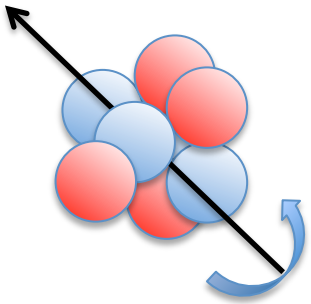
Spin-orbit decomposition of *ab initio* wavefunctions

a preliminary report



Calvin Johnson, San Diego State University

Supported by a grant from the U.S. Department of Energy

THE BIGSTICK CODE

Uses "factorization" algorithm: Johnson, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761(2013)

Arbitrary single-particle radial waveforms
Allows local or nonlocal two-body interaction
Three-body forces implemented and validated
Applies to both nuclear and atomic cases

Runs on both desktop and parallel machines
--can run at least dimension 100M+ on desktop
(20 Lanczos iterations in 300 CPU minutes)

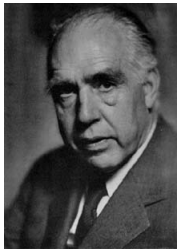
20-30k lines of codes
Fortran 90 + MPI + OpenMP

Atoms :

L=0,1,2

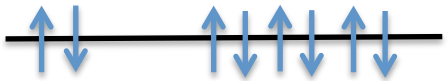
L=0,1

L=0



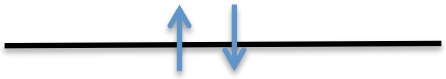
Atoms :

L=0,1,2



L=0,1

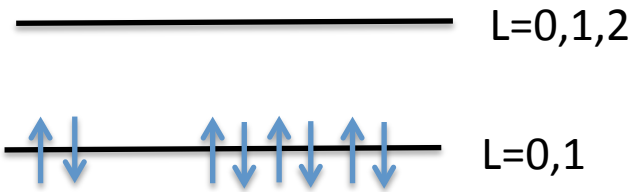
Spin is minor in atomic physics…



L=0

(Niels Bohr) (E. Schrodinger)

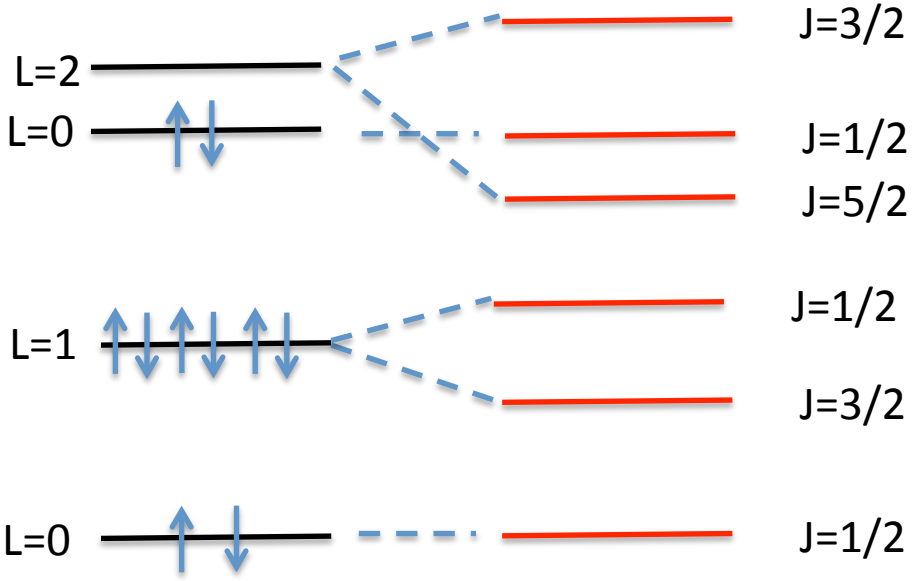
Atoms :



Spin is minor in atomic physics…

(Niels Bohr) (E. Schrodinger)

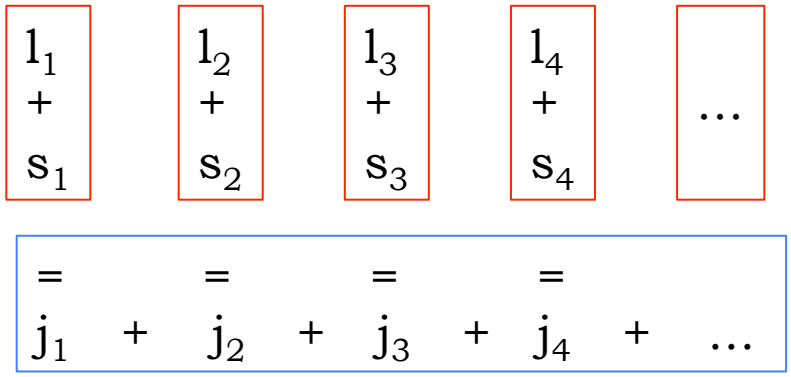
Nuclei:



…but crucial in nuclear physics…

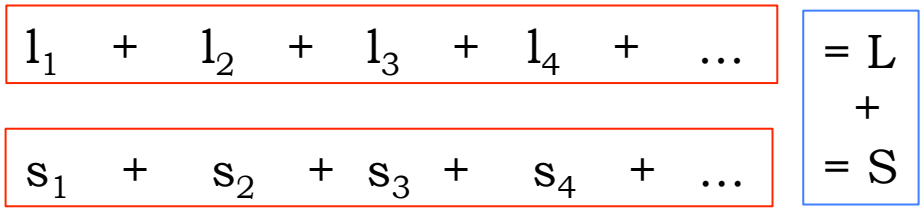
(Maria Goeppert-Mayer)

j-j versus L-S



$= J$

"j-j coupling"

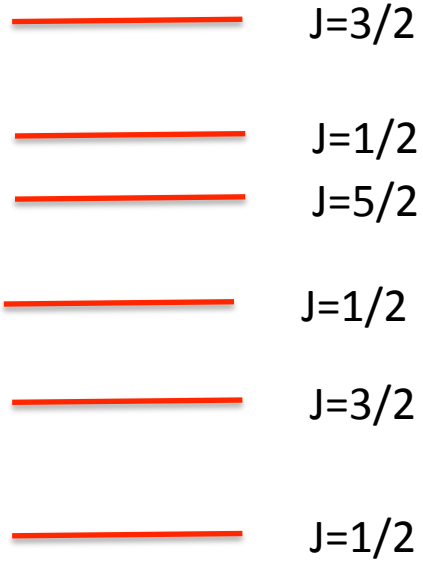


$= J$

"L-S coupling"

How good is j-j coupling?
How can we tell?

Nuclei:



Well, let's see how much a configuration-mixing calculation is approximated by a filled shell

(Maria Goeppert-Mayer)

Let's start with phenomenological forces

Nuclide	Model space	Interaction	g.s. =
^{48}Ca	pf	KB3G	90 % $(0f_{7/2})^8$
^{24}O	sd	USDB	91% $(0d_{5/2})^6$ $(1s_{1/2})^2$
^{22}O	sd	USDB	75% $(0d_{5/2})^6$

(Calculations are standard configuration-mixing: diagonalization of Hamiltonian in *m*-scheme Slater determinants, in single major harmonic oscillator shell)

Pretty good!

(Maria Goeppert-Mayer)

Let's start with phenomenological forces

Nuclide	Model space	Interaction	g.s. =
^{48}Ca	pf	KB3G	90 % $(0f_{7/2})^8$
^{24}O	sd	USDB	91% $(0d_{5/2})^6 (1s_{1/2})^2$
^{22}O	sd	USDB	75% $(0d_{5/2})^6$
^{8}He	p	Cohen-Kurath	53 % $(0p_{3/2})^4$

(Calculations are standard configuration-mixing: diagonalization of Hamiltonian in *m*-scheme Slater determinants, in single major harmonic oscillator shell)

...except that last one!

(Maria Goeppert-Mayer)

It gets worse!

Nuclide	Model space	Interaction	g.s. =
^{32}S	sd	USDB	29 % $(0d_{5/2})^{12}$ $(1s_{1/2})^{4}$
^{28}Si	sd	USDB	21% $(0d_{5/2})^{12}$
^{12}C	p	Cohen-Kurath	37% $(0p_{3/2})^{8}$

Oh no! I guess there *is* a lot of configuration mixing!

