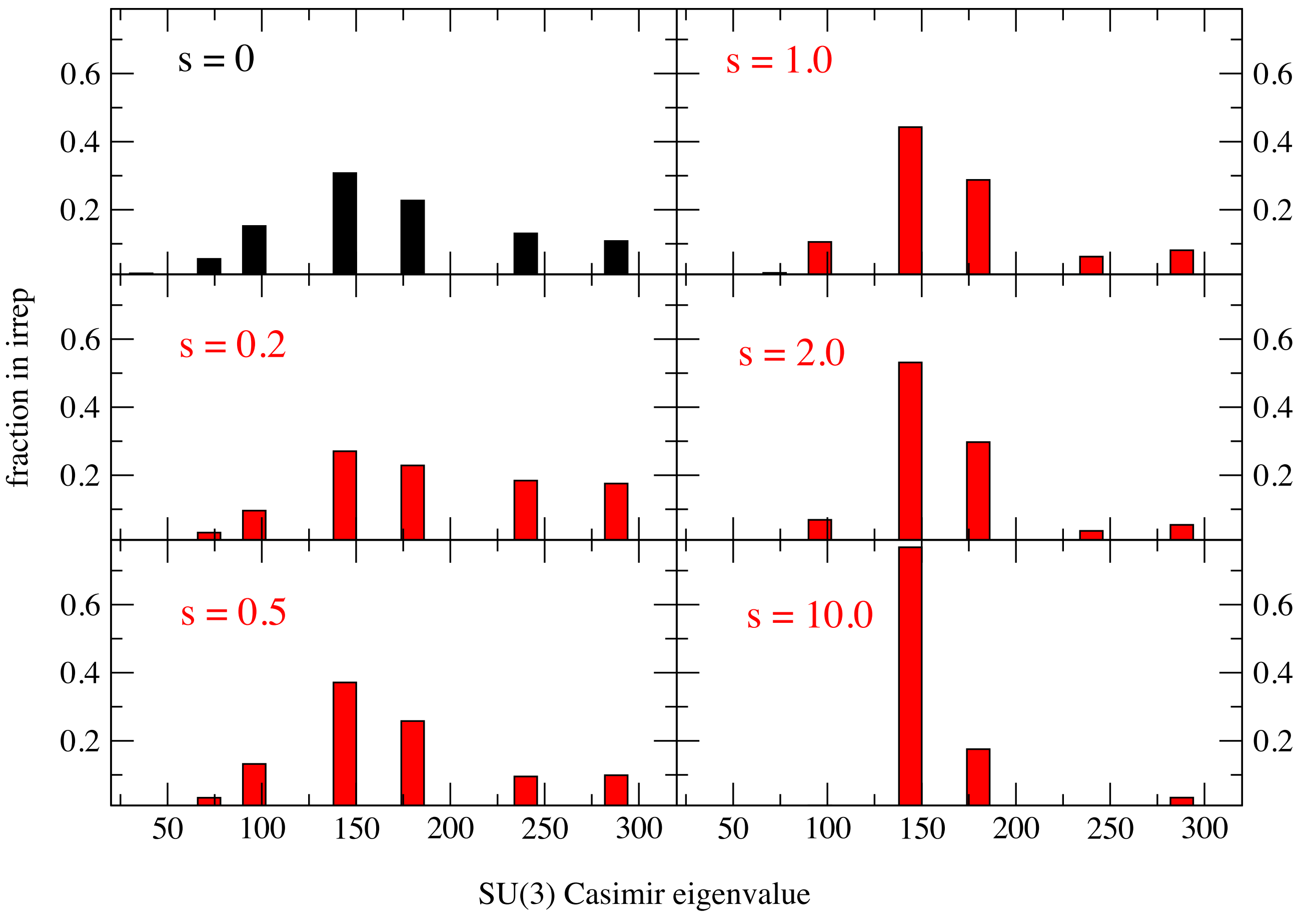


^{28}Ne

USDB interaction

2_2 state

standard SRG



^{28}Ne

USDB interaction

2_2 state

new SRG

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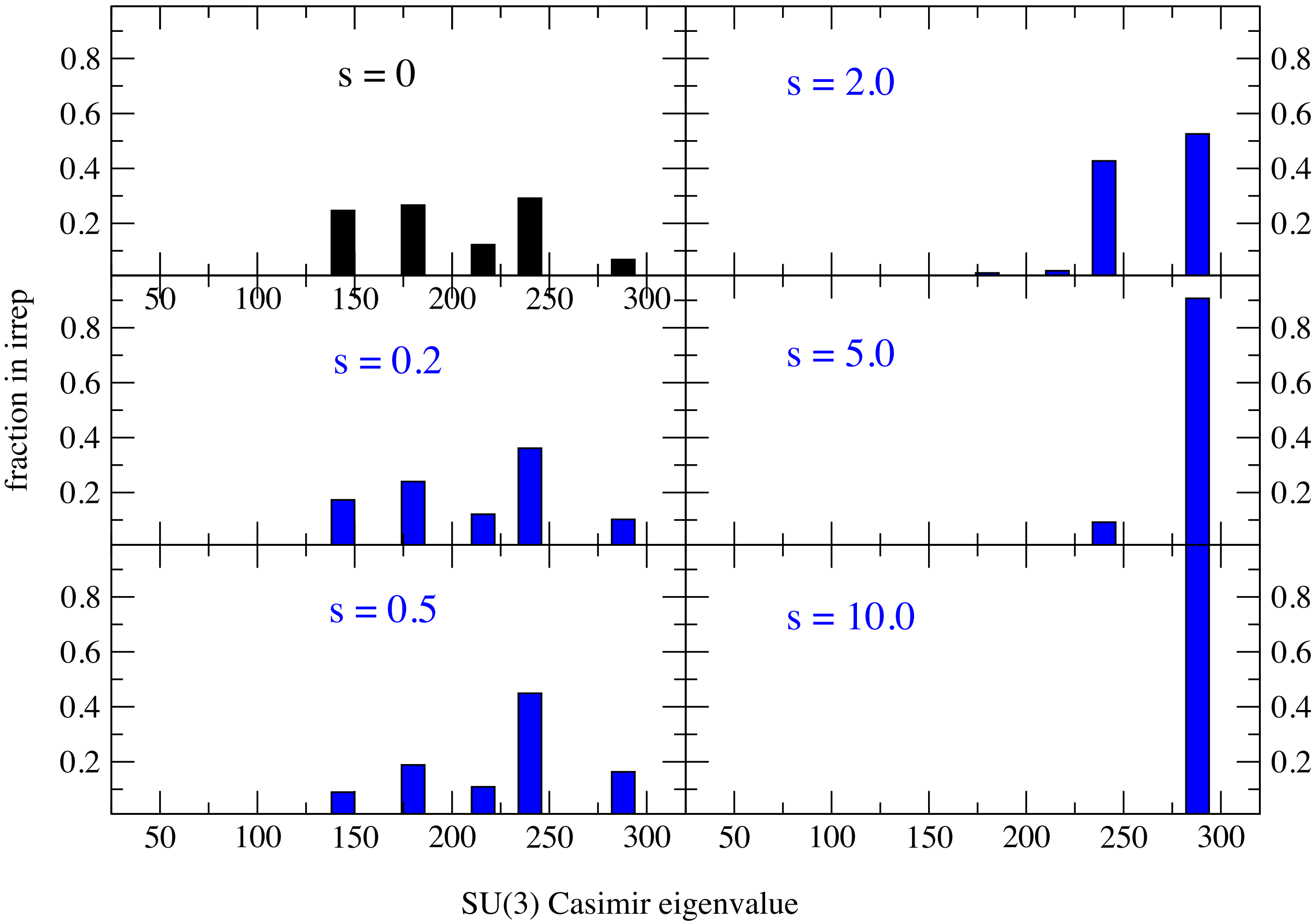

^{28}Ne

USDB interaction

6_1 state

standard SRG

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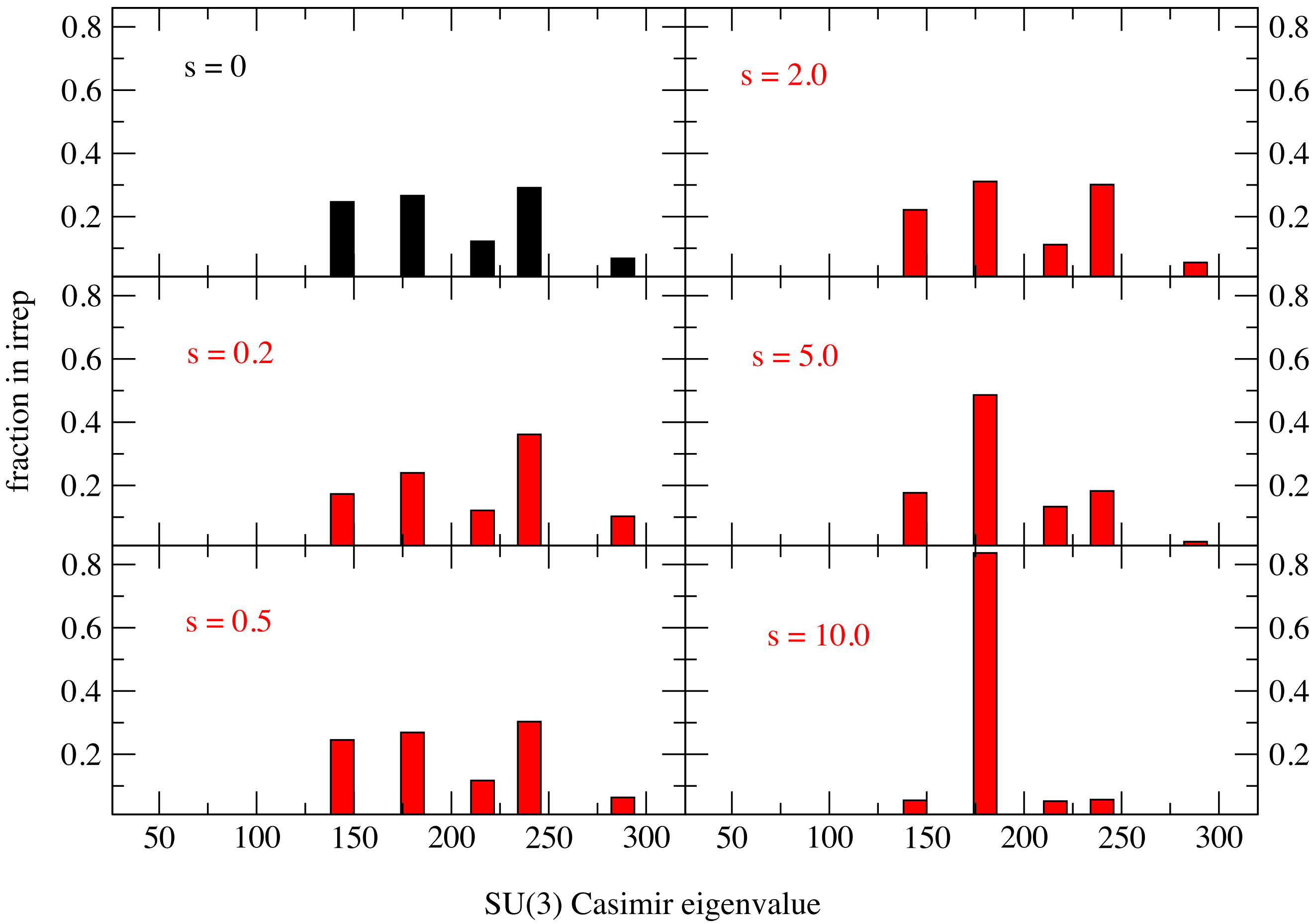