(Maria Goeppert-Mayer)

Let's see if there is a simpler picture, such as L-S coupling.

$$\begin{array}{|c|}\hline l_1 \\ + \\ s_1 \\ \hline \end{array} \quad \begin{array}{|c|}\hline l_2 \\ + \\ s_2 \\ \hline \end{array} \quad \begin{array}{|c|}\hline l_3 \\ + \\ s_3 \\ \hline \end{array} \quad \begin{array}{|c|}\hline l_4 \\ + \\ s_4 \\ \hline \end{array} \quad \begin{array}{|c|}\hline \ldots \\ \hline \end{array}$$

$$\boxed{= \quad + \quad = \quad + \quad = \quad + \quad = \quad + \quad \ldots \\ j_1 \quad + \quad j_2 \quad + \quad j_3 \quad + \quad j_4 \quad + \quad \ldots} \quad = J$$

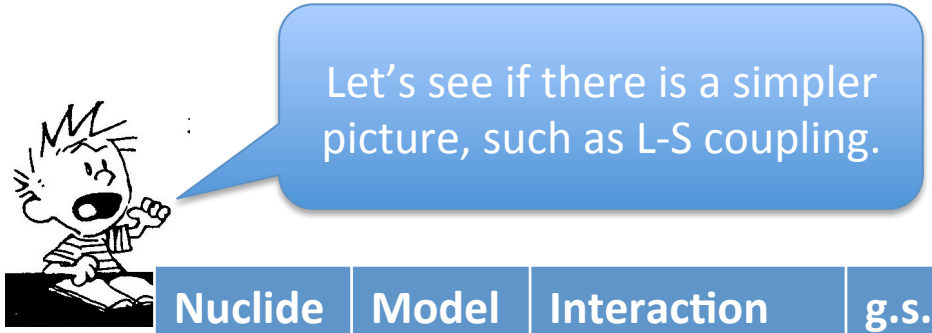
"j-j coupling"

$$\boxed{l_1 + l_2 + l_3 + l_4 + \ldots}$$

$$\boxed{s_1 + s_2 + s_3 + s_4 + \ldots}$$

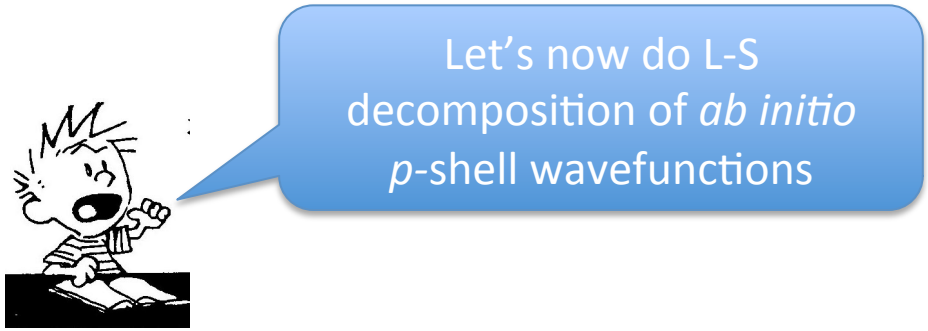
$$\boxed{\begin{array}{c} = L \\ + \\ = S \end{array}} \quad = J$$

"L-S coupling"



Nuclide	Model space	Interaction	g.s. =	g.s. =
^{48}Ca	pf	KB3G	90 % $(0f_{7/2})^8$	20% L = 0
^{24}O	sd	USDB	91% $(0d_{5/2})^6 (1s_{½})^2$	34% L = 0
^{22}O	sd	USDB	75% $(0d_{5/2})^6$	38% L = 0
^{8}He	p	Cohen-Kurath	53 % $(0p_{3/2})^4$	96% L = 0
^{32}S	sd	USDB	29 % $(0d_{5/2})^{12} (1s_{½})^4$	34% L = 0
^{28}Si	sd	USDB	21% $(0d_{5/2})^{12}$	36% L = 0
^{12}C	p	Cohen-Kurath	37% $(0p_{3/2})^8$	82% L = 0

This illustrates a (once) well-known fact: that L-S coupling is a better approximation in the *p*-shell than *j-j* coupling.



Why?

-- To see if this pattern holds for *ab initio* interactions
   -- How well do phenomenological interactions match *ab initio*?

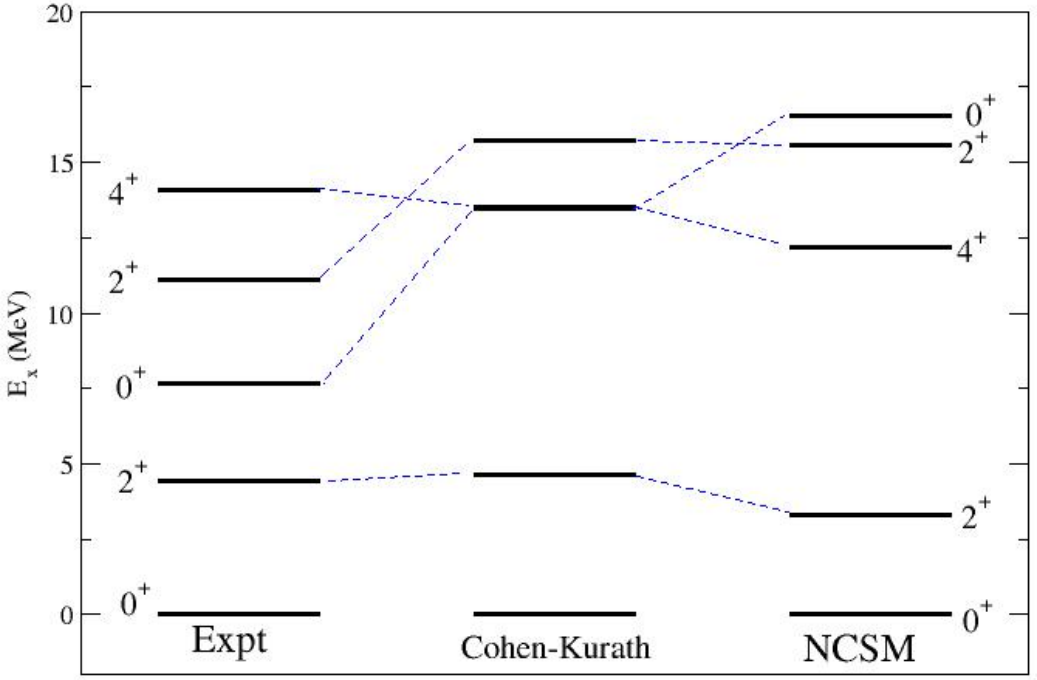
-- Crucially, we know the 3-body forces strongly affects the spin-orbit force. Can we see this happen directly?

Note: In this talk I only give 2-body results. Need 3-body forces…

^{12}C

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

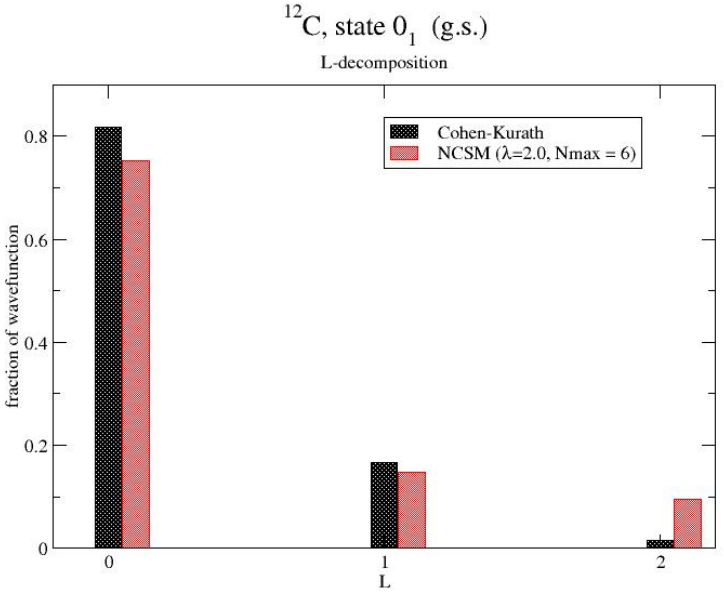
NCSM: N3LO chiral 2-body force SRG evolved* to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 35 million

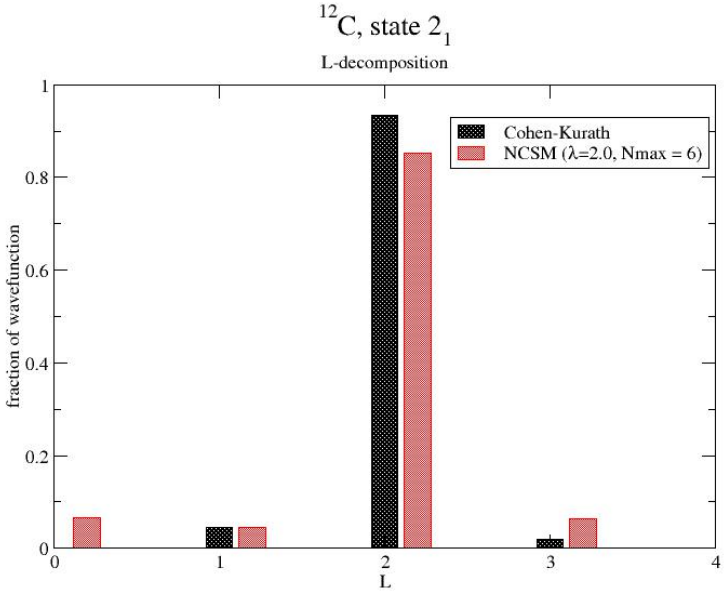


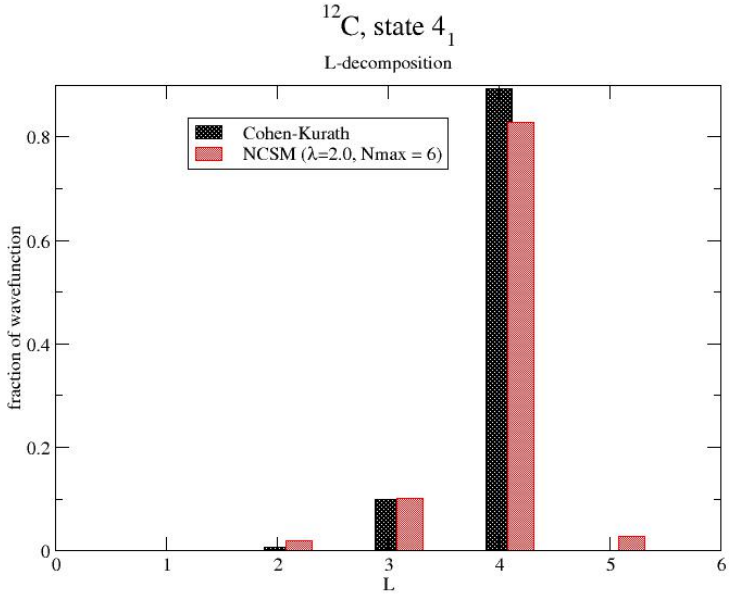
(Calculations carried out using BIGSTICK shell-model code: Johnson, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761 (2013).)

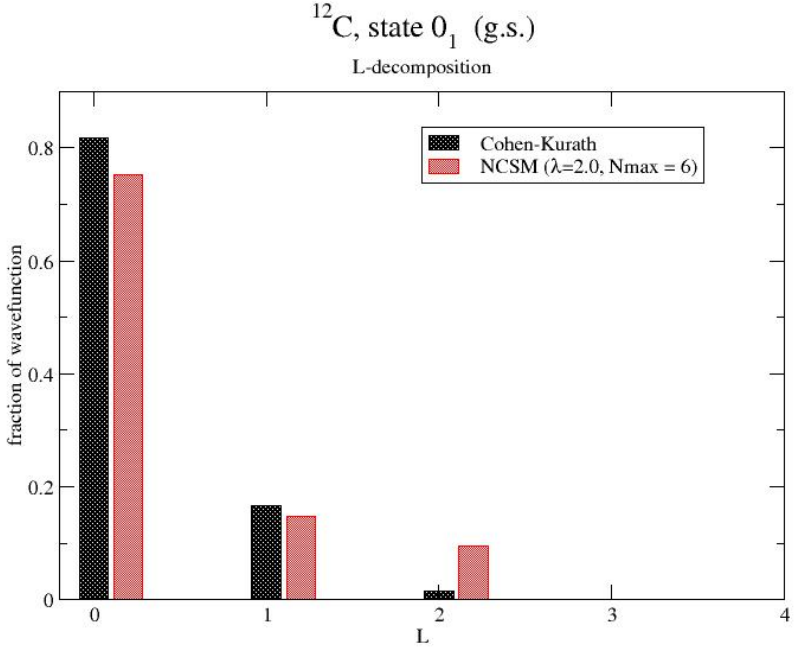
*code courtesy of P. Navratil, any mistakes in using it are mine!

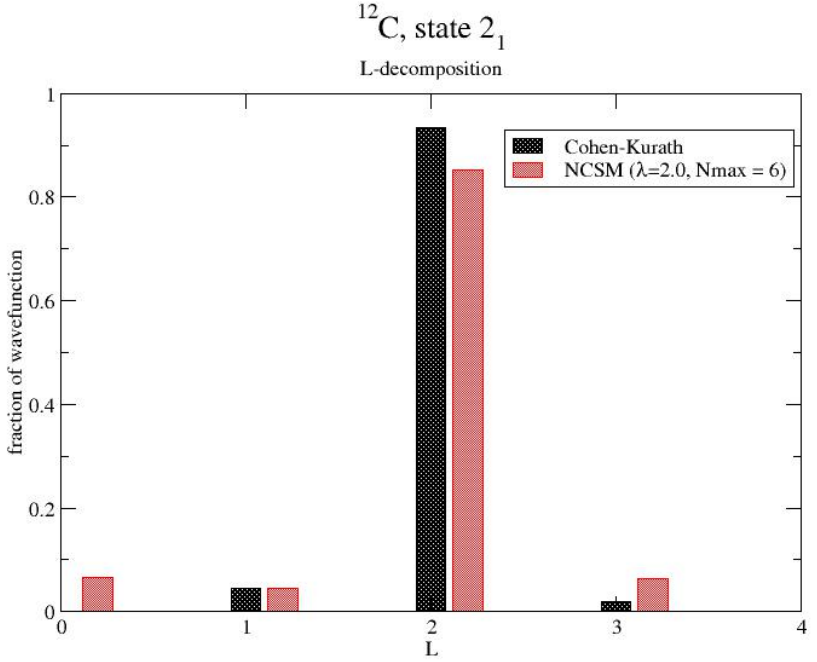
And the (rotational) band played on...

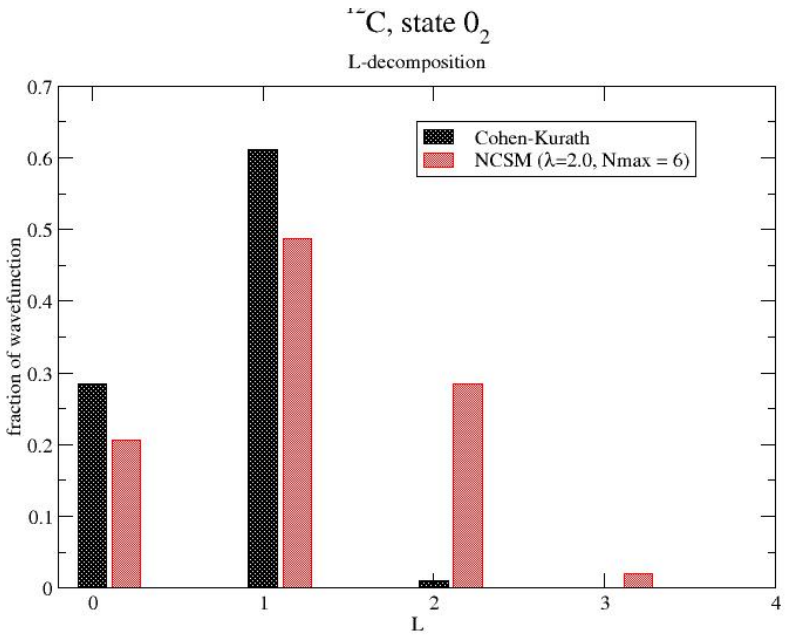


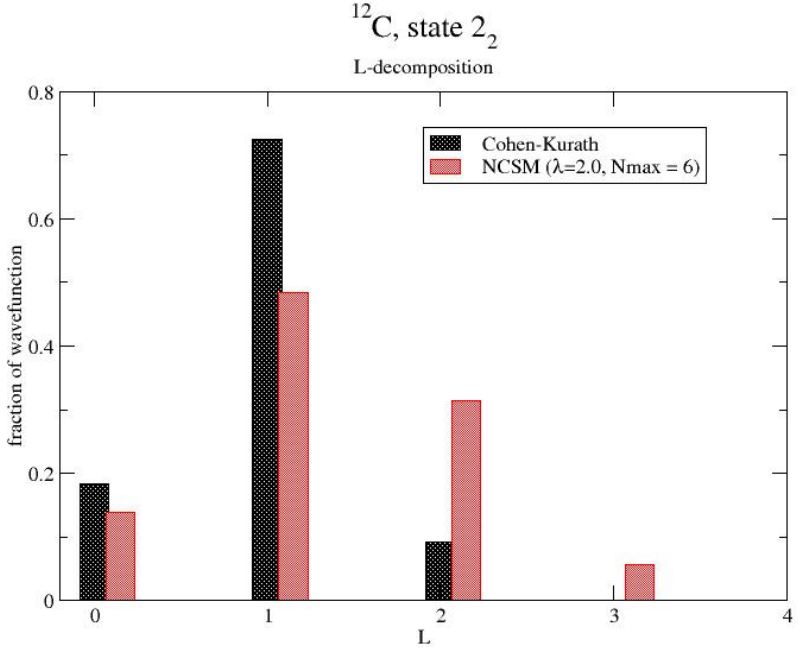


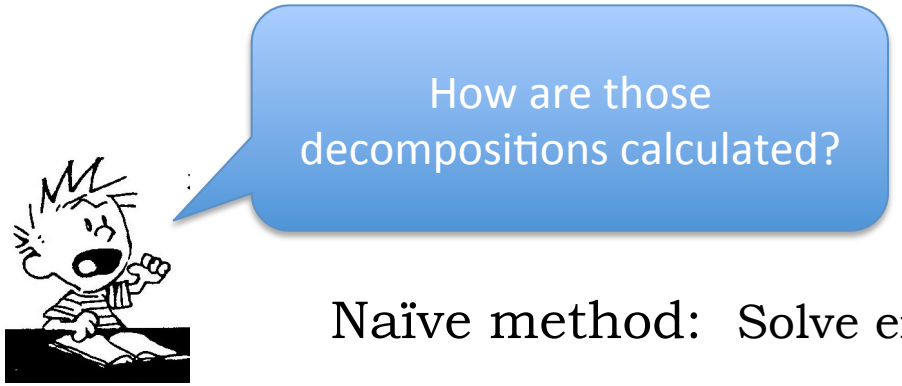



^{12}C, state 0_1 (g.s.)
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L


^{12}C, state 2_1
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L


^{12}C, state 0_2
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L


^{12}C, state 2_2
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L



Naïve method: Solve eigenpair problems, e.g.