^{28}Ne

USDB interaction

6_1 state

new SRG

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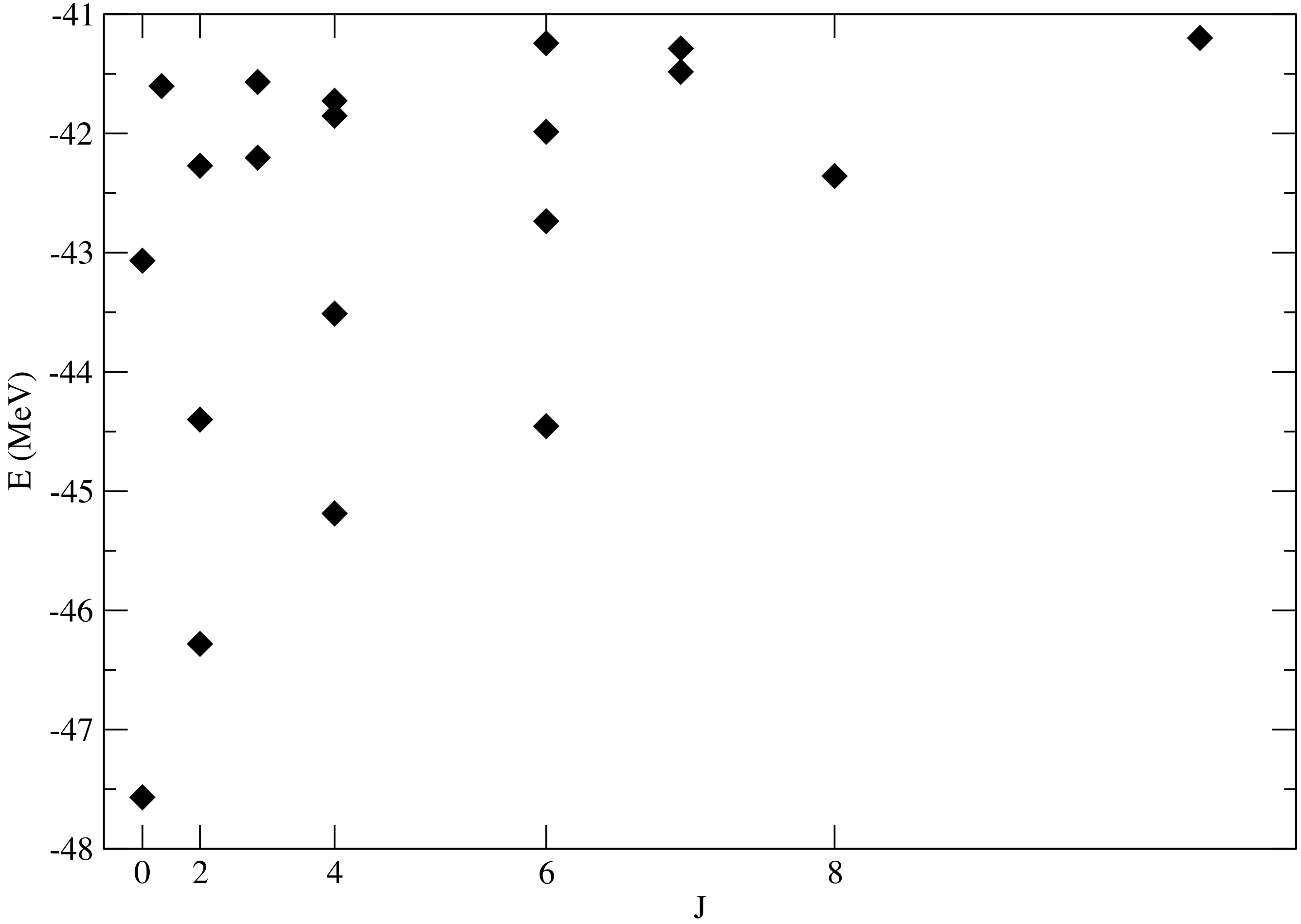

^{44}Ti

GX1A interaction

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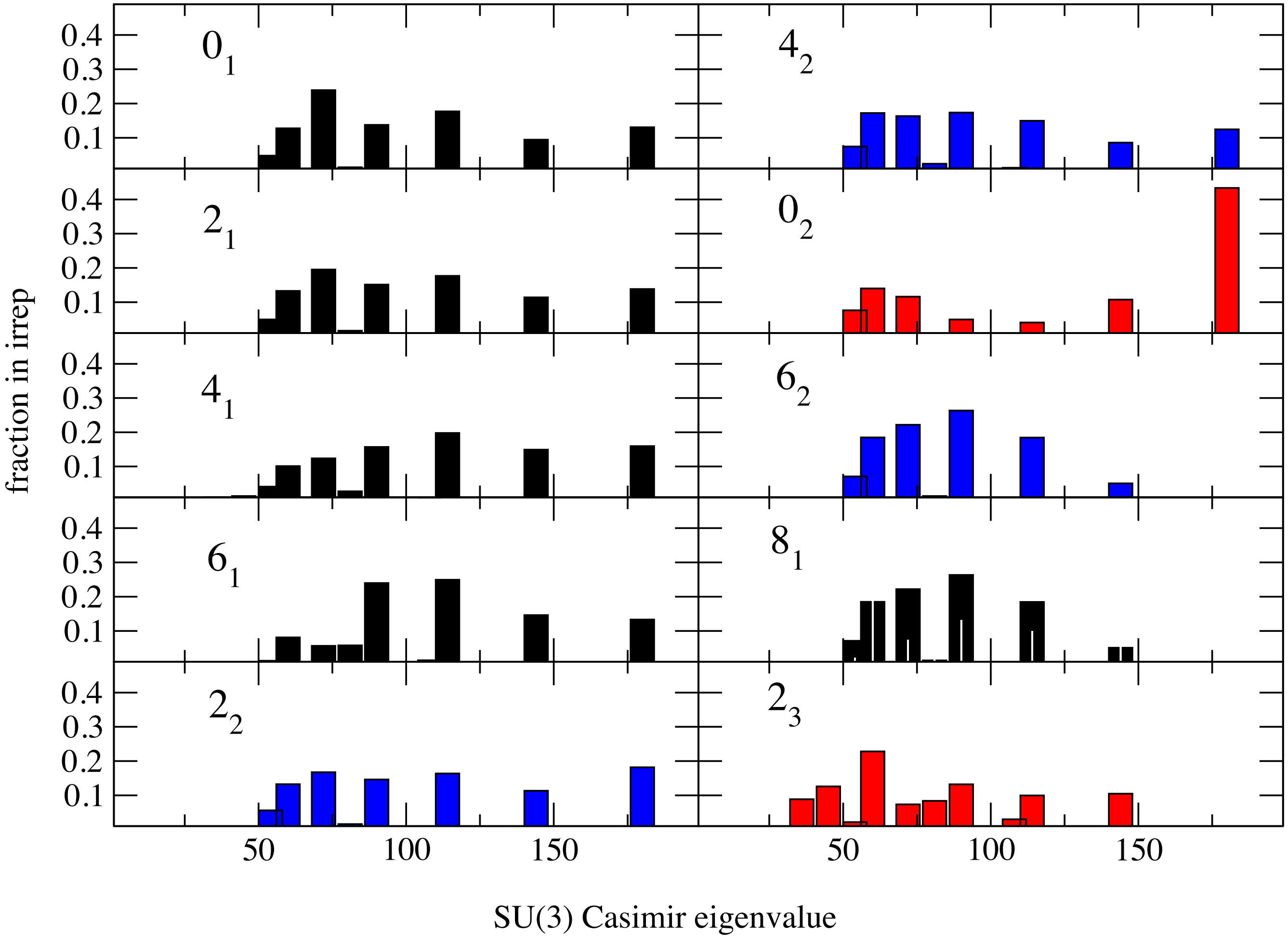
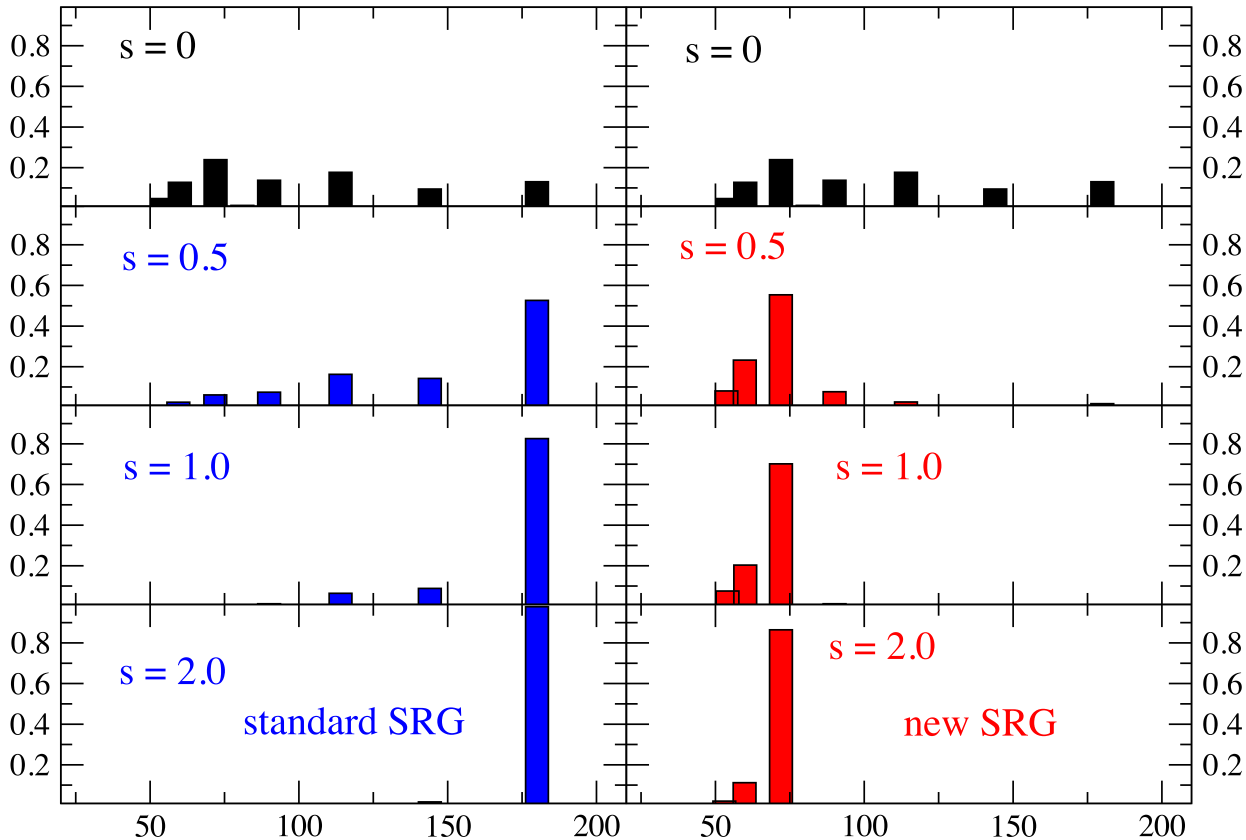