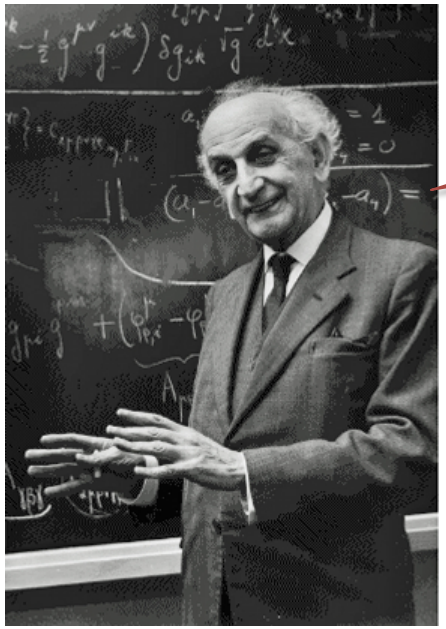
$$\mathbf{H} \mid \Psi_n > = E_n \mid \Psi_n >$$

and

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

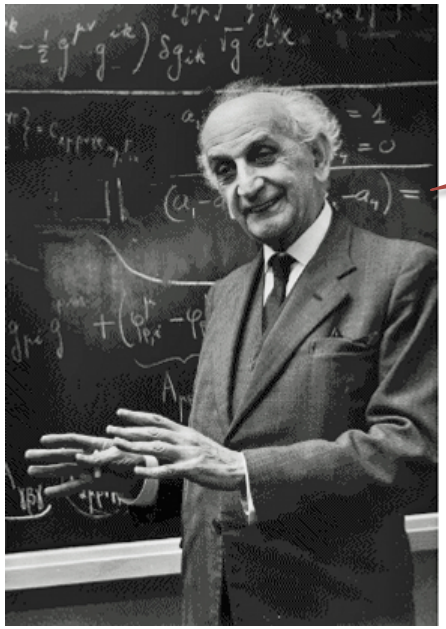
…and then take overlaps, $|< l; \alpha \mid \Psi_n >|^2$

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



There is another way

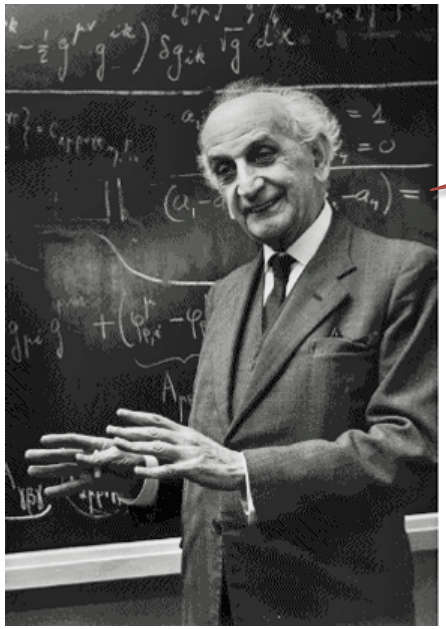
(Cornelius Lanczos)



(Cornelius Lanczos)

There is another way

The Lanczos Algorithm!



(Cornelius Lanczos)

There is another way

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

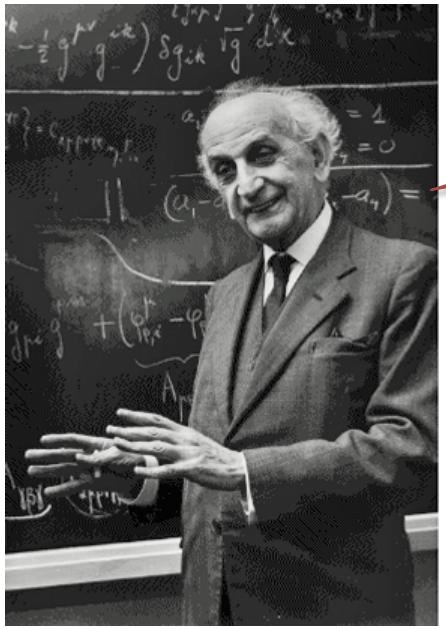
$$\mathbf{A}\vec{v}_2 = \beta_1\vec{v}_1 + \alpha_2\vec{v}_2 + \beta_2\vec{v}_3$$

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

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

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)

There is another way

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

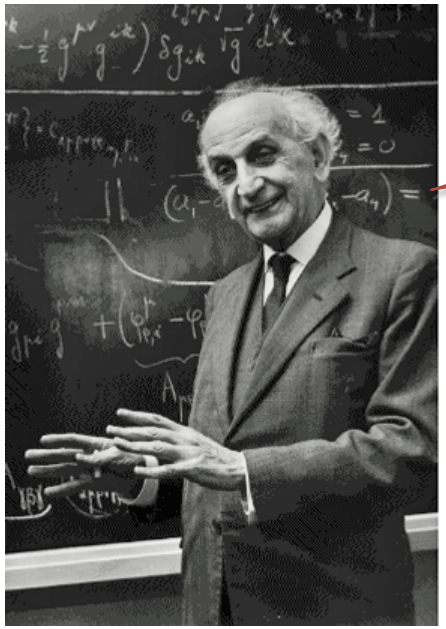
$$|\psi\rangle = c_1 |v_1\rangle + c_2 |v_2\rangle + c_3 |v_3\rangle + \ldots$$

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

$$|\langle v_1 | \psi \rangle|^2 = c_1^2$$

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

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



(Cornelius Lanczos)

There is another way

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)

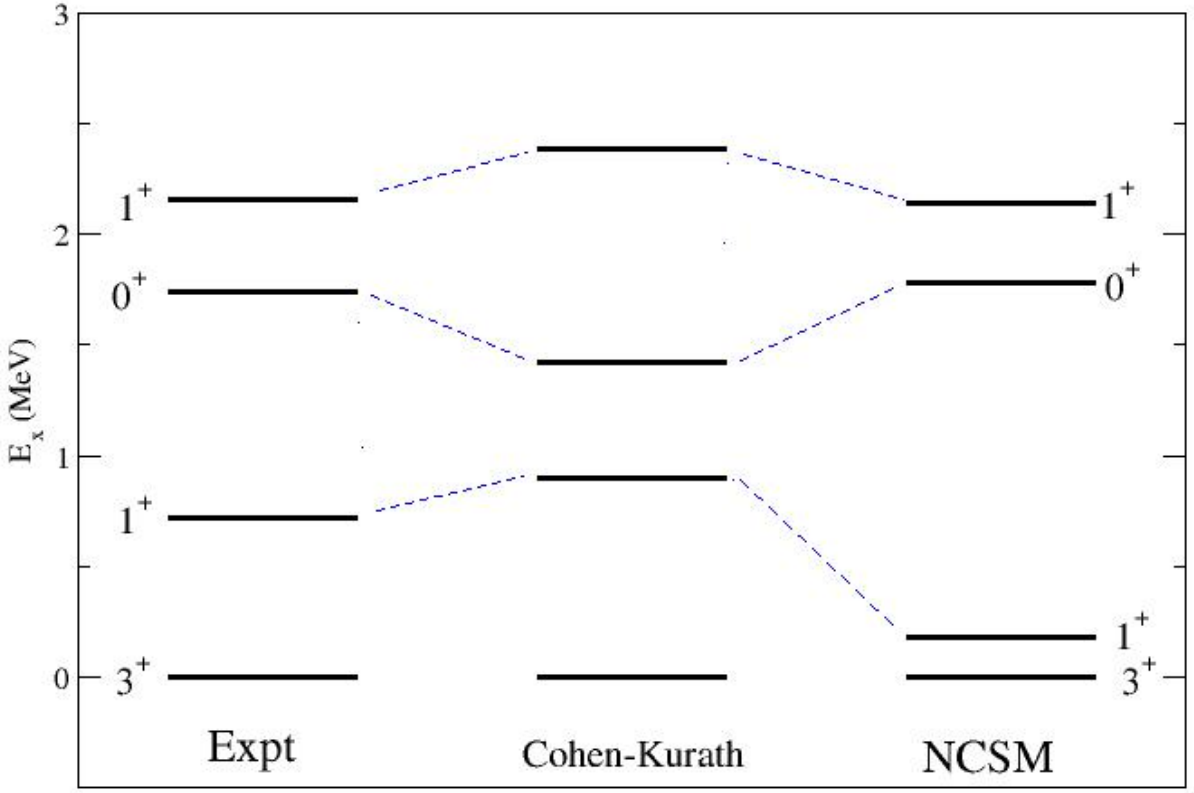
Decomposition of wavefunction into SU(3) components, looking at effect of spin-orbit force:
V. Gueorguiev, J. P Draayer, and C. W. J., PRC **63**, 014318 (2000).

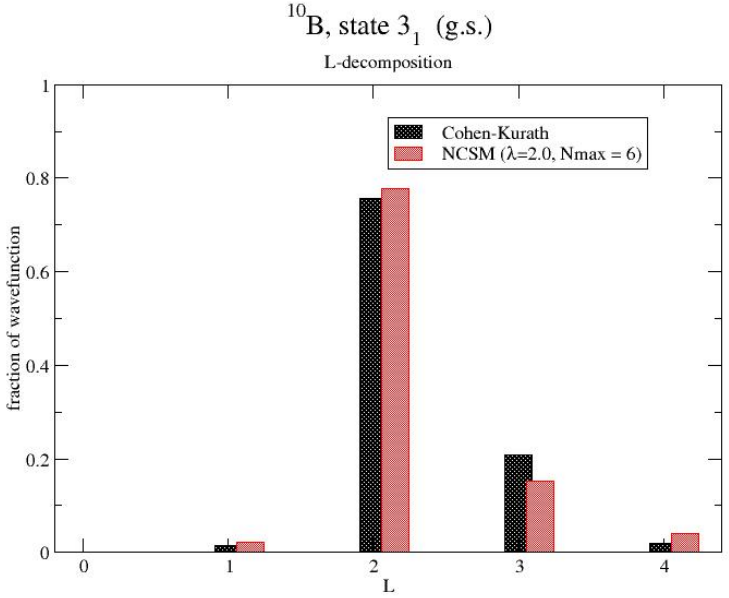
Present calculations carried out using BIGSTICK shell-model code:
Johnson, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761 (2013).

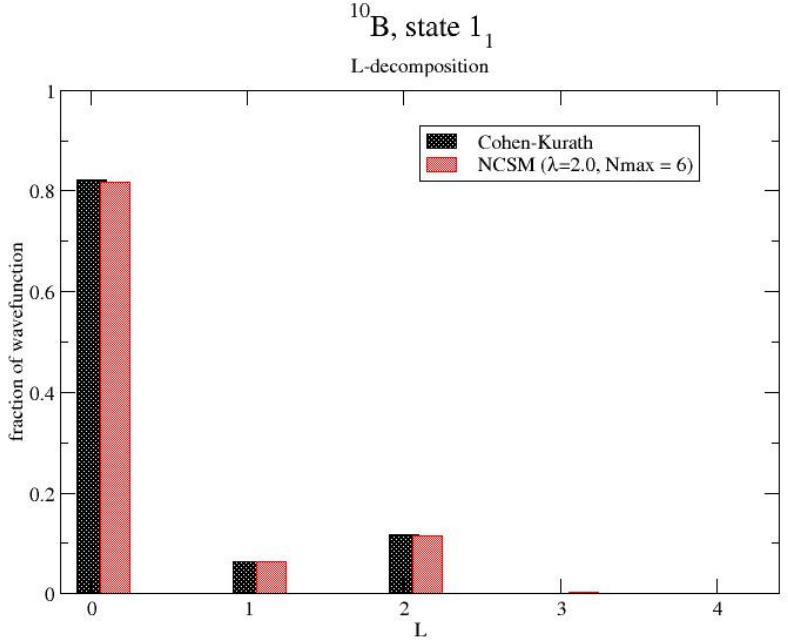
^{10}B

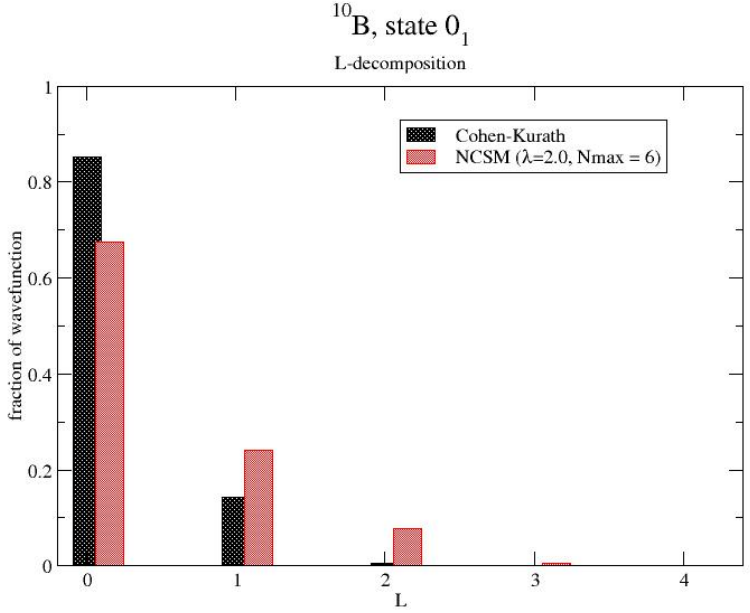
Phenomenological Cohen-Kurath *m*-scheme dimension: 84

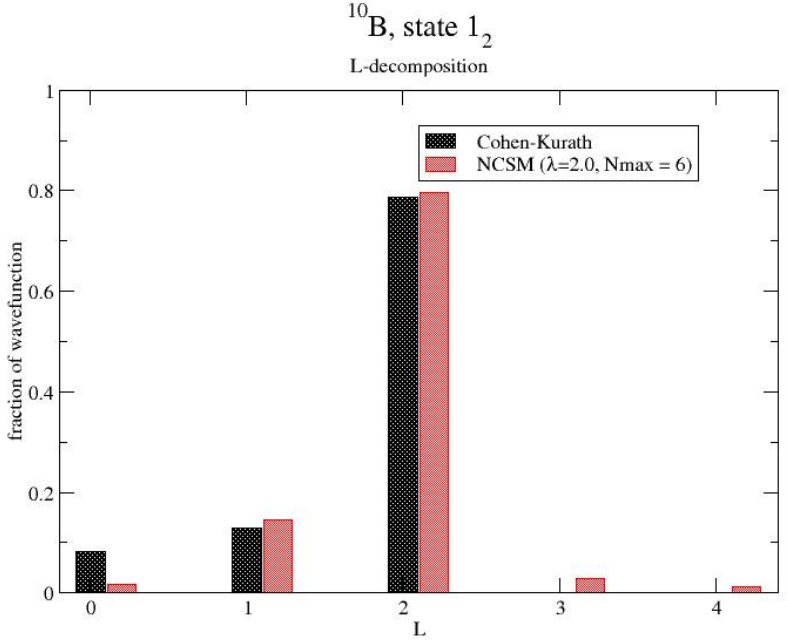
NCSM: N3LO chiral 2-body force SRG evolved to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 12 million