^{44}Ti

GX1A interaction

SAN DIEGO STATE UNIVERSITY



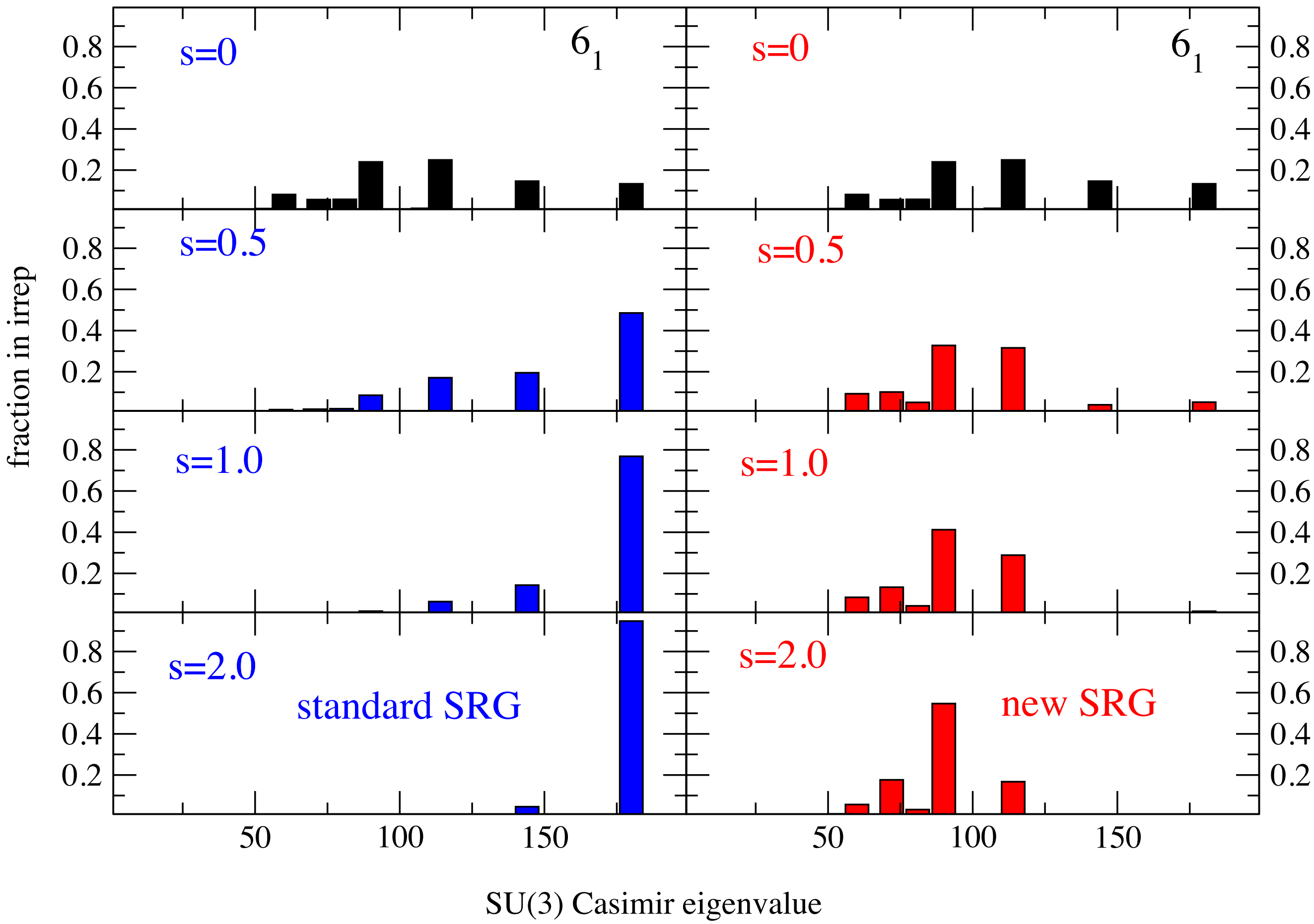
^{44}Ti

GX1A interaction

0_1 g.s.