^{10}B, state 3_1 (g.s.)
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L


^{10}B, state 1_1
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L

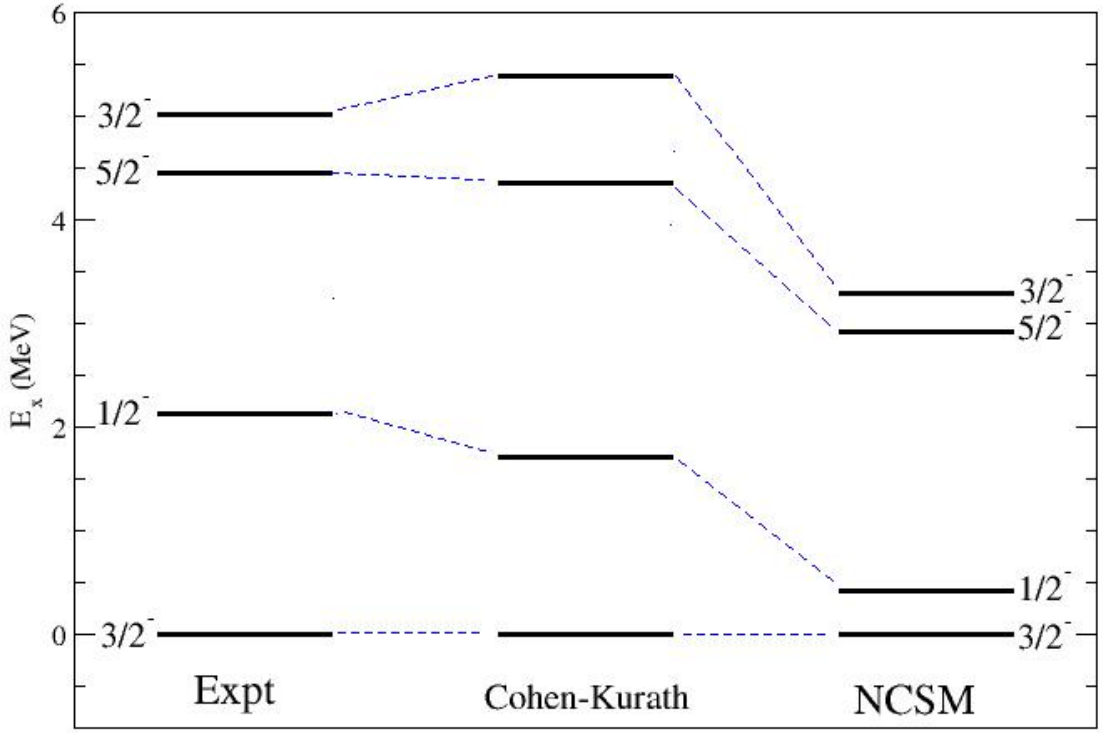

^{10}B, state 0_1
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L

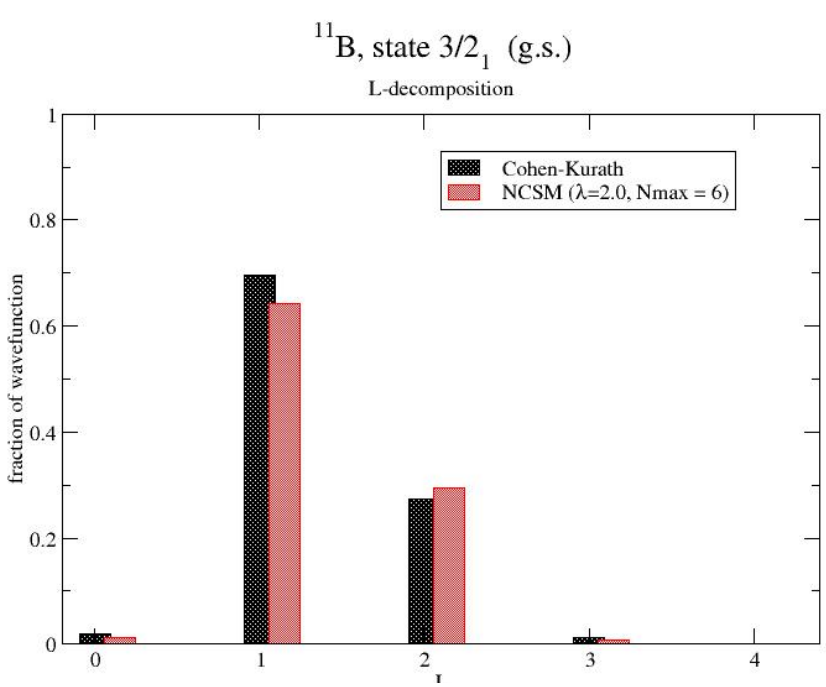

^{10}B, state 1_2
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L

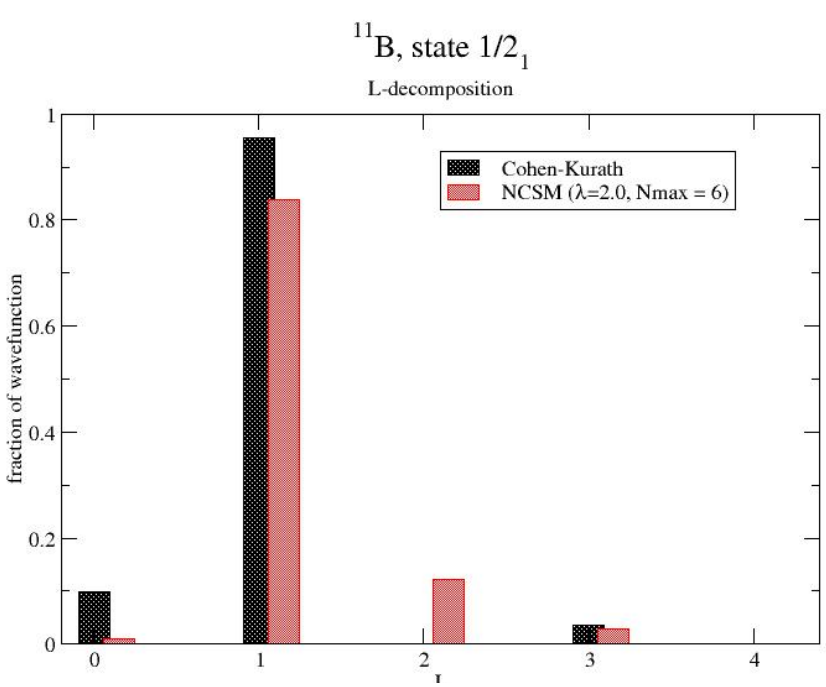
^{11}B

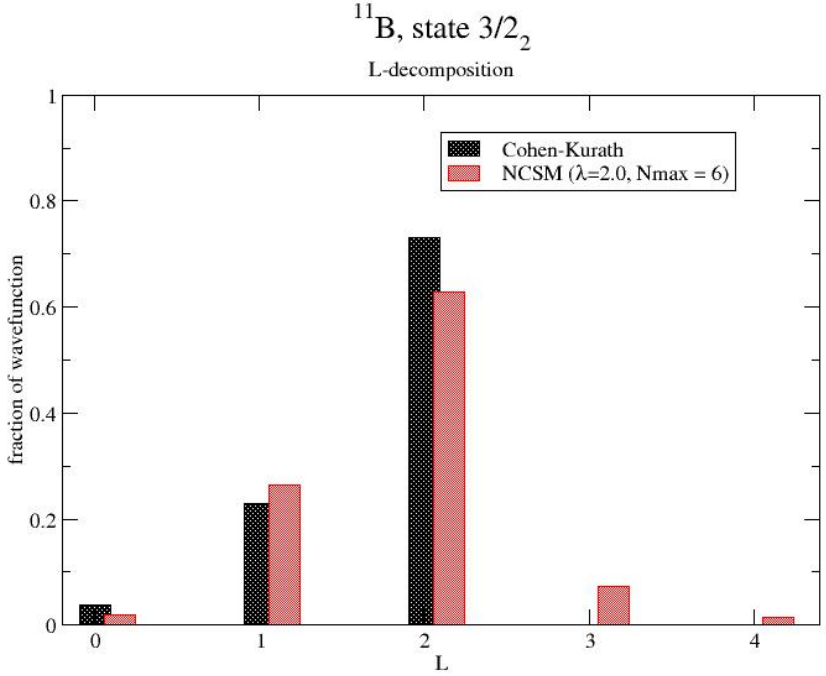
Phenomenological Cohen-Kurath *m*-scheme dimension: 62

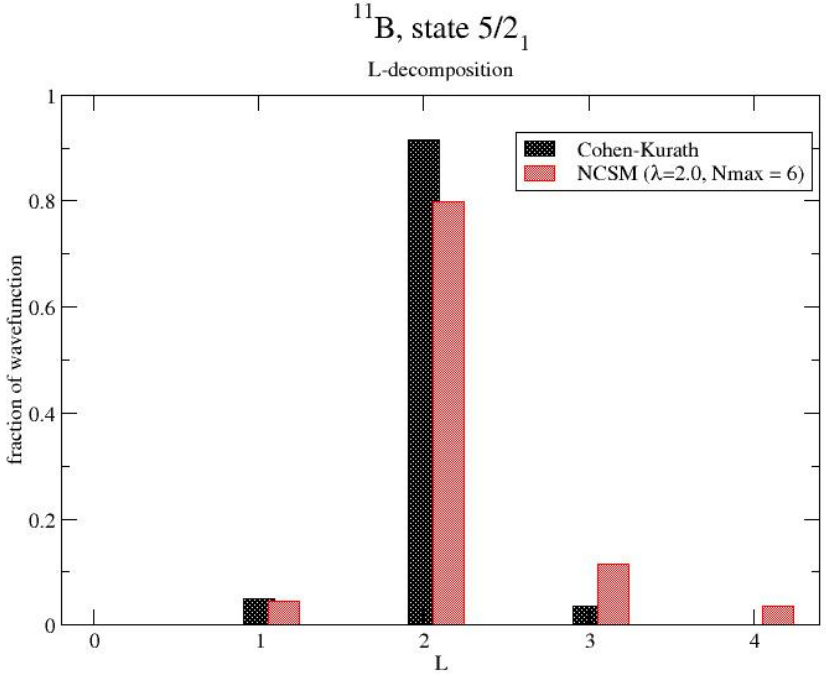
NCSM: N3LO chiral 2-body force SRG evolved to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 20 million




^{11}B, state 3/2$_1$ (g.s.)
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4