Increasing evolution

San Diego State University

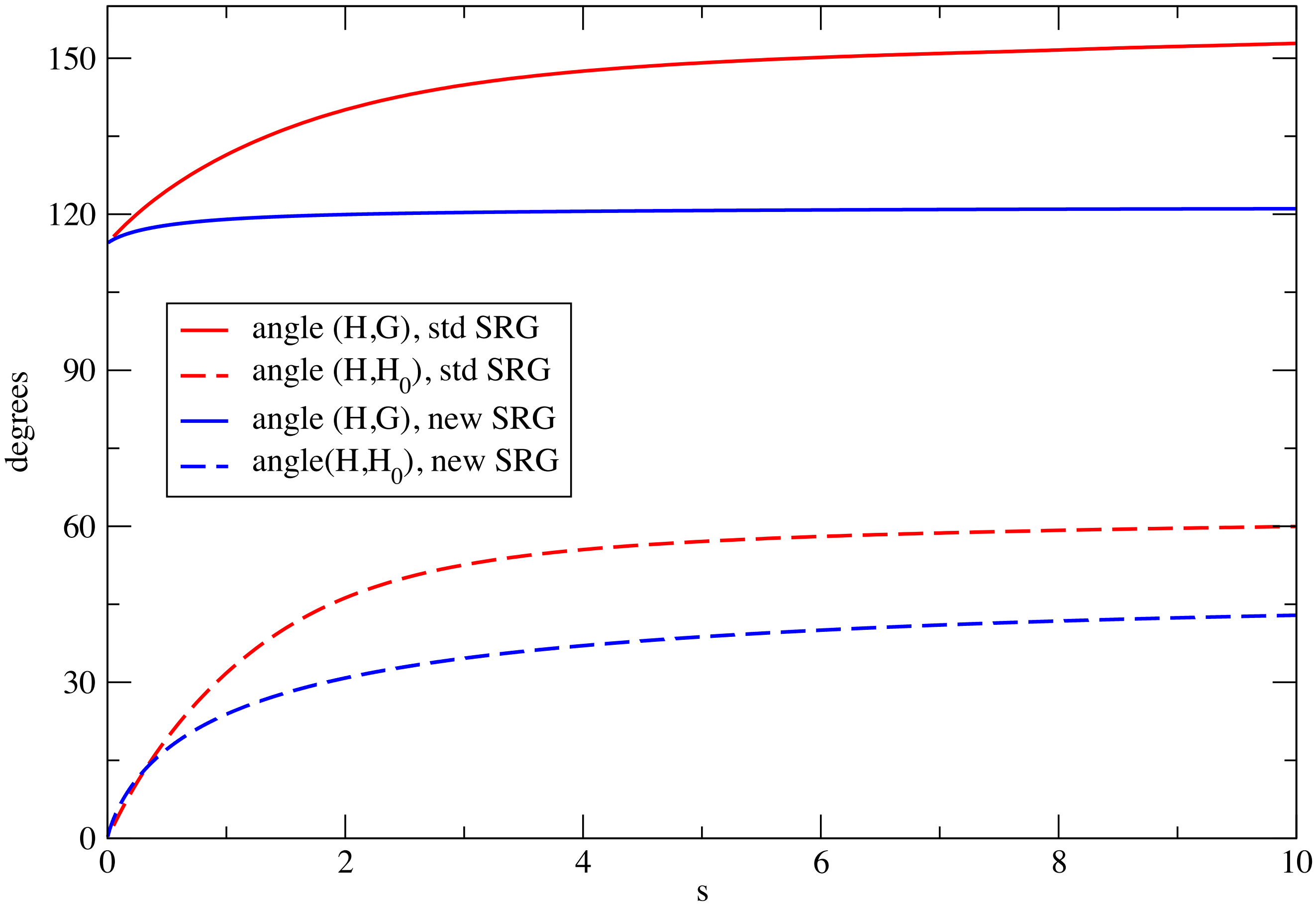


^{44}Ti

GX1A interaction

6_1 state

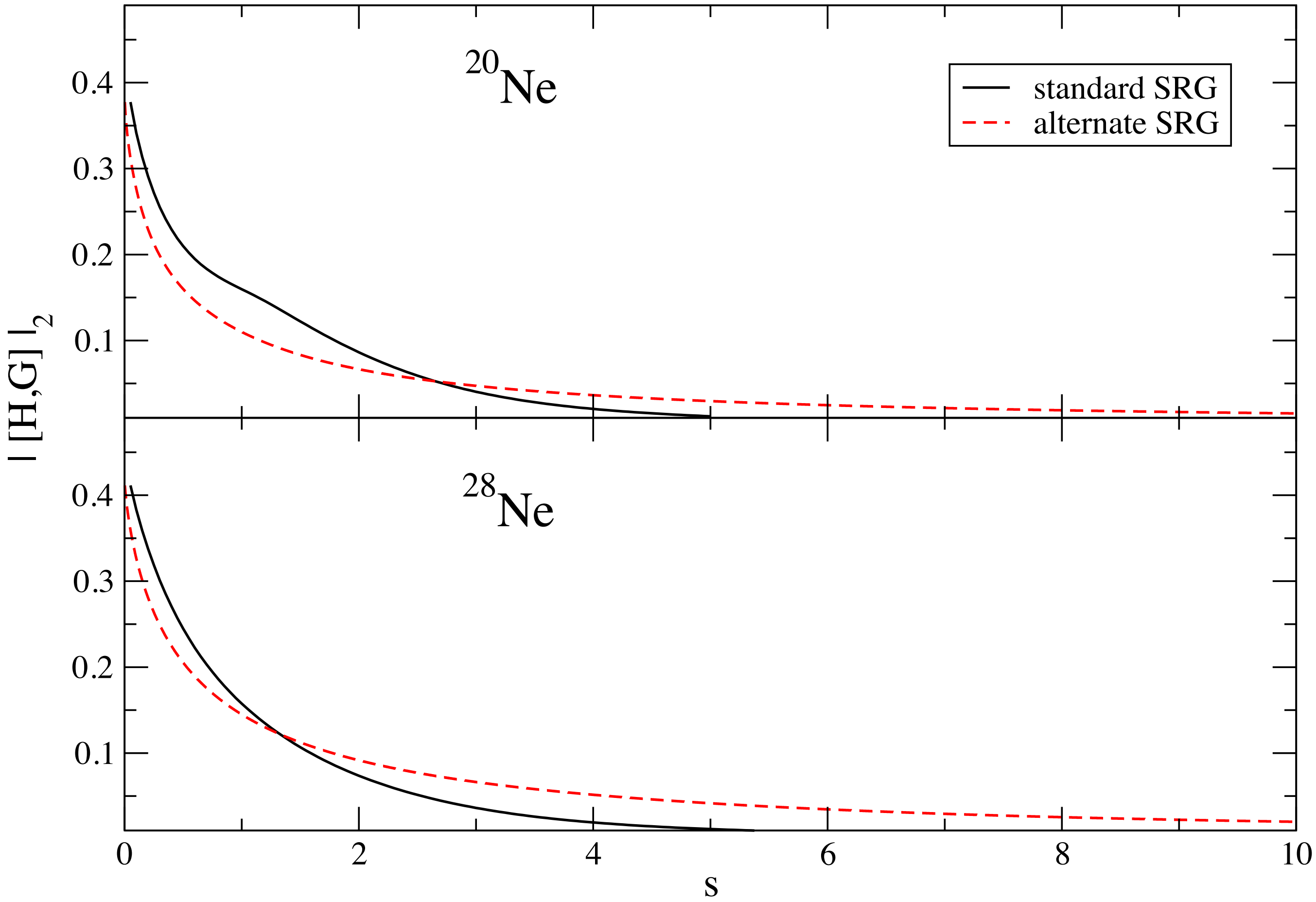
Increasing evolution



^{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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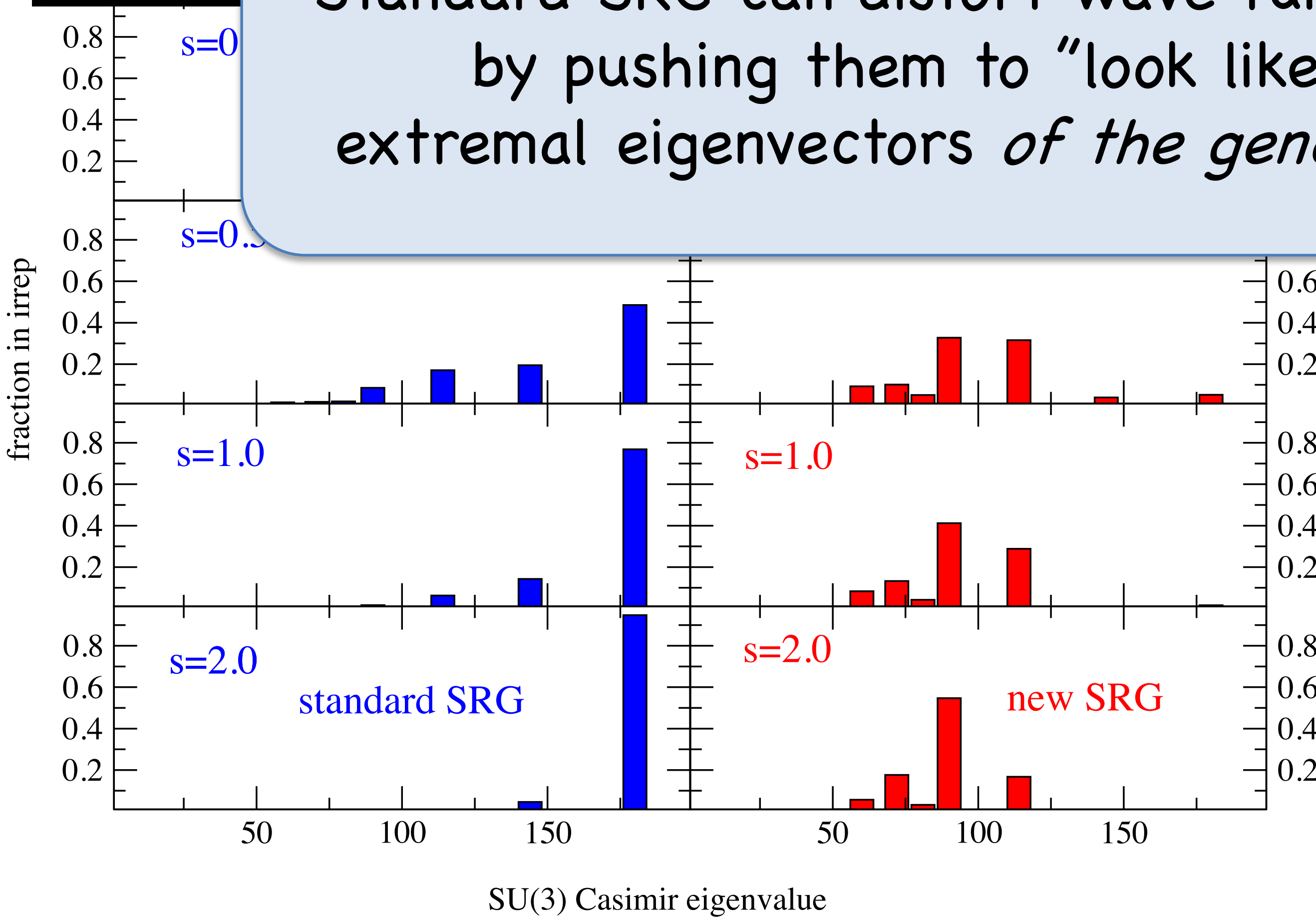
The story here:

Standard SRG can distort wave functions by pushing them to "look like" extremal eigenvectors *of the generator*

...teraction

6_1 state



SAN DIEGO STATE UNIVERSITY

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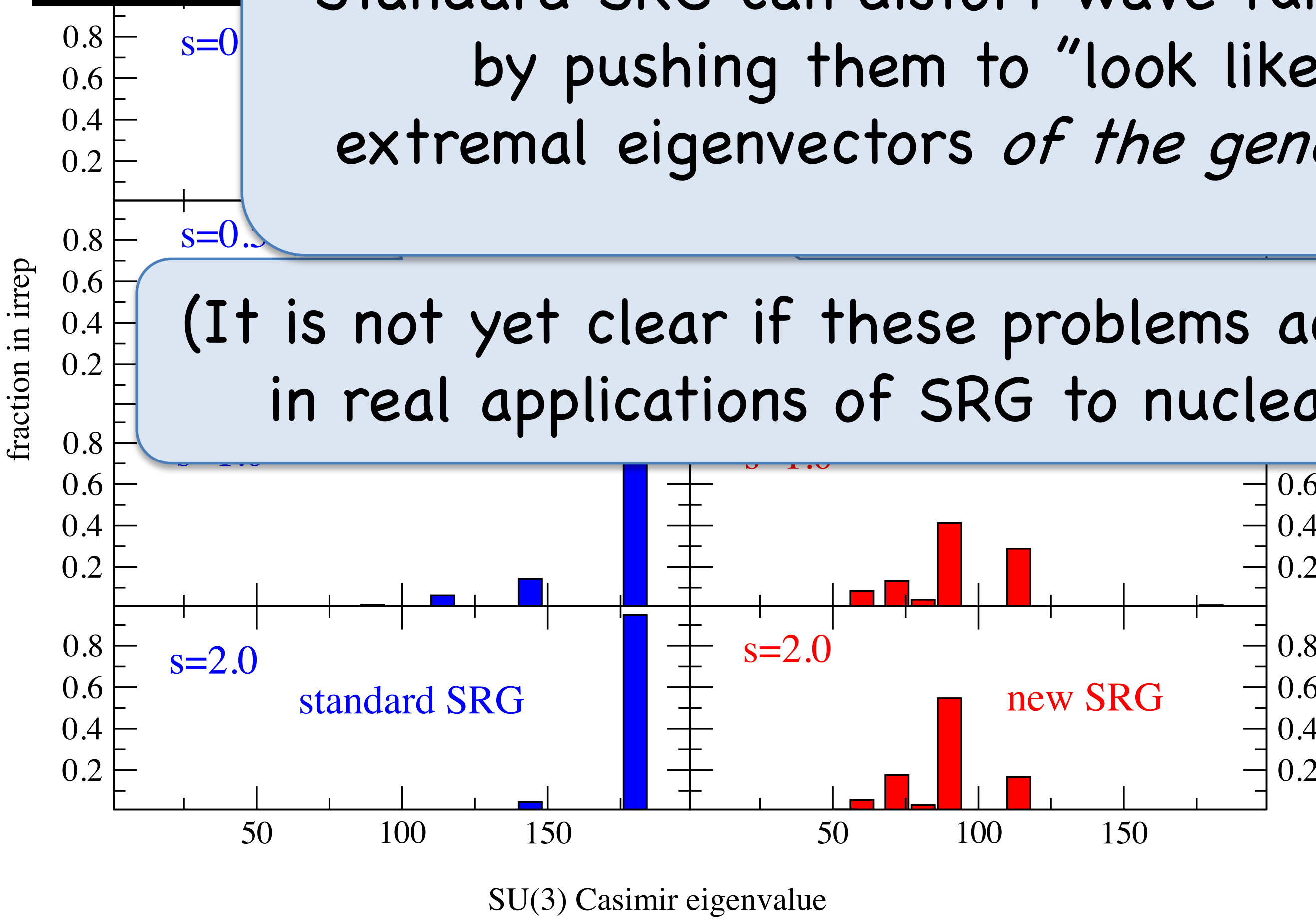
Standard SRG can distort wave functions by pushing them to "look like" extremal eigenvectors *of the generator*

teraction

(It is not yet clear if these problems actually occur in real applications of SRG to nuclear physics)



SAN DIEGO STATE UNIVERSITY

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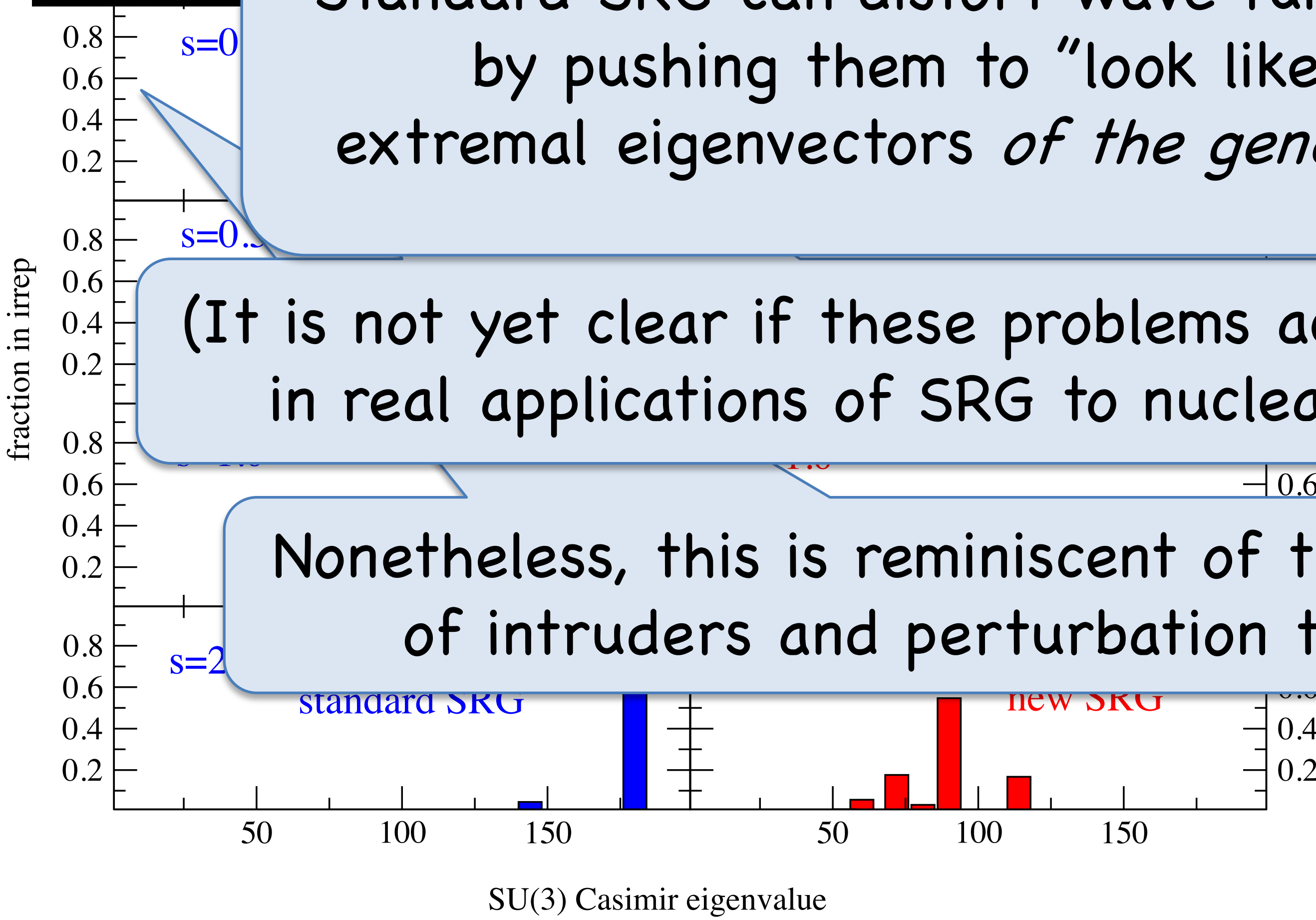
Nonetheless, this is reminiscent of the problem of intruders and perturbation theory.



SAN DIEGO STATE UNIVERSITY

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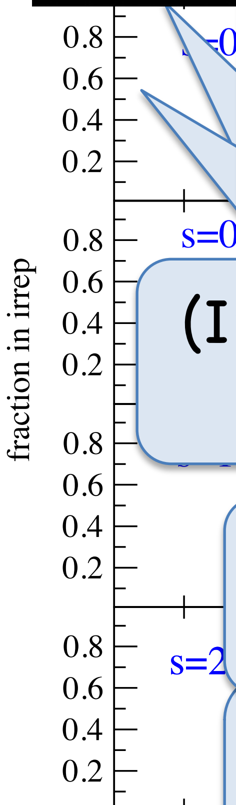
Standard SRG can distort wave functions by pushing them to "look like" extremal eigenvectors *of the generator*



(It is not yet clear if these problems actually occur in real applications of SRG to nuclear physics)

Nonetheless, this is reminiscent of the problem of intruders and perturbation theory.

The "new" SRG tends to have larger overlaps between the original and evolved wave functions

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?

Thank you!

Additional slides

for curious people

Intruders and perturbation theory

Divide up the Hilbert space into the model space P and the excluded space Q.

The Feshbach effective interaction in the model space is

$$P\,H\,P + P\,H\,Q\,(E - QHQ)^{-1}\,Q\,H\,P$$

For wave functions mostly in P, the second term can be well approximated in perturbation theory

For wave functions mostly in Q ("intruders"), the second term does not converge well in perturbation theory

(Barrett and Kirson, early 1970s)

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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?

Ca

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

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?

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 $\mid \Psi_n >$!

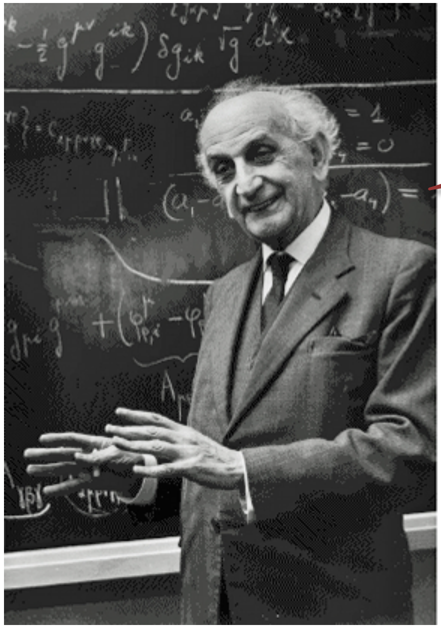
Casi

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

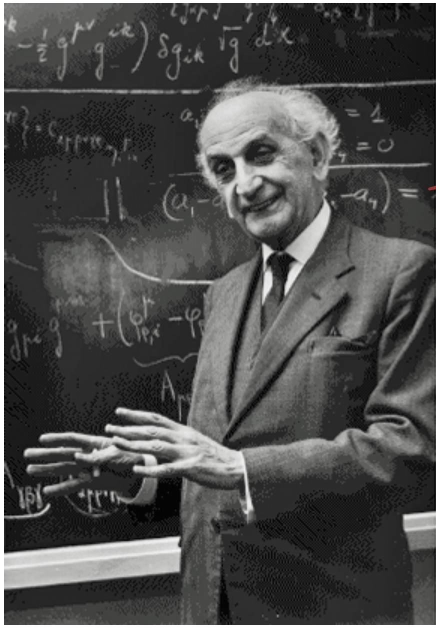
Fo
th

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

There is another way

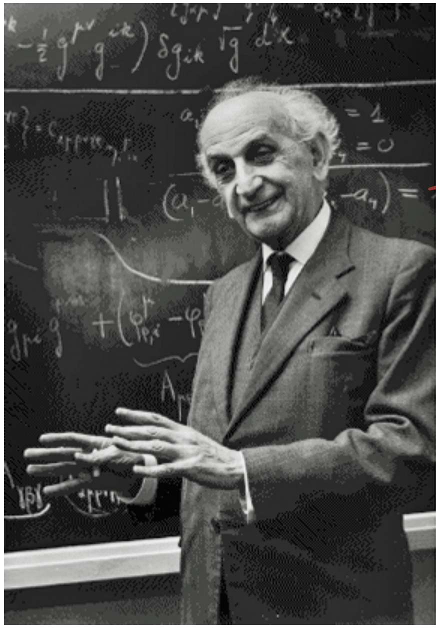


(Cornelius Lanczos)



(Cornelius Lanczos)

The Lanczos Algorithm!