^{11}B, state 1/2$_1$
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4

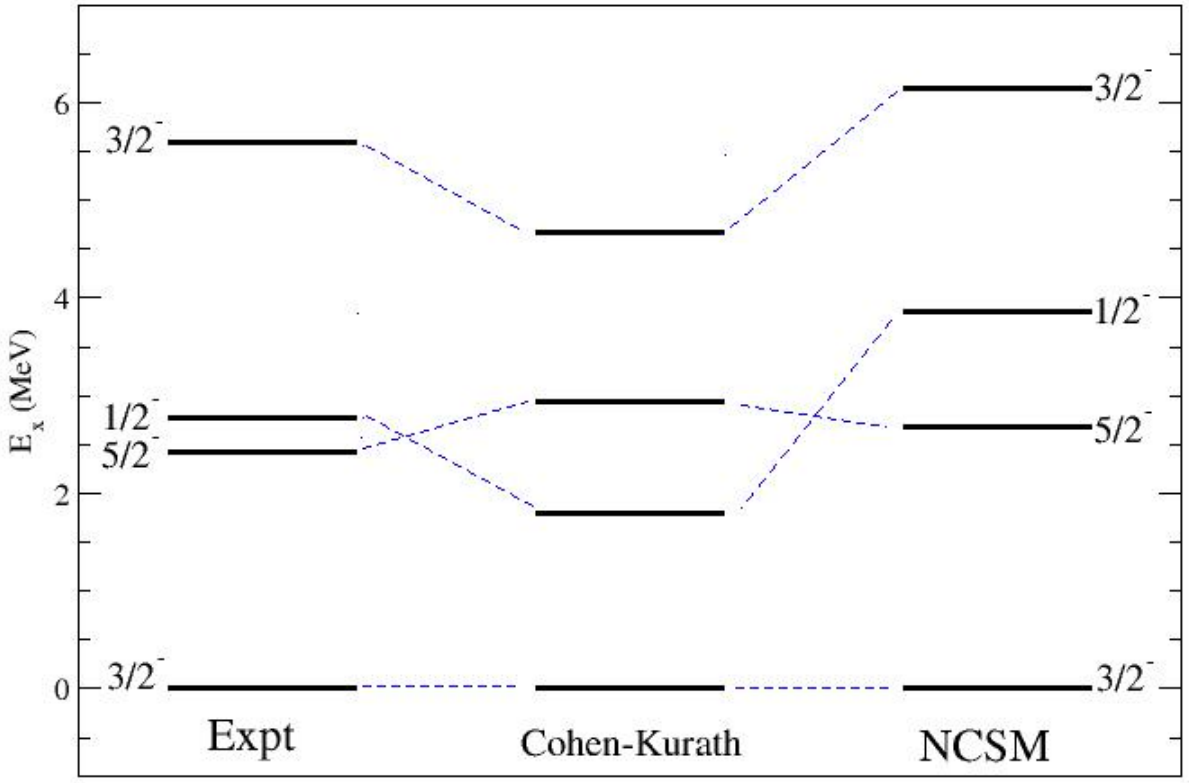

^{11}B, state 3/2$_2$
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
L

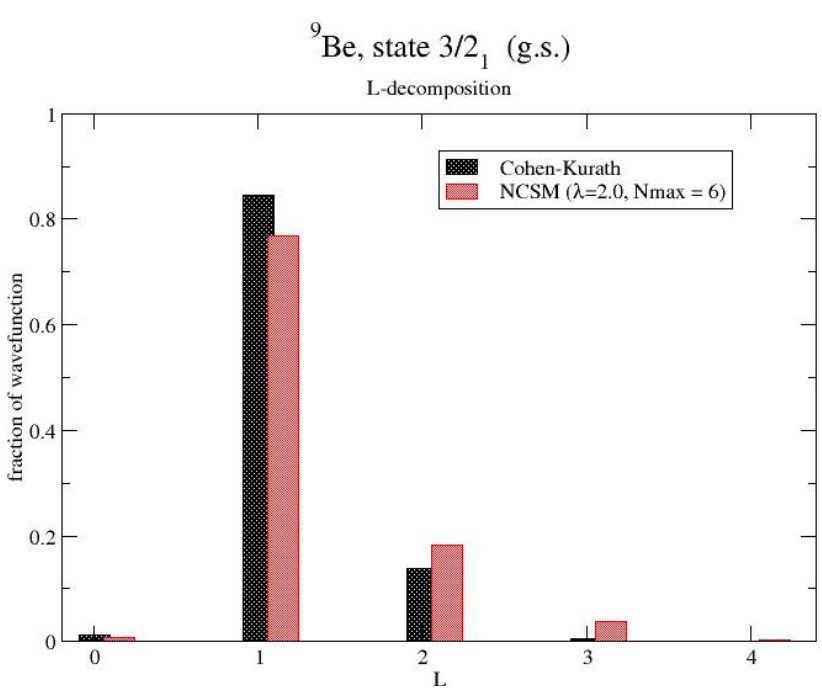

^{11}B, state 5/2$_1$
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
L

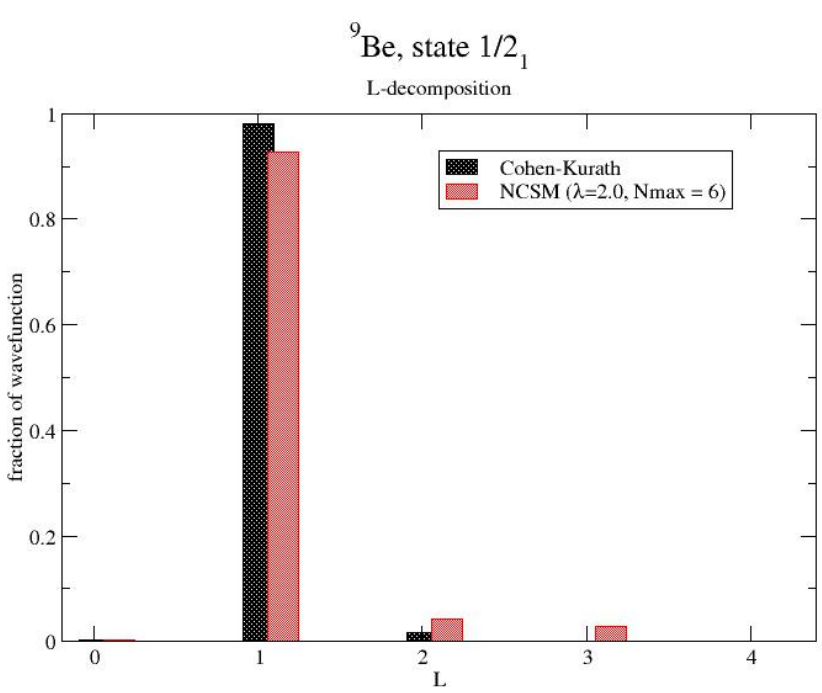
^{9}Be

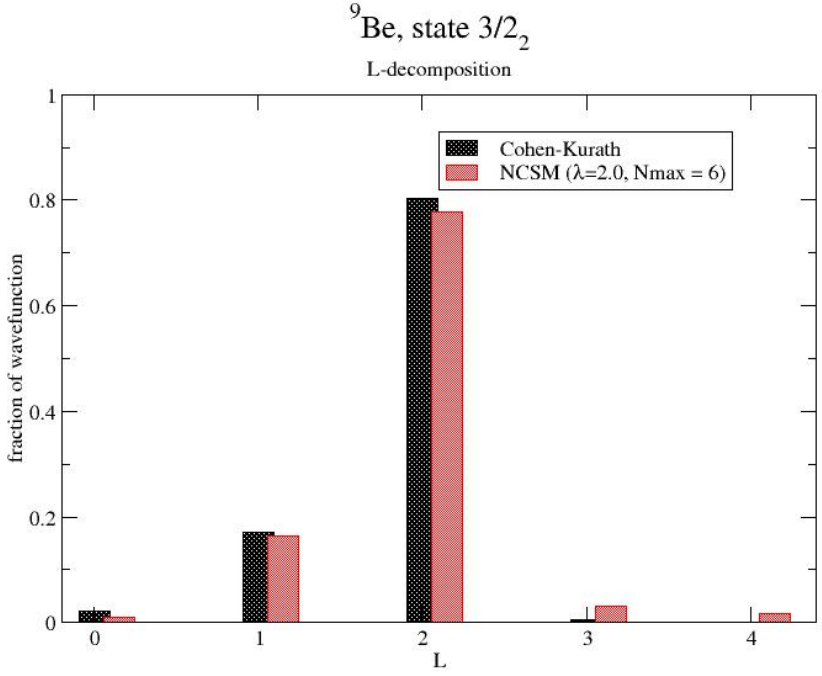
Phenomenological Cohen-Kurath *m*-scheme dimension: 62

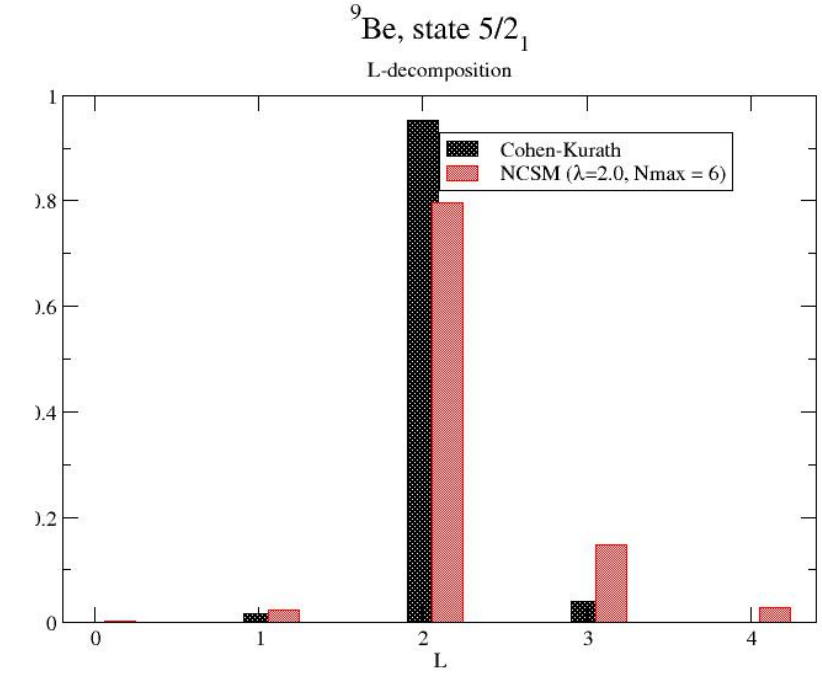
NCSM: N3LO chiral 2-body force SRG evolved to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 5.2 million