(Cornelius Lanczos)

There is another way

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

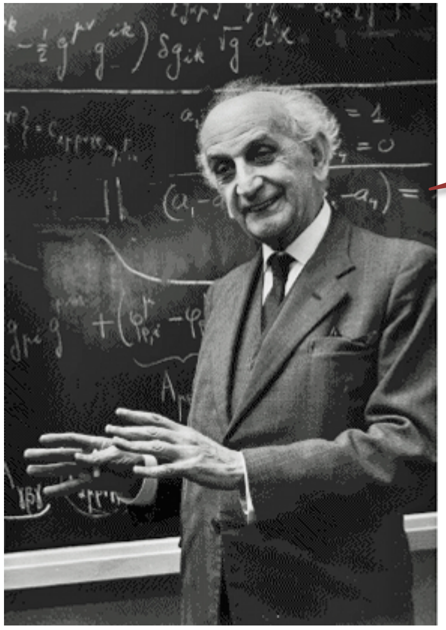
$$\mathbf{A}\vec{v}_2 = \beta_1\vec{v}_1 + \alpha_2\vec{v}_2 + \beta_2\vec{v}_3$$

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

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

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



(Cornelius Lanczos)

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

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

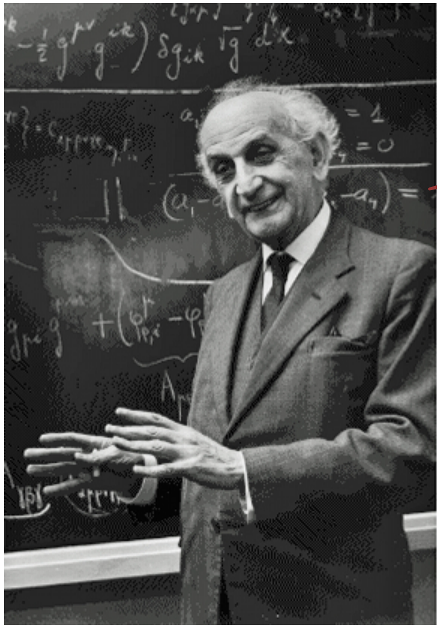
It is easy to read off the overlap of an eigenstate with the "pivot" :

$$|< v_1\ |\psi >|^2 = c_1^2$$

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.

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).

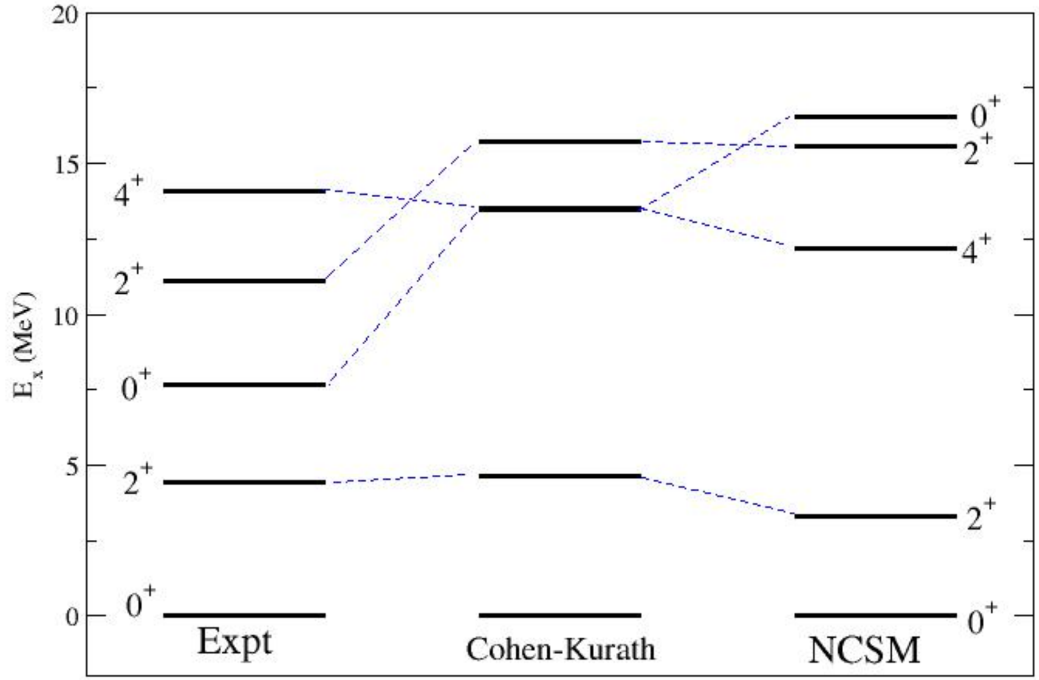
Present calculations carried out using BIGSTICK shell-model code:
Johnson, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761 (2013).

^{12}C

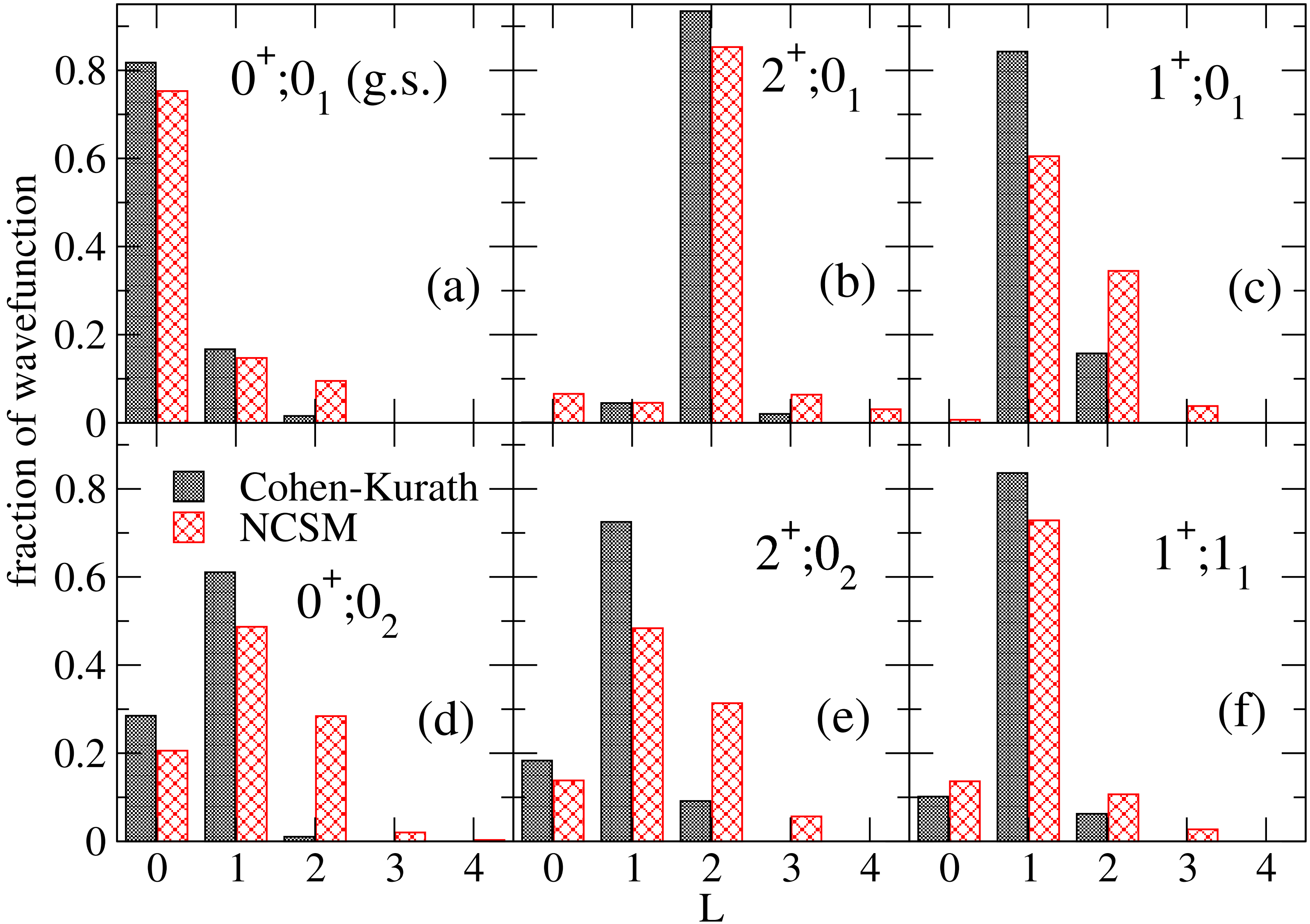
Phenomenological Cohen-Kurath force (1965) in 0*p* shell
m-scheme dimension: 51

NCSM: N3LO chiral 2-body force SRG evolved* to λ = 2.0 fm^{-1}, N_{max} = 6, ħω=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!

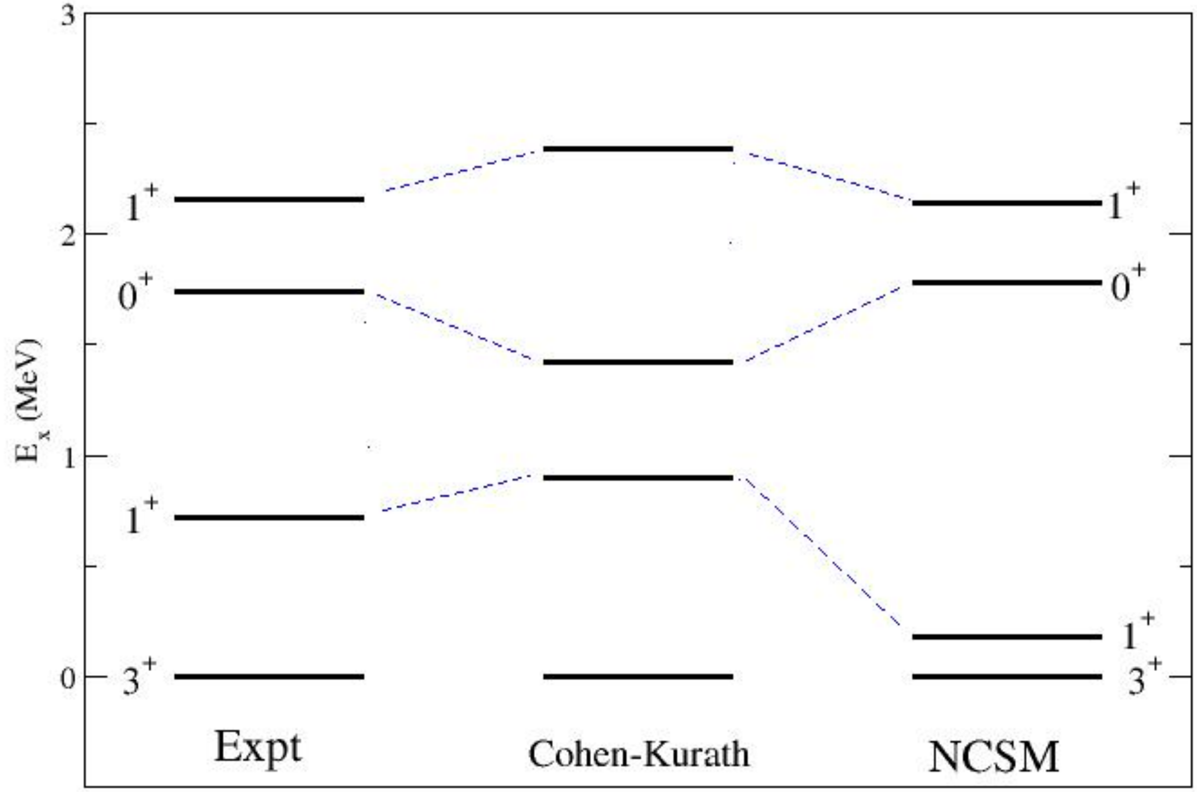


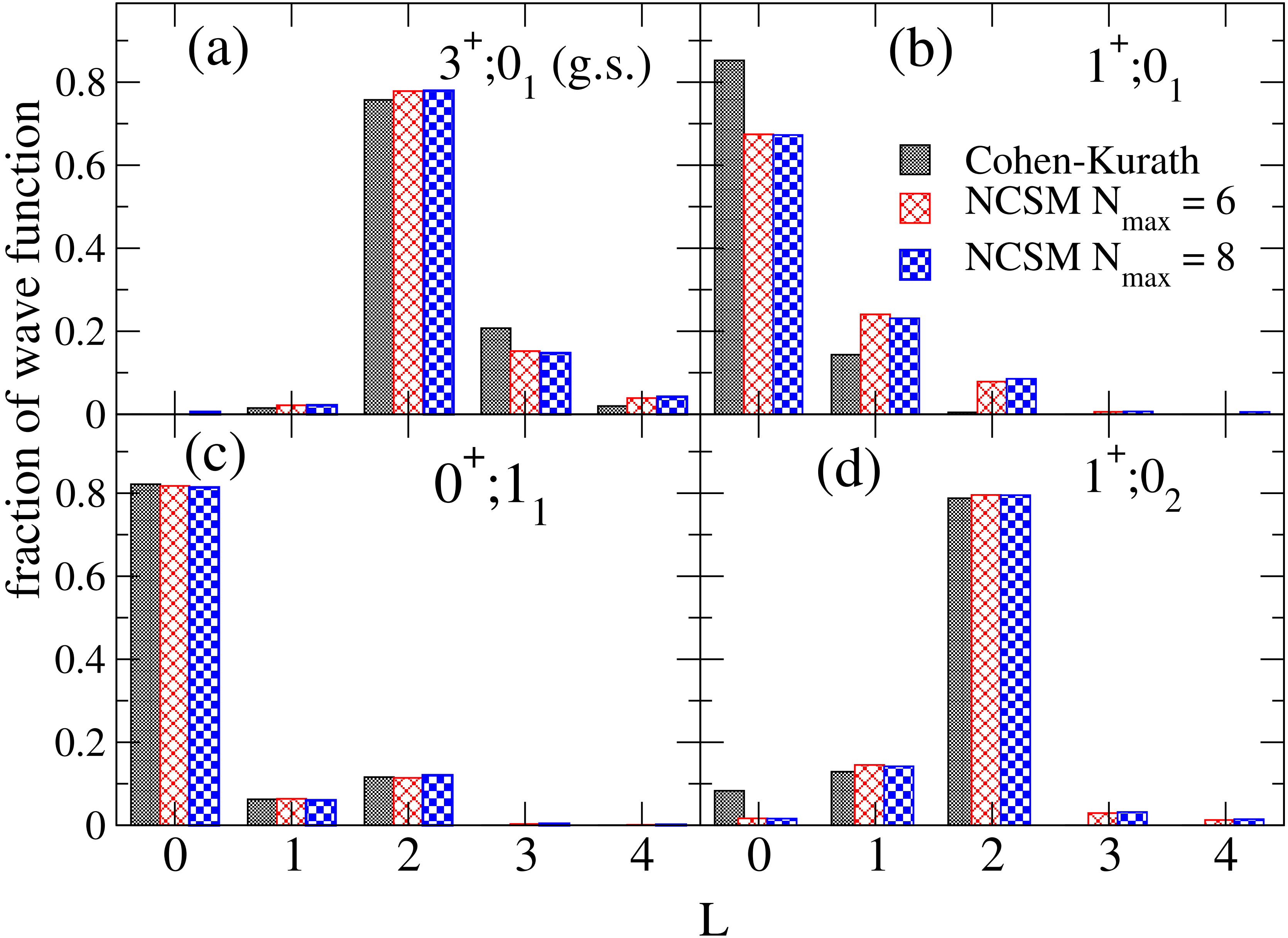
fraction of wavefunction
0
0.2
0.4
0.6
0.8
$0^+;0_1$ (g.s.)
(a)
$2^+;0_1$
(b)
$1^+;0_1$
(c)
Cohen-Kurath
NCSM
$0^+;0_2$
(d)
$2^+;0_2$
(e)
$1^+;1_1$
(f)
0
1
2
3
4
L

^{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, ħω=22 MeV
m-scheme dimension: 12 million