^{9}Be, state $3/2_1$ (g.s.)
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L

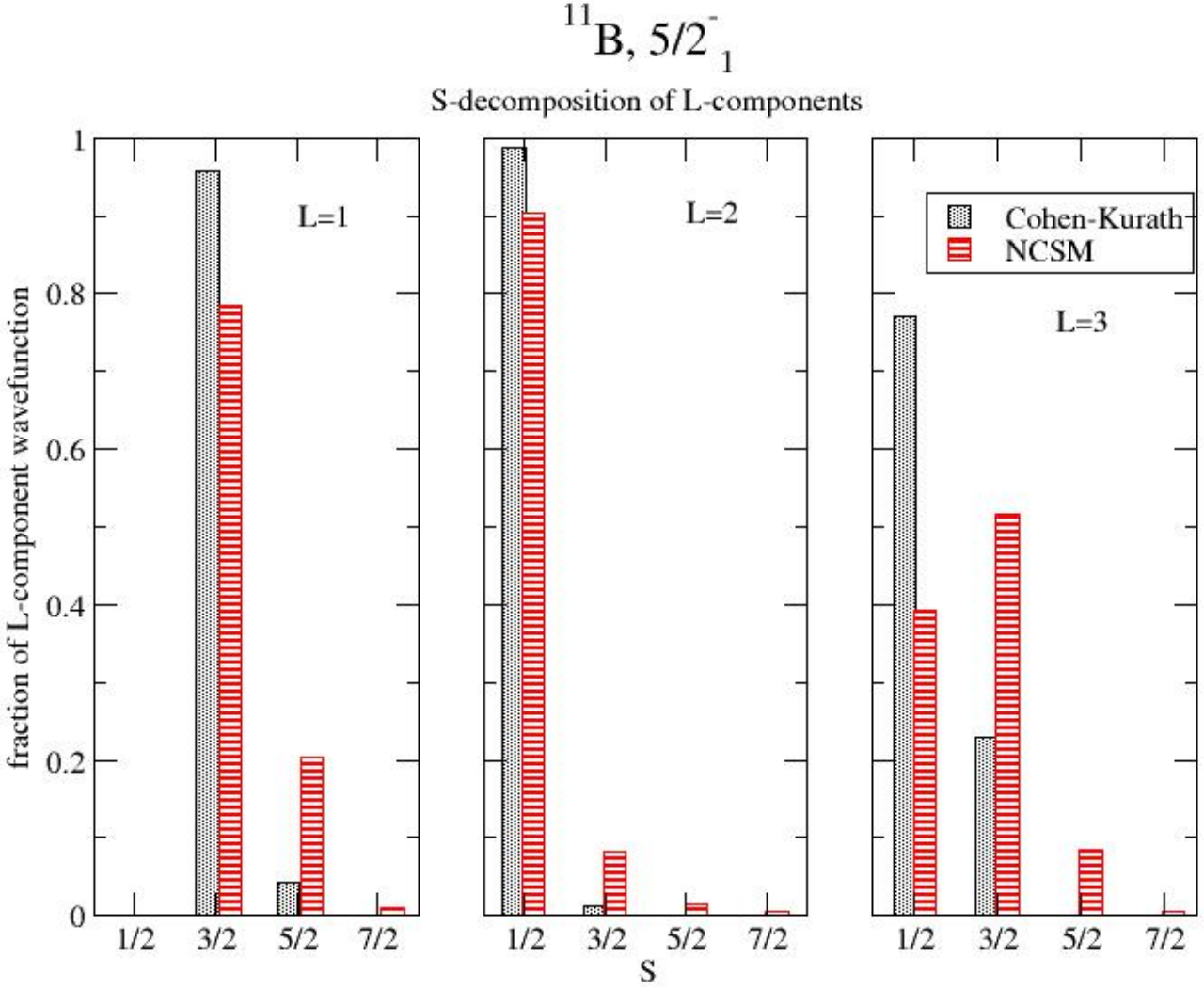

^{9}Be, state $1/2_1$
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L

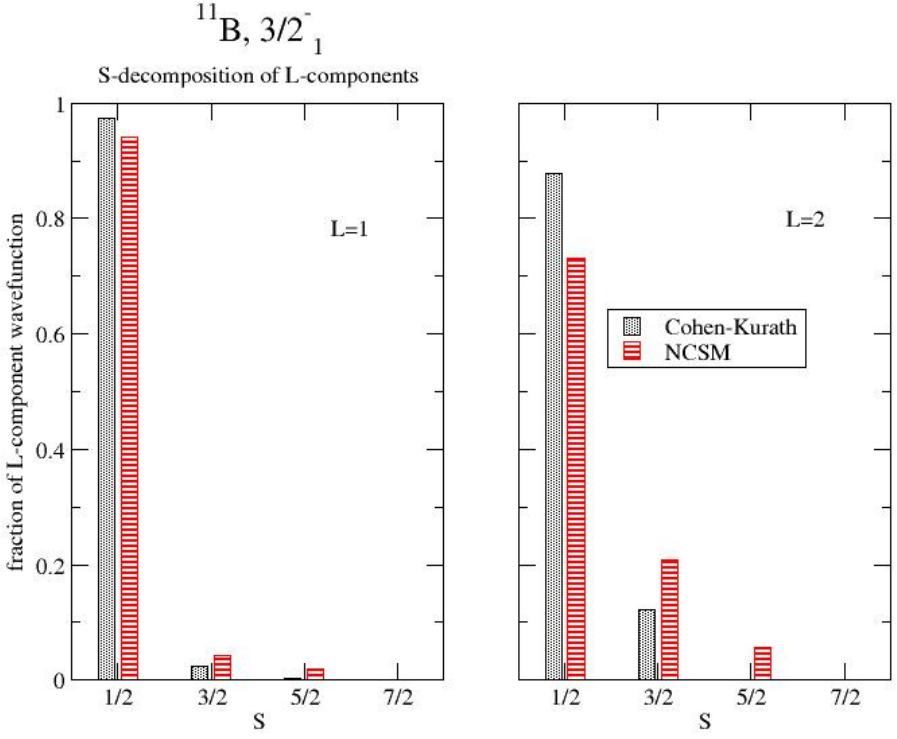

^{9}Be, state $3/2_2$
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
fraction of wavefunction
L

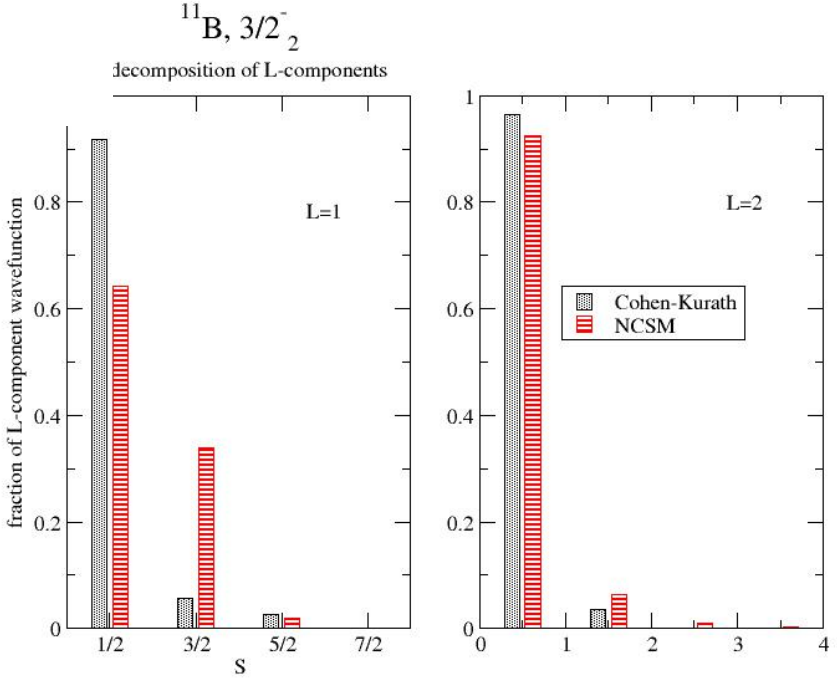

^{9}Be, state $5/2_1$
L-decomposition
Cohen-Kurath
NCSM (λ=2.0, Nmax = 6)
L

I can further decompose each component of good L
into components of good S…. I just choose a few cases from ^{11}B.

I can further decompose each component of good L
into components of good S…. I just choose a few cases from ^{11}B.




^{11}B, 3/2$^-_1$
S-decomposition of L-components
fraction of L-component wavefunction
L=1
L=2
Cohen-Kurath
NCSM
1/2
3/2
5/2
7/2
S


^{11}B, 3/2$^-_2$
decomposition of L-components
fraction of L-component wavefunction
L=1
L=2
Cohen-Kurath
NCSM
1/2
3/2
5/2
7/2
S

Summary and future work:

*We can decompose shell-model wavefunctions
into L-S components (in particular using the Lanczos trick)

* Both phenomenological interactions in the *p*-shell
(Cohen-Kurath, 1965) and *ab initio* forces yield
very similar results, especially in L-components.
Full LS-decomposition may show more differences.

* The next step is to add in 3-body forces and see
(a) what states change the most and
(b) if they bring any states closer to phenomenology

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