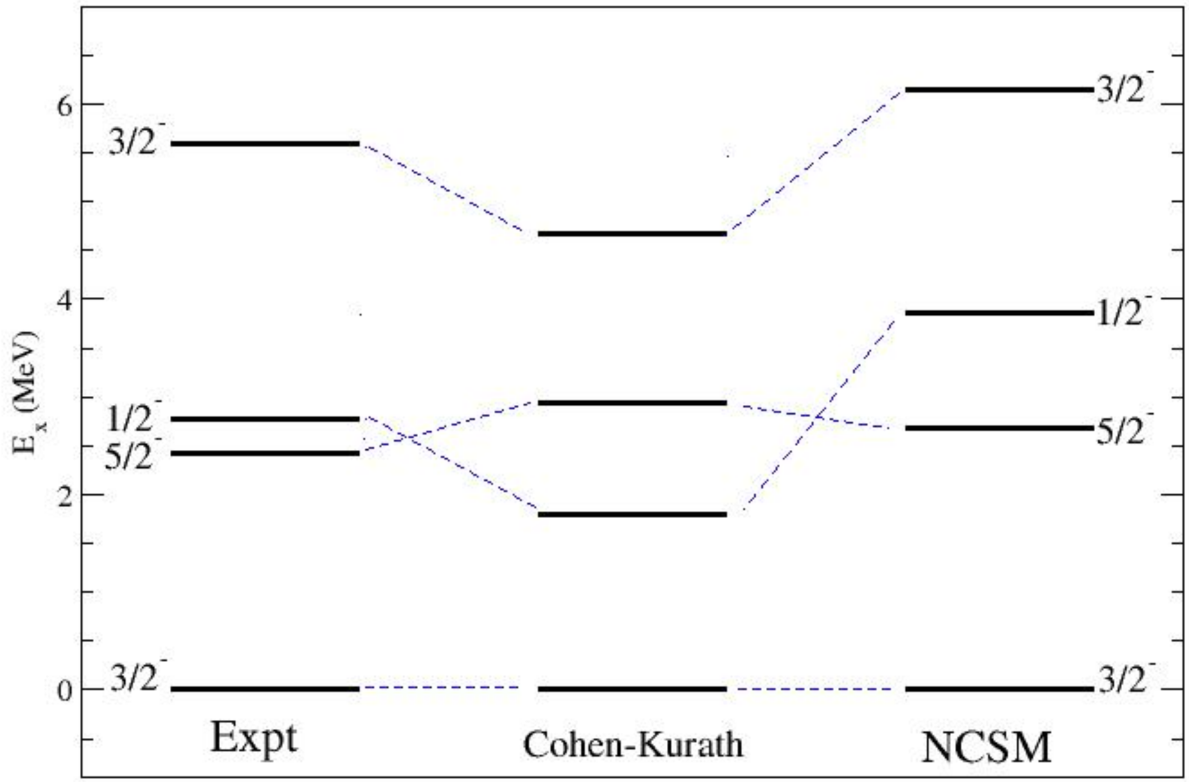


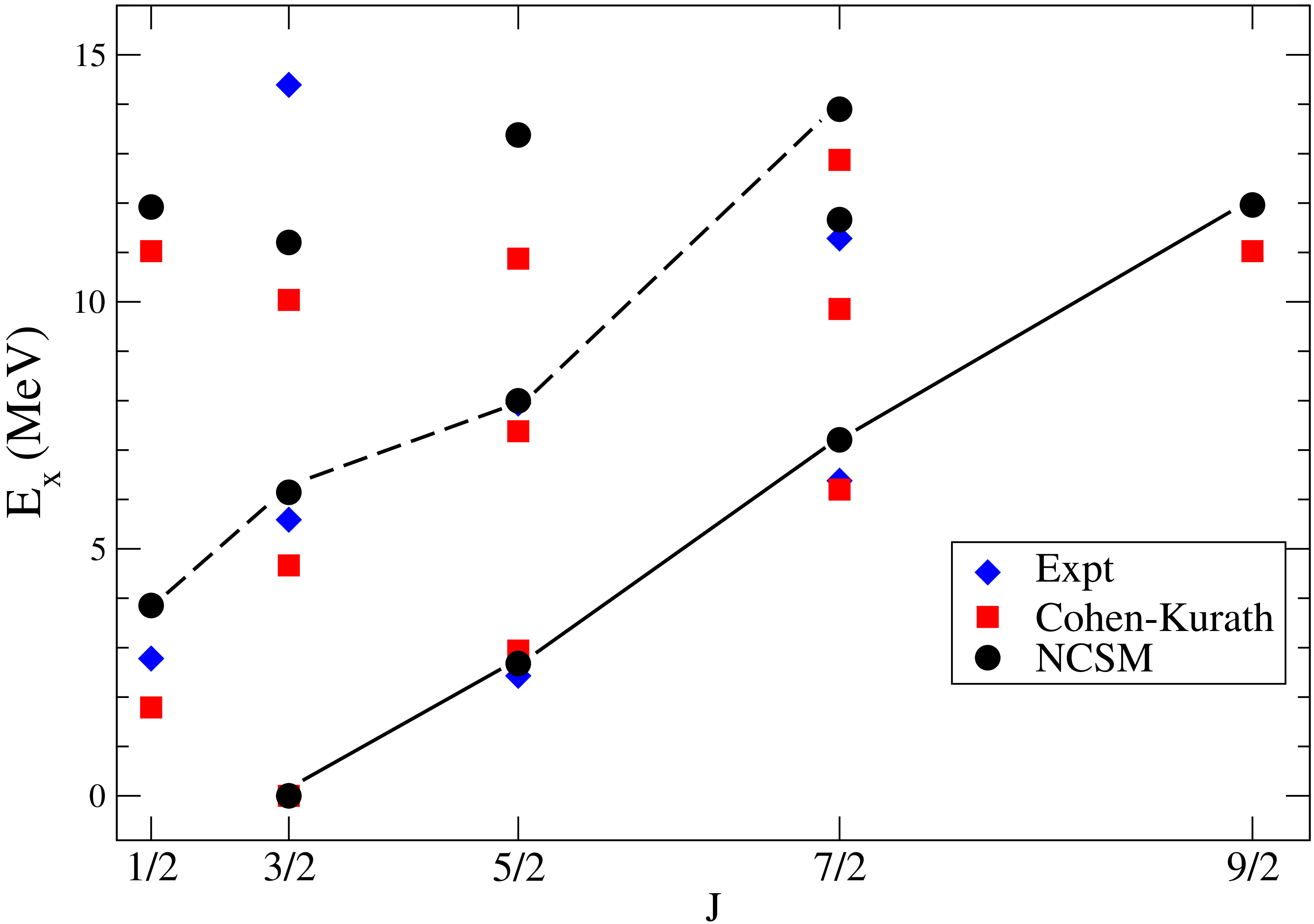

(a)
$3^+;0_1$ (g.s.)
(b)
$1^+;0_1$
(c)
$0^+;1_1$
(d)
$1^+;0_2$
Cohen-Kurath
NCSM N_{max} = 6
NCSM N_{max} = 8
fraction of wave function
0
0.2
0.4
0.6
0.8
0
1
2
3
4
L

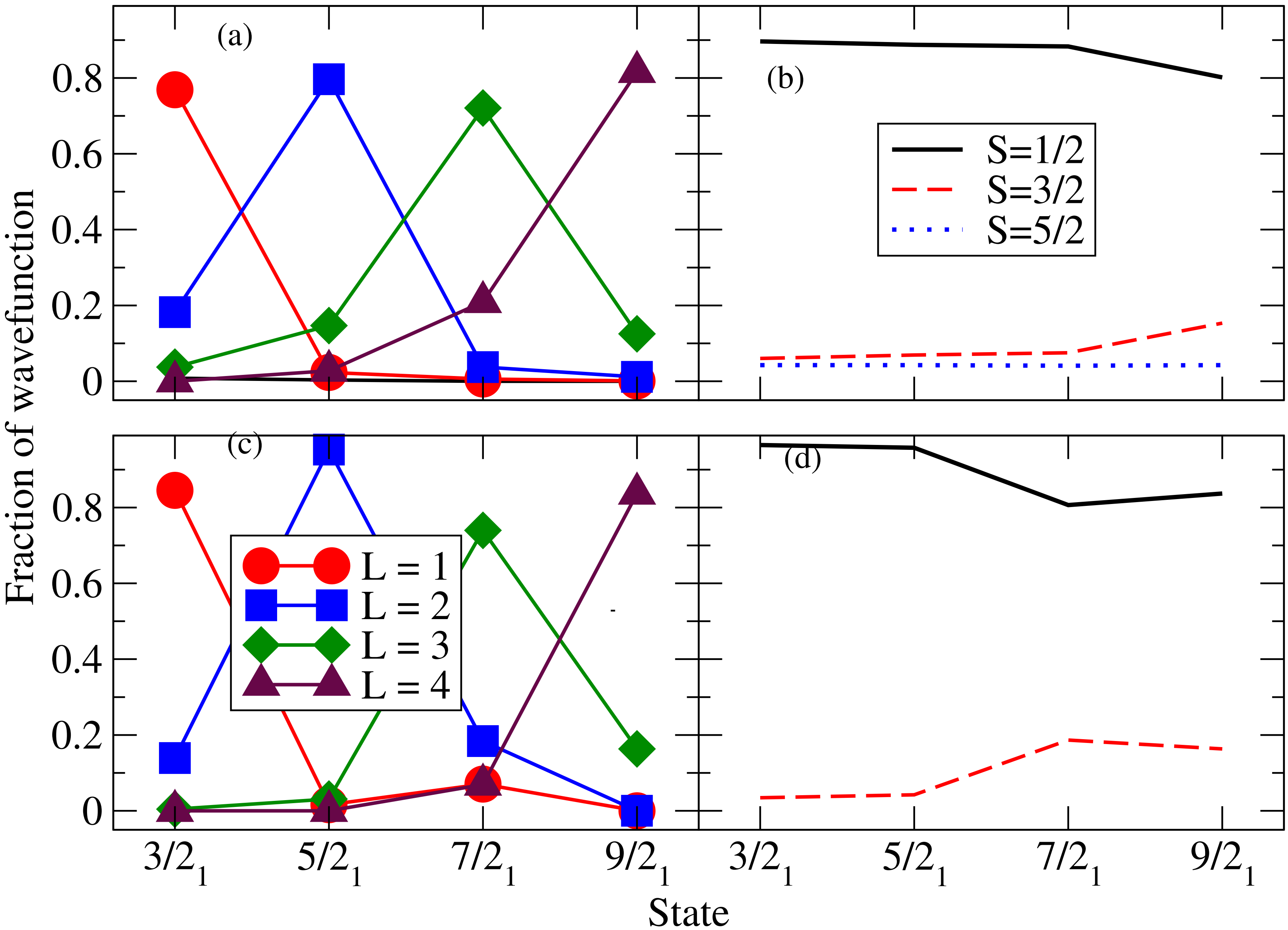
^{9}Be

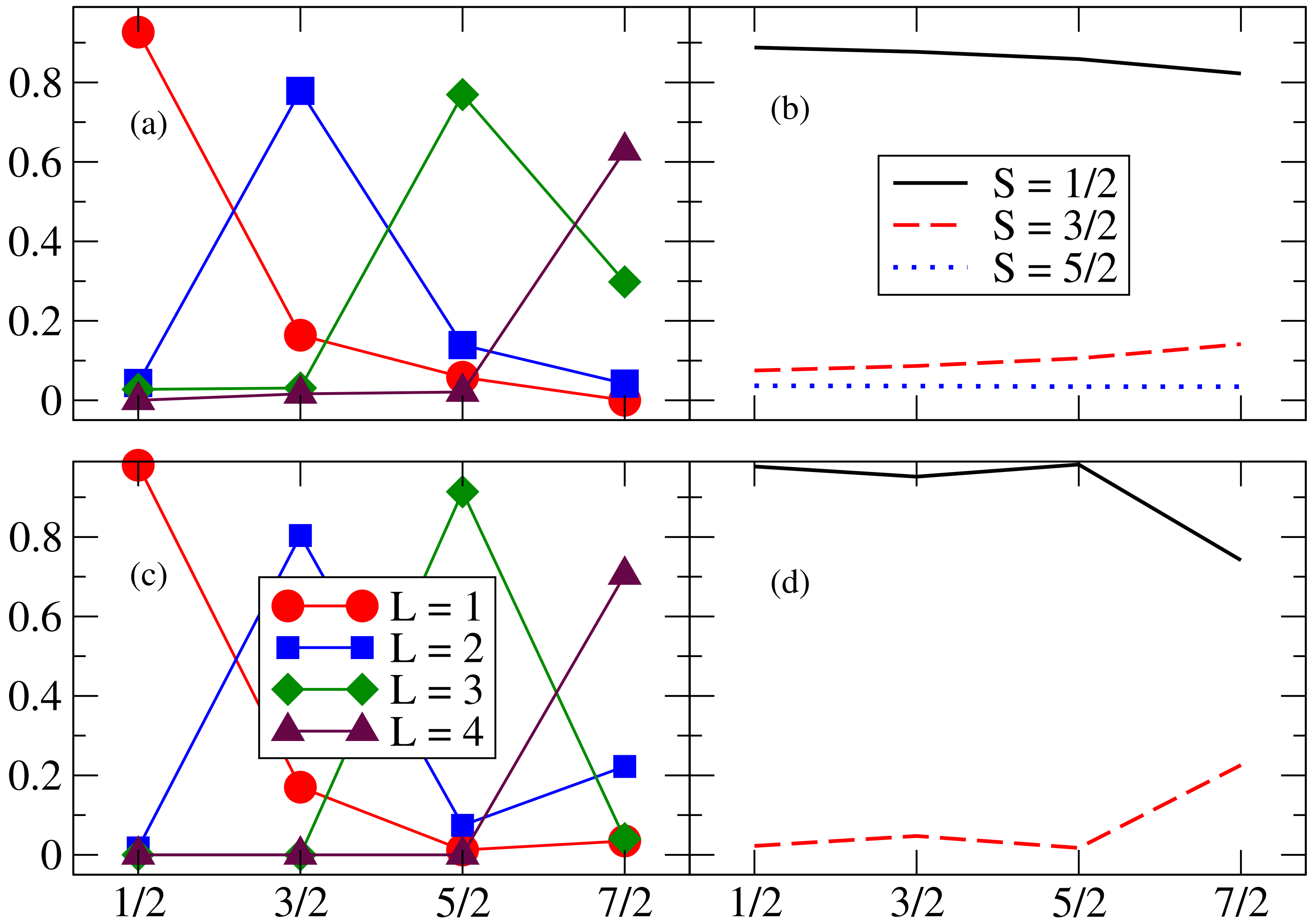
Phenomenological Cohen-Kurath *m*-scheme dimension: 62

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